APS March Meeting 2013
Baltimore, Maryland
http://www.aps.org/meetings/march/
8:00AM A1.00001 Longitudinal Spin Seebeck Effect EIJI SAITO, Institute for Materials Research, Tohoku University — The spin Seebeck effect (SSE) refers to the generation of a spin voltage as a result of a temperature gradient in magnetic materials [1-7]. Here, a spin voltage is a potential for electron spins to drive a nonequilibrium spin current; when a conductor is attached to a magnet with a finite spin voltage, it induces a spin injection into the conductor. The SSE is of crucial importance in spintronics and spin caloritronics, since it enables simple and versatile generation of a spin current from heat. The simplest and most straightforward setup of the SSE is the longitudinal configuration [4], in which a spin current flowing parallel to a temperature gradient is measured via the inverse spin Hall effect (ISHE). The longitudinal SSE device consists of a ferromagnetic or ferrimagnetic insulator (FI, e.g., YIG) covered with a paramagnetic metal (PM, e.g., Pt) film. When a temperature gradient is applied perpendicular to the FI/PM interface, an ISHE-induced voltage is generated in the PM layer. In this talk, we report the observation of the longitudinal SSE in various FI/PM systems and provide evidence that the longitudinal SSE is free from thermoelectric artefact [7], i.e., the anomalous Nernst effect caused by extrinsic magnetic proximity [8]. Then, we discuss the longitudinal SSE from an application point of view [6]. We thank E. Saitoh, S. Maekawa, G. E. W. Bauer, X.-F. Jin, H. Adachi, D. Hou, D. Tian, T. Kikkawa, A. Kirihara, and M. Ishida for their support and valuable discussions.


8:36AM A1.00002 Transport Magnetic Proximity Effects in Platinum, SSU-YEN HUANG, The Johns Hopkins University, National Tsing Hua University — Platinum (Pt) metal, being non-magnetic and having a strong spin-orbit coupling interaction, has been central in detecting pure spin current and establishing most of the recent spin-based phenomena. Thus, it is important to ascertain the transport and magnetic characteristics of thin Pt films in contact with a ferromagnet. In this work, we use both electric and thermal means to conclusively show the transport magnetic proximity effects (MPE) of thin Pt film in contact with ferromagnetic insulator YIG. At thicknesses comparable to, and less than, the spin diffusion length, the strong ferromagnetic characteristics in Pt films on YIG are indistinguishable from those of ferromagnetic permalloy on YIG. [1] The MPE occurs at the interface and decreases exponentially away from the interface, in contrast with a few monolayers. As a result, the pure spin current detected by a thin Pt is tainted with a spin polarized current. The pure spin current phenomena, such as the inverse spin Hall effect and the spin Seebeck effect, have been contaminated with the anomalous Hall effect and the anomalous Nernst effect respectively. These results raise serious questions about the suitability, and the validity, of using Pt in establishing pure spin current phenomena; on the other hand, a much stronger spin-based effect can be induced by the MPE at the interface. This research is in collaboration with X. Fin, Y. P. Chen, J. Wu, and J. Q. Xiao (University of Delaware), T. Y. Chen (Arizona State University) and D. Qu, W. G. Wang, and C. L. Chien (The Johns Hopkins University).


9:12AM A1.00003 Observation of the planar Nernst effect in Permalloy and Nickel Thin Films with In-plane Thermal Gradients¹, BARRY ZINK, University of Denver — The reliable generation of pure spin currents is an important ingredient in future spintronic devices that may offer lower power consumption and greater processing capabilities than current technology. Over the past few years some groups have reported that such a spin current can be generated simply by applying a thermal gradient to a ferromagnetic material. This effect, called the spin Seebeck effect (SSE), has generated tremendous interest in the interaction of heat, charge and spin in ferromagnetic systems. In this talk we will present our own recent measurements of thermoelectric and thermomagnetic effects in thin film metallic ferromagnets. These are enabled by a micromachined thermal isolation platform that removes potentially confounding effects introduced in such measurements by the presence of a highly thermally conductive bulk substrate. One of the main results is the observation of a transverse thermopower, called the planar Nernst effect (PNE), that is caused by spin-dependent scattering. This PNE should therefore be present in any attempted measurement of the SSE in a metal system where spin-dependent scattering of electrons occurs. Furthermore our “zero substrate” experiment shows no signal with the expected symmetry of the SSE, suggesting that the presence of the substrate is required to cause such a signal. Further experiments are required to determine if a pure spin current is actually involved in the generation of the signal associated with the SSE in ferromagnetic metal films. This work was performed in collaboration with A. D. Avery, and M. R. Pufall.

¹This work is supported by the NSF CAREER award (DMR-0847796).

9:48AM A1.00004 Non-universal shot noise in quasiequilibrium spin valves, TERO HEIKKILA, Aalto University — Shot noise can be used as a diagnostic tool characterizing mesoscopic wires, especially the inelastic scattering in them. This characterization is based on the fact that in the absence of inelastic scattering that carries the energy away from the system, disordered wires are described by a universal Fano factor defined as the ratio of the noise power and the average current. In particular, we predict that the Fano factor gets strongly suppressed for the antiparallel configuration of magnetizations. T.T. Heikkilä and K.E. Nagaev, arXiv:1302.1372
10:24 AM A1.00005 Charge Transitions from Magnetization Dynamics

The main challenge of spin caloritronics is to establish a connection between heat currents and spin currents. Towards this end, spin Hall effects have become very important, since they allow to convert a pure spin current into a transverse charge voltage. I will show how these spin Hall effects can be characterized with great accuracy using spin pumping, where the excitation of ferromagnetic resonance generates a pure spin current in an adjacent non-magnetic conductor. The change in the line-width of the ferromagnetic resonance determines the spin-mixing conductance and thus after proper calibration, charge current measurements can be achieved. Furthermore, the concomitant opening angles of the magnetization precession can be used to determine the magnitude of the spin current. The charge current generated from inverse spin Hall effect is measured through the associated electrical voltage and the ratio of spin and charge current directly determines the spin Hall angle. Furthermore, I will present an alternative approach for converting magnetization dynamics into measurable charge voltages. Namely, the dissipation of magnetization dynamics in thin films generally also results in a temperature gradient perpendicular to the film, since the supporting substrate acts as a heat sink. This in turn can generate a transverse voltage through the anomalous Nernst effect. Interestingly, this allows to detect spin waves with very good signal to noise ratio and unlike optical or inductive detection techniques, there is practically no lower limit for the wavelength of the detected spin waves.

Monday, March 18, 2013 8:00 AM - 11:00 AM
Session A2 DCMP: Invited Session: Novel Superconductivity in FE Selenide Superconductors
Ballroom II - Douglas Scalapino, University of California at Santa Barbara

8:00 AM A2.00001 Ab initio calculations and crystal symmetry considerations for novel FeSe-based superconductors

IGOR MAZIN, NRL — Density functional calculations disagree with the ARPES measurements on both K0.3Fe2Se2 superconducting phase and FeSe/SrTiO3 monolayers. Yet they can still be dramatically useful for the reason that they respect full crystallographic symmetry and take good account of electron-ion interaction. Using just symmetry analysis, it is shown that nodeless d-wave superconductivity is not an option in these systems, and a microscopic framework is derived that leads to a novel s-wave sign-reversal state, qualitatively different from the already familiar s± state in pnictides and bulk binary selenides. Regarding the FeSe monolayer, bonding and charge transfer between the film and the substrate is analyzed and it is shown that the former is weaker and the latter negligible, which sets important restrictions on possible mechanisms of doping and superconductivity in these monolayers. In particular, the role of the so-called “Se etching,” necessary for superconductivity in FeSe monolayers, is analyzed in terms of electronic structure and bonding with the substrate.

8:36 AM A2.00002 Scanning tunneling microscopy study on superconductivity of FeSe thin films

XUCUN MA, Institute of Physics, Chinese Academy of Sciences — Searching for superconducting materials with high transition temperature (Tc) is one of the most exciting and challenging fields in physics and materials science. By using MBE technique, we are able to prepare stoichiometric and superconducting FeSe single crystalline films on various substrates, which enables us to investigate superconductivity mechanism of FeSe thin films in well-controlled way [1-3]. Most importantly, by using low temperature scanning tunneling spectroscopy, a superconductive gap as large as 20 meV and the vortex state under high magnetic field are revealed in the single unit-cell thick FeSe films on SrTiO3(001) substrate [4]. Such a high Tc superconductor is further confirmed by recent transport measurement. The study not only demonstrates a powerful way for finding new superconductors and for raising Tc, but also provides a well-defined platform for systematic study of the mechanism of unconventional superconductivity by using different superconducting materials and substrates. The study is collaborated with Professor Qi-Kun Xue, Department of Physics, Tsinghua University, China.

References:

9:12 AM A2.00003 Phase Diagram and High Temperature Superconductivity at 65K in the Single-Layer FeSe Films Revealed by ARPES

SHAOULONG HE, National Lab for Superconductivity, Institute of Physics, CAS, Beijing — The discovery of the iron-based superconductors in 2008 not only provides another venue to understand the origin of high-Tc superconductivity but also a new playground to explore novel superconductors with higher superconducting transition temperature. The latest report of possible high temperature superconductivity in the single-layer FeSe films grown on SrTiO3 substrate is both surprising and interesting [1]. In this talk, we report the electronic structure and phase diagram of the single-layer FeSe films by angle-resolved photoemission spectroscopy (ARPES) [2,3]. Our high-resolution ARPES results show that it has a simple Fermi surface topology consisting only of electron pockets near the zone corner without indication of any Fermi surface around the zone center. In addition, our observation of large and nearly isotropic superconducting gap in this strictly two-dimensional system rules out existence of gap nodes in the superconducting gap. We also established a phase diagram in this single-layer FeSe films by an annealing procedure to tune the charge carrier concentration over a wide range. By optimizing the annealing process, we observed evidence of a record high Tc of ~ 65K in the single-layer FeSe films. The wide tunability of the system across different phases, and its high-Tc, make the single-layer FeSe film ideal not only to investigate the superconductivity physics and mechanism, but also to study novel quantum phenomena and for potential applications.

References:

9:48AM A3.00004 Pairing and Fermiology in iron-chalcogenide superconductors, DUNG-HAI LEE, Dept. Physics, University of California, Berkeley — “Stripe”-type magnetic fluctuations has been postulated as the trigger of Cooper pairing in iron-based superconductors. In iron pnictides the matching of the peak magnetic fluctuations wavevector and the Fermiology lands support to the above idea. However recent ARPES results on high $T_c$ $A_xFe_{1-x}Se_2$ and FeSe/SrTiO$_3$ and neutron results on $A_xFe_{1-x}Se_2$ pose challenges to the above picture. In this talk we will take a fresh new look at the purported pairing mechanism of iron-based superconductors.

10:24AM A2.00005 $S_4$ Symmetric Microscopic Model for Iron Based Superconductors, JIANGPING HU, Institute of Physics, CAS, China and Department of Physics, Purdue University — How are cuprates and iron-based high temperature superconductors correlated? What is the common mechanism behind two different families of iron-based superconductors, iron-pnictides and iron-chalcogenides? These two questions are two major challenges in the today’s field of high temperature superconductors. In this talk, we will show when the lattice symmetry, the $S_4$ symmetry of the building block, the tri-layer structure of FeAs or FeSe, is properly considered, the low energy physics of iron-based superconductors is governed by a two-orbital Hamiltonian near half filling that can be divided into two weakly coupled one-orbital models. We will discuss the microscopic origin and some unique properties of the model, including magnetism and pairing symmetry. The model provides a unified understanding of iron pnictides and iron-chalcogenides, and suggests that cuprates and iron-based superconductors share an identical high-$T_c$ superconducting mechanism. The model leads to a natural classification of pairing symmetry according to $S_4$ symmetry. When the pairing is driven by antiferromagnetic exchange couplings, there are two different s-wave states. One s-wave is the well-studied s$_z$ pairing which is in the A phase of $S_4$ symmetry (even under $S_4$ symmetry operation), and the other is a new type of extended s-wave pairing which is in the B phase of $S_4$ symmetry (odd under $S_4$ symmetry operation). The superconductivity order in the B phase are characterized by opposite signs between up and bottom As(Se) layers in the trilayer FeAs(Se) structure. The 122 Iron-chalcogenides and the single layer FeSe are most likely in the B-phase. We believe that the model establishes a new foundation for exploring novel properties of iron based superconductors.


Monday, March 18, 2013 8:00AM - 11:00AM –

8:00AM A3.00001 Evidence of low-lying gapped excitations in the $\nu = 5/2$ quantum fluid$^1$. URSULA WURSTBAUER, Columbia University — The competition between quantum phases that dictate the physics in the second Landau level (SLL) results in striking phenomena. A highly fascinating state is the even denominator fractional quantum Hall (FQHE) state at filling $\nu = 5/2$ that is widely believed to support non-Abelian quasi-particle excitations. Our work explores the low-lying neutral excitation modes in the SLL by resonant inelastic light scattering measurements. At $5/2$ the spectra reveal a band of gapped modes with peak intensity at energy of 0.07meV. These modes are interpreted as a roton minimum in the wave vector dispersion of spin-conserving excitations. The intensity of the roton band significantly diminishes by increasing the temperature to 250mK and it fully collapses for $T > 250$mK. This temperature dependence is consistent with activated magneto-transport of the incompressible quantum fluid at $5/2$. A long wavelength spin wave mode ($SW$) is seen at the bare Zeeman energy, indicating that there is non-zero spin-polarization. Both, roton and SW modes appear only in a very narrow filling factor range of less than $\nu < 5/2 \pm 0.1$. A gapless continuum of low-lying excitations emerges at filling factors slightly away from $5/2$. This demonstrates a transition from an incompressible quantum fluid at exactly $\nu = 5/2$ to compressible states at very close filling factors. This work is in collaboration with A. Pinczuk, A. Levy, K. West, L. Pfeiffer, S. Mondal, J. Watson and M. Manfra.

$^1$Supported by the U.S. National Science Foundation and the Alexander von Humboldt Foundation.

8:36AM A3.00002 Spin transition in the second Landau level$^1$. W. PAN, Sandia National Labs — The fractional quantum Hall effect (FQHE) states in the second Landau level have attracted growing interest and intensive theoretical and experimental investigations due to their being non-Abelian states. Recently, we systematically examined the spin polarization of the 8/3 and 12/5 states in a series of high quality two dimensional electron systems. Evidence of spin transition was observed for both states, suggesting a more complicated nature of the FQHE ground states in the second Landau level.

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

9:12AM A3.00003 Quantum Hall Interferometry and Detection of Anyonic Braiding Statistics, STEVEN SIMON, Oxford University — In two spatial dimensions quantum mechanical particles are not limited to being bosons or fermions as they are in three dimensions, but can be particles known as anyons. Such anyons come in two major varieties — Abelian and non-Abelian — both of which were long ago predicted to be realized in certain Fractional Quantum Hall (FQH) systems. However, experimental demonstration of anyonic braiding properties has remained elusive and very controversial. New results by Willett et. al. and Kang et. al. have been interpreted as evidence of anyonic braiding in Fabry Perot interferometers in the second Landau level. In this talk, I will discuss my current understanding of these works based on a number of recent publications.

References:

9:48AM A3.00004 Quantifying disorder and its impact in the 2nd Landau level$^1$. MICHAEL MANFRA, Purdue University — Strong electronic correlations are evident in the 2nd Landau level (LL) of an ultra-high quality GaAs/AlGaAs two-dimensional electron gas (2DEG). The exotic fractional quantum Hall states at filling factors $\nu = 5/2$ and $12/5$, as well as the reentrant integer quantum Hall states flanking half-filling, are a few examples presently under intense investigation. While it is generally accepted that samples must be of extremely low disorder to exhibit correlations in the 2nd LL, our understanding of how to quantify residual disorder and its impact on the states of interest remains primitive. In this talk we will critically examine how disorder is quantified for the 2DEG both at zero magnetic field and in the quantum Hall regime, and then compare the results of this analysis with measurements of the excitation gap at $\nu = 5/2$ in samples in which disorder is varied in a well-defined manner. Our results highlight the very different impact on the excitation gap generated by different types of disorder and the limitations of presently employed characterization methods.

$^1$Work done in collaboration with the Csathy group, Purdue University
surfaces will be mentioned. Accessed by tuning a single parameter, has striking consequences such as an exact relation between the correlation functions of fermions and those of the order arguments and are verified by numerical DMRG solution of a lattice model that mimics the physics of the phase transition. The emergent supersymmetry, at low energies. The magnetic order parameter field is identified as the superpartner of the Majorana fermions. These results are obtained using field theoretical to spontaneous magnetic order at the boundary. We show that the associated quantum phase transition, if continuous, has emergent space-time supersymmetry . We also show that in the asymptotic limit FMFs can encode quantum information. Quasi-energy analysis shows that a stable FMF zero mode and two other satellite modes exist in a wide parameter space with large quasi-energy gaps, which prevents transitions to other Floquet states under adiabatic driving. We also show that in the asymptotic limit FMFs can encode quantum information. Quasi-energy analysis shows that a stable FMF zero mode and two other satellite modes exist in a wide parameter space with large quasi-energy gaps, which prevents transitions to other Floquet states under adiabatic driving.

Institute for Theoretical Physics, DONNA SHENG, Cal State University Northridge, ASHVIN VISHWANATH, University of California Berkeley — In the absence of disorder regime. Our formula doesn’t involve gauge or twisted boundary condition, hence can be computational effective.

This research is supported by NSF grants DMS-1066045 and DMR-1056168

Monday, March 18, 2013 8:00AM - 11:00AM – Session A6 DCMP: Topological Insulators: Novel States in Topological Insulators 302 - Tudor Stanescu, West Virginia University

8:00AM A6.00001 Noncommutative Magneto-Electric Responses of Topological Insulators1. BRYAN LEUNG, Rutgers University, EMIL PRODAN, Yeshiva University — Topological magneto-electric response, constructed on a Brillouin torus, defines a \( Z_2 \) invariant and classifies topological phases. In the presence of disorder or B field, the notion of Brillouin torus is destroyed. This problem can be overcome by using noncommutative geometry. Starting from a generic 3D lattice model, we derive the magneto-electric response on a noncommutative Brillouin torus. Our result is a noncommutative topological formula. We show that its topological stability requires only mobility gap, therefore the robustness extends to strong disorder regime. Our formula doesn’t involve gauge or twisted boundary condition, hence can be computational effective.

8:12AM A6.00002 Heavy Adatoms on Magnetic Surfaces: A Search for Chern Insulators, KEVIN GARRITY, DAVID VANDERBILT, Rutgers University — The theoretical possibility of a quantum anomalous Hall (QAH) insulator, or Chern insulator, has been known for many years, and several strategies for achieving this topological phase have been proposed. However, no unambiguous experimental realization is yet in hand. In this work, we propose a new QAH search strategy and verify its viability with first-principles calculations. We propose constructing a QAH insulator by depositing a layer of adatoms with large spin-orbit coupling (e.g., Pb, Bi) on the surface of a magnetic insulator. We argue that such systems will typically have surface bands with non-zero Chern numbers, so that if metallic, they will typically have a large anomalous Hall conductivity. Thus, the search for Chern insulators reduces to looking for examples exhibiting a global gap across the entire BZ. Using first-principles calculations, we search through many examples of heavy elements on MnTe, MnSe, and EuS surfaces. Our search reveals several Chern insulators with band gaps of up to 0.14 eV, which may be promising targets for future experimental investigations.

8:24AM A6.00003 Topology, Delocalization via Average Symmetry and the Symplectic Anderson Transition, CHARLES KANE, University of Pennsylvania, LIANG FU, Massachusetts Institute of Technology — A field theory of the Anderson transition in two dimensional disordered systems with spin-orbit interactions and time-reversal symmetry is developed, in which localization is driven by the proliferation of vortex-like topological defects. The sign of the vortex fugacity determines the \( Z_2 \) topological class of the localized phase. There are two distinct fixed points with the same critical exponents, corresponding to transitions from a metal to an insulator and a topological insulator respectively. The critical conductivity and correlation length exponent of these transitions are computed in a \( N = 1 - \epsilon \) expansion in the number of replicas, where for small \( \epsilon \) the critical points are perturbatively connected to the Kosterlitz Thouless critical point. Delocalized states, which arise at the surface of weak topological insulators and topological crystalline insulators, occur because vortex proliferation is forbidden due to the presence of symmetries that are violated by disorder, but are restored by disorder averaging.

8:36AM A6.00004 Floquet Majorana Fermions for Topological Qubits, D.E. LIU, Duke University, A. LEVCHENKO, Michigan State University, H.U. BARANGER, Duke University — We develop an approach to realizing a topological phase transition and non-Abelian statistics with dynamically induced Floquet Majorana Fermions (FMFs). When the periodic driving potential does not break fermion parity conservation, FMFs can encode quantum information. Quasi-energy analysis shows that a stable FMF zero mode and two other satellite modes exist in a wide parameter space with large quasi-energy gaps, which prevents transitions to other Floquet states under adiabatic driving. We also show that in the asymptotic limit FMFs preserve non-Abelian statistics and, thus, behave like their equilibrium counterparts.

8:48AM A6.00005 ABSTRACT WITHDRAWN

9:00AM A6.00006 Emergent Supersymmetry in Topological Superconductors, TARUN GROVER, Kavli Institute for Theoretical Physics, DONNA SHENG, Cal State University Northridge, ASHVIN VISHWANATH, University of California Berkeley — In the absence of interactions, topological superconductors (TSC) host helical Majorana fermion edge states protected by time reversal symmetry. Increasing interactions can lead to spontaneous magnetic order at the boundary. We show that the associated quantum phase transition, if continuous, has emergent space-time supersymmetry at low energies. The magnetic order parameter field is identified as the superpartner of the Majorana fermions. These results are obtained using field theoretical arguments and are verified by numerical DMRG solution of a lattice model that mimics the physics of the phase transition. The emergent supersymmetry, accessed by tuning a single parameter, has striking consequences such as an exact relation between the correlation functions of fermions and those of the order parameter. Similar results are argued to hold for the 2+1 dimensional boundary of a bulk topological superconductor. Generalization to topological insulator surfaces will be mentioned.

\[2\] G. J. Sreejith, Y.-H. Wu, A. Wojs and J.K. Jain, unpublished.
\[3\] S. Mukherjee, S. S. Mandal, A. Wojs, J.K. Jain, unpublished.
\[4\] A. Babam, Y.-H. Wu, G. J. Sreejith, A. Wojs, J. K. Jain, unpublished.

1Department of Energy and National Science Foundation

\[1\] A. C. Balram, Y.-H. Wu, G. J. Sreejith, A. Wojs, J.K. Jain, unpublished.
9:12AM A6.00007 Dynamical manipulation of 2D topological insulator edge states for Majorana fermion braiding1, SHU-PING LEE, JASON ALICEA, caltech — Edge states of 2D topological insulators such as HgTe provide a promising platform for realizing Majorana modes. Networks required for braiding Majoranas along the edge channels can be obtained by adjoining HgTe quantum wells to form corner junctions. Physically cutting quantum wells for this purpose, however, presents technical challenges. Here we propose a more accessible means of forming networks that relies on dynamically manipulating the location of edge states inside of a single HgTe sheet. In particular, we show that edge states can effectively be dragged into the system’s interior by gating a region near the edge into a metallic regime and then removing the resulting gapless carriers via proximity-induced superconductivity. This method allows one to construct rather general quasi-1D networks along which Majorana modes can be shuttled and exchanged by electrostatic means.

1Supported by NSF grant DMR-105522 and the Alfred P. Sloan Foundation.

9:24AM A6.00008 Topological Excitonic Superfluids in Three Dimensions1, MATTHEW GILBERT, University of Illinois - Urbana-Champaign, EWELINA HANKIEWICZ, Universitaet Wuerzburg, YOUNGSEOK KIM, University of Illinois - Urbana-Champaign — We study the equilibrium and non-equilibrium properties of topological dipolar intersurface exciton condensates within time-reversal invariant topological insulators in three spatial dimensions without a magnetic field. We elucidate that, in order to correctly identify the proper pairing symmetry within the condensate order parameter, the full three-dimensional Hamiltonian must be considered. As a corollary, we demonstrate that only particles with similar chirality play a significant role in condensate formation. Furthermore, we find that the intersurface exciton condensation is not suppressed by the interconnection of surfaces in three-dimensional topological insulators as the intersurface polarizability vanishes in the condensed phase. This eliminates the surface current flow leaving only intersurface current flow through the bulk. We conclude by illustrating how the excitonic superfluidity may be identified through an examination of the terminal currents above and below the condensate critical current.

1Army Research Office (ARO) under contract number W911NF-09-1-0347, the Office of Naval Research (ONR) under contract number N0014-11-1-0728, and the Air Force Office of Scientific Research (AFOSR) under contract number FA9550-10-1-0459, DFG Grant HA 5893

9:36AM A6.00009 Quantum interference and quantum oscillation on the surface of mirror symmetric topological insulators1, CHEN FANG, University of Illinois at Urbana Champaign, ARIS ALEXANDRADINATA, Princeton University, MATTHEW GILBERT, University of Illinois at Urbana Champaign, SU-YANG XIU, ZAHID HASAN, ANDREI BERNEVIG, Princeton University — We first study the quasiparticle interference (QPI) of the surface states in crystalline topological insulators which possess mirror symmetry and time-reversal symmetry, by analyzing the Fourier transformed local density of states (FT-LDOS), \( \rho(b, \omega) \) around a single static impurity on the surface. The topological characters of the surface states of these new materials lead to QPI patterns distinct from those of 2D metals and of surface states on 3D time-reversal TI’s. We apply the general analysis to the QPI on the \( \langle 001 \rangle \)-surface of Pb\(_{1-x}\)Sn\(_x\)Te and predict all vanishing singularities in \( \rho(b, \omega) \). We also demonstrate that QPI can also be used to probe the Lifshitz transition of the surface states observed in recent ARPES experiment. We next study the Shubnikov de Hass oscillation of these surface states and show that the oscillation has a single period before the Lifshitz transition and two distinct periods after the transition. Adding in-plane magnetic field before the Lifshitz transition leads to splitting of the period into two close periods and a beating thereof.

1ONR - N00014-11-1-0635. AFOSR FA9550-10-1-0459, ONR N0014-11-1-0728. NSF CAREER DMR-095242, ONR - N00014-11-1-0635, Darpa - N66001-11- 14110

9:48AM A6.00010 Chern and Majorana Modes in QuasiCrystals, INDUBALA SATIJA, George Mason University, GERARDO NAUMIS, Universidad Nacional Autonoma de Mexico — The topology of quasicrystals is found to have a novel manifestation in the spatial profile of band edge states as topological invariants transform peaks into doublets of size equals the Chern number. The Chern-dressed peaks form a self-similar pattern encoding topological fingerprints at all length scales. For quasicrystals exhibiting localized states, fluctuations about exponentially localized zero modes describe the onset to topological transition where Majorana modes delocalize. These exotic modes can be captured in their entirety using \( U(1) \) symmetry breaking perturbation that supports both the Chern and the Majorana modes. Here topological transition is accompanied by localization as edge-localized modes move to the interior, loosing topological protection.

10:00AM A6.00011 Vortex zero modes, chiral anomaly and effective field theory for odd parity topological superconductor in three dimensional Dirac materials1, BITAN ROY, PALLAB GOSWAMI, National High Magnetic Field Laboratory — The low energy quasiparticle dispersion of various narrow gap and gapless semiconductors are respectively described by three dimensional massive and massless Dirac fermions. The three dimensional Dirac spinor structure admits an interesting time-reversal invariant, odd parity and Lorentz pseudo-scalar topological superconducting state. In this talk we demonstrate the existence of fermion zero energy states in the vortex core of this odd parity topological superconductor under generic conditions. Guided by the existence of the zero modes and its intimate connection with the chiral anomaly and the index theorem, we derive an effective topological field theory for such a superconducting state. We also discuss the experimental consequences of the zero modes and the topological field theory for the low temperature unconventional superconducting states of copper intercalated bismuth selenide, and indium doped tin telluride.

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10:12AM A6.00012 Ab initio study of topological insulating property in the heterojunction of Bi (111) bilayer and Bi\(_2\)Te\(_2\)Se, KYUNG-HWAN JIN, SEUNG-HOON JHI, Department of Physics, POSTECH — Study of topological insulator (TI) is showing rapid progress in both theory and experiment, particularly on three dimensional materials. Examples of two dimensional TI (quantum spin Hall) materials are, on the other hand, comparatively less common. As such, theoretical predictions of single Bi (111) bilayers as TI draw great attention from experiment. A recent report of ARPES measurements claims verification of the 2D TI property of Bi bilayer, but analysis leaves much room for further clarification. Because Bi (111) bilayers grown on 3D TI substrates such as Bi\(_2\)Te\(_2\)Se and Bi\(_2\)Te\(_2\)Se; understanding the details of the interface between the Bi bilayer and 3D TI substrates is essentially required. We study the electronic structures of Bi bilayer-Bi\(_2\)Te\(_2\)Se heterojunction from first-principles calculations. We find a substantial shift of Dirac cone from the TI substrates into Bi bilayer that thus becomes metallic on TI substrates. It is shown that the origin of this change is the inversion-symmetry breaking in Bi bilayer due to TI substrate. By comparing our calculations of Bi bilayer nanoribbons on Bi\(_2\)Te\(_2\)Se with STM/STS measurements, we successfully resolve and locate the edge states of a single Bi bilayer and confirm its 2D TI character.
10:24AM A6.00013 Topological indices, defects, and Majorana fermions in chiral superconductors, DAICHI ASAHI, NAOTO NAGAOYA, Department of Applied Physics, University of Tokyo — We study theoretically the role of topological invariants to protect the Majorana fermions in a model of two-dimensional (2D) chiral superconductors which belong to class D of the topological periodic table. A rich phase diagram is revealed. Each phase is characterized by the topological invariants for 2D (Z) and 1D (Z2), which lead to the Majorana fermion at the edge dislocation and the core of the vortex. The topological invariants are determined by the hopping integrals along x and y directions. Interference of the Majorana fermions originating from the different topological invariants is studied. The interaction between zero-energy states at edge dislocations and at vortex cores eliminates the zero-energy states when they coexist at the same position. The stability of the Majorana fermion with respect to the interlayer coupling, i.e., in 3D, is also examined. We found that the zero-energy state survive a finite hopping integral along the z-direction unless the energy gap closes.

10:36AM A6.00014 On the possibility of the fractional ac Josephson effect and doubled Shapiro steps in non-topological Josephson junctions1, JAY SAU, Harvard University, EREZ BERG, Weizmann Institute of science, BERTRAND HALPERIN, Harvard University — Topological superconductors supporting Majorana Fermions with non-abelian statistics are presently a subject of intense theoretical and experimental effort. It has been proposed that the observation of a half-frequency or a fractional Josephson effect is a more reliable test for topological superconductivity than the search for end zero modes. In fact, the fractional Josephson effect has been observed for the semiconductor nanowire system in the form of doubled Shapiro states. Here we consider the possibility of seeing such a fractional ac Josephson and doubled Shapiro steps from a superconducting nanowire in the non-topological phase. Using a semiclassical treatment we find that both the fractional ac Josephson effect and the doubled Shapiro step can, in principle, occur in the non-topological phase because of non-dynamical Landau Zener processes associated with the Andreev bound state spectrum of the junction. Therefore, while the observation of doubled Shapiro steps can be taken as indicative of a topological phase, it may not be a smoking gun signature for topological superconductivity and Majorana fermions.

1 JS thanks the Harvard Quantum Optics Center for support

10:48AM A6.00015 Majorana Flat Bands and Uni-directional Majorana Edge States in Gapless Topological Superconductors1, KAM TUEN LAW, CHRIS L.M. WONG, JIE LIU, Hong Kong University of Science and Technology, PATRICK A. LEE, Massachusetts Institute of Technology — In this work, we show that an in-plane magnetic field can drive a fully gapped $p \pm ip$ topological superconductor into a gapless phase which supports Majorana flat bands (MFBs). Unlike previous examples, the MFBs in the gapless regime are protected from disorder by a chiral symmetry. In addition, novel uni-directional Majorana edge states (MESs) which propagate in the same direction on opposite edges appear when the chiral symmetry is broken by Rashba terms. Unlike the usual chiral or helical edge states, uni-directional MESs appear only in systems with a gapless bulk. We show that the MFBs and the uni-directional MESs induce nearly quantized zero bias conductance in tunneling experiments.

1 The authors thank Hong Kong GRC and DOE of United States for financial support.

Monday, March 18, 2013 8:00AM - 11:00AM – Session A8 DCMP: Graphene: Quantum Hall Effect 307 - Herb Fertig, Indiana University

8:00AM A8.00001 Four-flux fractional quantum Hall states in suspended graphene, ANDREI LEVIN, BENJAMIN FELDMAN, Harvard University, BENJAMIN KRAUSS, JURGEN SMET, Max-Planck-Institut fur Festkorperforschung, AMIR YACOBY, Harvard University — The interactions between charge carriers in ultraclean graphene subject to a perpendicular magnetic field can drive the system to condense into one of a set of incompressible fractional quantum Hall (FQH) states. We use a scanning single-electron transistor to measure the local electronic compressibility of suspended graphene. In addition to observing incompressible behavior at fractional filling factors in the two-flux composite fermion sequence, we also observe FQH states arising from four-flux composite fermions, including states at filling factors $\nu = 1/5, 2/7, 2/9, 3/11, 5/7$ and $6/5$. We measure the energy gaps of these states as a function of magnetic field, most display approximately linear scaling. Interestingly, several four-flux FQH states are conspicuously absent near filling factors $\nu = 1$ and $2$, despite the robust appearance of their counterparts near $\nu = 0$.

8:12AM A8.00002 Measurements of Chiral Heat Current in the Quantum Hall Regime, SEUNG-GEOL NAM, Department of Physics, Pohang University of Science and Technology, Korea, E.H. HWANG, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon, Korea, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Korea — Heat transport measurements can offer a new window to probe the low-energy physics in quantum-Hall systems, which cannot be provided by the electronic transport measurements. In this presentation, we report chiral heat transport measurements in monolayer graphene in the integer quantum Hall regime. We inject charge carriers at a higher temperature than the system bulk and measure the thermoelectric voltage corresponding to the local electron temperature at a distance from the injection point. We find that in graphene heat transport at the edge in the quantum Hall regime is chiral and its direction is dependent on both the carrier type and the magnetic field direction. Measured thermoelectric signals in unipolar regions can be understood by the Mott relation, but a severe deviation of the signals from the Mott relation is found at a p-n junction. Thermoelectric signal decays with distance from the heater and saturates with increasing heating power even though it increases linearly at low powers, which indicates that a part of heat is transferred out of the edge current.

8:24AM A8.00003 Drude weight, cyclotron resonance, and the Dicke model of graphene cavity QED, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, LUCA CHIROLLI, VITTORIO GIOVANNETTI, NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, ALLAN MACDONALD, Department of Physics, University of Texas at Austin, Austin, Texas 78712, USA — The unique optoelectronic properties of graphene make this two-dimensional (2D) material an ideal platform for fundamental studies of cavity quantum electrodynamics (QED) in the strong-coupling regime. The celebrated Dicke model of cavity QED can be approximately realized in this material when the cyclotron transition of its 2D massless Dirac fermion carriers is nearly resonant with a cavity photon mode. In this talk I will discuss the theory of strong matter-photon coupling in this circumstance, emphasizing the essential role of a dynamically generated matter energy term that is quadratic in the photon field and absent in graphene’s low-energy Dirac model.

1 Work supported by MIUR-FIRB grants RBID08B3FM and RBFR10MSBT, Welch Foundation grant TBF1473, and by DOE Division of Materials Sciences and Engineering grant DE-FG03-02ER45608.
8:36AM A8.00004 Theory of unconventional quantum Hall effect in strained graphene\textsuperscript{1} ZI-XIANG HU, Chongqing University, China and Princeton University, USA, BITAN ROY, KUN YANG, National High Magnetic Field Laboratory, Florida State University, USA — We show graphene discurs an unconventional sequence of quantized Hall conductivity, when subject to both magnetic fields (B) and strain through both theoretical arguments and numerical calculations. The strain produces time-reversal symmetric pseudo/axial magnetic fields (\textit{b}). The single electron spectrum is composed of two inter-penetrating sets of Landau levels (LLs), located at \(\pm \sqrt{2n(b \pm B)}\), \(n = 0, 1, 2, \ldots\). For \(b > B\), these two sets of LLs have opposite chiralities, resulting in oscillating Hall conductivity between 0 and \(\pm \Delta\). 

\begin{itemize}
  \item \textbf{Tokyo, Japan, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, TOMOKI MACHIDA, Institute of Industrial Science,}
  \item SATORU MASUBUCHI, MASAHIRO ONUKI, MIHO ARAI, Institute of Industrial Science, University of 
  \item 1 magnetic field and gate electric fields. 
  \item Moreover, our results suggest possibilities to visualize the resulting texture via measuring the charge density difference between the two graphene layers, 
  \item that the Coulomb interaction opens a gap between the two lowest-lying states near the Fermi level, and yields a smooth valley texture throughout the domain walls. Moreover, our results suggest possibilities to visualize the resulting texture via measuring the charge density difference between the two graphene layers, 
  \item which is predicted to exhibit a charge density wave. The width of the smooth texture and the resulting pattern can be tuned by the interplay between the magnetic field and gate electric fields. 
  \item \textbf{USA} — We investigate the interaction-induced valley textured domain walls in bilayer graphene at the \(\nu = 0\) quantum Hall state, subject to a kink-like perpendicular electric field. Such a state can be realized in a double-gated suspended sample, where the electronic charge densities sign a line in the middle of the sample. Using the Hartree-Fock approximation, we find that the Coulomb interaction opens a gap between the two lowest-lying states near the Fermi level, and yields a smooth valley texture throughout the domain walls. Moreover, our results suggest possibilities to visualize the resulting texture via measuring the charge density difference between the two graphene layers, 
  \item which is predicted to exhibit a charge density wave. The width of the smooth texture and the resulting pattern can be tuned by the interplay between the magnetic field and gate electric fields. 
\end{itemize}

\textsuperscript{1}Supported by NSF No. DMR-0654118, DMR-1004545, NSFC No. 11274403, and DOE No. de-sc0002140.

8:48AM A8.00005 Valley-kink in Bilayer Graphene at \(\nu = 0\): A Charge Density Signature for Quantum Hall Ferromagnetism\textsuperscript{1} CHIA-WEI HUANG, EFRAT SHIMSHONI, Department of Physics, Bar-Ilan University, Ramat Gan, 52900, Israel, HERBERT FERTIG, Department of Physics, Indiana University, Bloomington, IN 47405, USA — We investigate the interaction-induced valley patterns in bilayer graphene at the \(\nu = 0\) quantum Hall state, subject to a kink-like perpendicular electric field. Such a state can be realized in a double-gated suspended sample, where the electronic charge densities sign a line in the middle of the sample. Using the Hartree-Fock approximation, we find that the Coulomb interaction opens a gap between the two lowest-lying states near the Fermi level, and yields a smooth valley texture throughout the domain walls. Moreover, our results suggest possibilities to visualize the resulting texture via measuring the charge density difference between the two graphene layers, 

\begin{itemize}
  \item which is predicted to exhibit a charge density wave. The width of the smooth texture and the resulting pattern can be tuned by the interplay between the magnetic field and gate electric fields. 
\end{itemize}

\textsuperscript{1}We thank financial support from the US-Israel Binaitional Science Foundation (BSF)

9:00AM A8.00006 Cyclotron-resonance-induced photovoltaic effect in high-mobility graphene in the quantum Hall regime, SATORU MASUBUCHI, MASAKI OYAMA, MIHAO OARAI, Institute of Industrial Science, University of Tokyo, Japan, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Material Science, Japan, TOMOKI MACHIDA, Institute of Industrial Science, University of Tokyo, Japan — We have investigated the infrared photodetected voltage \(\Delta V\) in high-mobility graphene on hexagonal boron nitride in the quantum Hall regime. We observed \(\Delta V\) of up to several \(eV\) at \(\nu = \pm 2\) quantum Hall states under the cyclotron resonance conditions. The dependence of \(\Delta V\) on the bias current indicates that \(\Delta V\) signals derive from the photovoltaic effect rather than the bolometric effect. The dependence of \(\Delta V\) on the magnetic field direction and measurement geometry suggest the edge channel transport as an origin of photovoltaic effect. \(\Delta V\) signals were robust up to \(T = 180\) K, indicating that \(\Delta V\) signals can be used for developing novel terahertz photodetectors operating at high temperatures.

9:12AM A8.00007 Landau-level mixing in the fractional quantum Hall effect in graphene\textsuperscript{1}. MICHAEL PETERSON, California State University Long Beach, CHETAN NAYAK, Microsoft Research, University of California Santa Barbara — We study the effects of Landau level mixing on the fractional quantum Hall effect in graphene. Landau level mixing in graphene is especially important since the ratio of the Coulomb energy to the cyclotron energy is independent of magnetic field and of order one. In particular, we derive an effective Hamiltonian method that can be used to provide an accurate analytic description of the central Hofstadter band in the weak-field regime. One of the most important discoveries obtained in this work is that massless Dirac particles always exist inside the central Hofstadter band no matter how small the magnetic flux may become. In other words, with its bandwidth broadened by the lattice effect, the \(\nu = 0\) Landau level contains massless Dirac particles within itself. In fact, by carefully analyzing the self-similar recursive pattern of the central Hofstadter band, we conclude that massless Dirac particles should occur under arbitrary magnetic field. As a corollary, the central Hofstadter band also contains a self-similar structure of recursive Landau levels associated with such massless Dirac particles.

\textsuperscript{1}We acknowledge support from DARPA, Microsoft Station Q, and Cal State Long Beach Start-up.

9:24AM A8.00008 Self-similar occurrence of massless Dirac particles in graphene under magnetic field. JUN-WON RHIM, KWON PARK, Korea Institute for Advanced Study — Intricate interplay between the periodicity of the lattice structure and that of the cyclotron motion gives rise to a well-known self-similar fractal structure of the Hofstadter butterfly for an electron moving in lattice under magnetic field. Evolving from the \(n = 0\) Landau level, the central band of the Hofstadter butterfly is especially interesting since it may hold a key to the mysteries of the fractional quantum Hall effect in graphene. In this paper, we develop an effective Hamiltonian method that can be used to provide an accurate analytic description of the central Hofstadter band in the weak-field regime. One of the most important discoveries obtained in this work is that massless Dirac particles always exist inside the central Hofstadter band no matter how small the magnetic flux may become. In other words, with its bandwidth broadened by the lattice effect, the \(n = 0\) Landau level contains massless Dirac particles within itself. In fact, by carefully analyzing the self-similar recursive pattern of the central Hofstadter band, we conclude that massless Dirac particles should occur under arbitrary magnetic field. As a corollary, the central Hofstadter band also contains a self-similar structure of recursive Landau levels associated with such massless Dirac particles.

9:36AM A8.00009 Observation of the Hofstadter butterfly in graphene on boron nitride, PATRICK MAHER, CORY DEAN, CARLOS FORSYTHE, LEI WANG, FERESHTE GHAHARI, Columbia University, PILKYUNG MOON, MIKITO KOSHINO, Tohoku University, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, KEN SHEPARD, JAMES HONE, PHILIP KIM, Columbia University — In 1976, Douglas Hofstadter considered the general problem of 2D electrons subject to both a magnetic field and a periodic potential. His solution predicted a remarkably complex energy spectrum exhibiting self-similar fractal structure, termed the Hofstadter Butterfly. Experimental exploration of this problem has been limited by the difficulty of fabricating a system with a lattice constant on the order of the magnetic length. It has recently been shown that single layer graphene on hexagonal-BN develops a Moiré pattern with a length of up to 15 nm when the rotational angle between the two lattices approaches zero. We present data demonstrating that for bilayer graphene on hexagonal boron nitride, the effect of the modulation potential associated with the Moiré pattern is large enough to be observable by standard transport. Under large magnetic fields, additional gaps appear within the usual bilayer quantum Hall spectrum, consistent with calculations of the Hofstadter spectrum. We present the first direct experimental evidence of the longstanding theoretical prediction that the gaps arising from the superlattice are characterized by two integer quantum numbers.
9:48AM A8.00010 Symmetry Breaking in Hofstadter’s Butterfly in graphene1, CARLOS FORSYTHE, Department of Physics, Columbia University, CORY DEAN, LEI WANG, Department of Mechanical Engineering, Columbia University, PATRICK MAHER, FERESHTE GHAHARI, Department of Physics, Columbia University, PILKYUNG MOON, MIKIKO KOSHINO, Department of Physics, Tohoku University, TAKASHI TANIGUCHI, KENJI WATANABE, National Institute for Materials Science, KEN SHEPARD, Department of Electrical Engineering, Columbia University, JIM HONE, Department of Mechanical Engineering, Columbia University, PHILIP KIM, Department of Physics, Columbia University — We will present magnetotransport measurements in hBN encapsulated bilayer graphene devices where one of hBN substrates provides a weak modulation of lattice potential. Under a strong magnetic field, interplay between periodic electric potential and quantizing magnetic field lead to a fractal energy spectrum known as Hofstadter’s butterfly. In graphene, while spin and layer symmetry breakings are expected in dual gated devices under large magnetic fields, valley symmetry breaking in the Hofstadter regime is not so easily understood. We will present the observance of these measured gaps along with a discussion of symmetry breaking at these gaps. Through careful modulation of temperature and electron density, we have extracted a range of activation energies associated with symmetry breakings.

1the speaker acknowledges support from the Columbia Optics and Quantum Electronics IGERT under NSF grant DGE-1069420

10:00AM A8.00011 Andreev Reflections and Superconducting Proximity Effect in lateral BN/Graphene/NbSe2 Heterostructures in the Integer Quantum Hall Regime, DMITRI K. EFETOV, CLEVIN HANDSCHIN, CORY DEAN, LEI WANG, PHILIP KIM, Columbia University, KIM GROUP TEAM — Inducing Superconductivity (SC) via proximity effect into the topo logical edge states of a 2D conductor in the Quantum Hall Regime (QHE) has been a long standing proposition which has recently reinvigorated attention. Here the combination of SC and QHE has a wide range of predictions such as the appearance of additional edge-states in the integer QHE. With the recent development of high mobility graphene on h-BN with an extremely low onset of the QHE (0.5T) and its high compatibility with various superconductors the road to test these predictions is now open. In this study we present lateral magneto-transport and electronic spectroscopy measurements of BN/graphene/NbSe2 heterostructures. We find that the NbSe2/graphene superconductor-normal metal interface (SN) has a very high transparency with extremely low electrical resistances of R∼100ohm and gives rise to Andreev reflections and a strong SC proximity effect in graphene below the critical SC transition temperature Tc ∼ 7.2K. The high mobility of the graphene on h-BN and the relatively high SC upper critical magnetic field of NbSe2 Hc2 ∼ 5T allow for a wide magnetic field range of 1-5T in which the SC and the QHE coexist.

10:12AM A8.00012 Edge magnetoplasmons in graphene: determination of carrier drift velocity in Quantum Hall regime1, IVANA PETKOVIC, F.I.B. WILLIAMS, KEYAN BENNACEUR, FABRIQUE PORTIER, PATRICE ROCHE, D.C. GLATTLI, Service de Physique de l’Etat Condense/IRAMIS/DSM (CNRS URA 2464), CEA Saclay, F-91191 Gif-sur-Yvette — Edge Magneto-Plasmons (EMP) are gapless quasi 1D elementary excitations which are split off from the bulk magneto-plasmon modes by the sample boundary, and are a tool of choice to investigate the structure of the edge of a 2D electron systems. We give a first experimental demonstration of their presence in graphene in the quantum Hall regime and use our results to evaluate the carrier drift velocity along the edge [1]. The group velocity of these modes is a sum of the Hall conductivity contribution and the carrier drift velocity at the edge. In graphene, due to its particular dynamics and an abrupt edge, the drift velocity is expected to be of the order of the Fermi velocity, thus becoming experimentally accessible. We show EMP to exist by timing the travel of narrow wave-packets on picosecond time scales around exfoliated samples. They show chiral propagation with low attenuation at a velocity which is quantized on Hall plateaus. We extract the carrier drift contribution and find it to be slightly less than the Fermi velocity, as expected for an abrupt edge. We also extract the spatial spread of edge accumulated charge and find it to be narrower than for soft edge systems.

1We acknowledge ERC Grant # 228273 and RTRA “Ganet” Grant.

10:24AM A8.00013 Quantum spin Hall effect in the graphene zero energy Landau level - Part I, ANDREA F. YOUNG, JAVIER D. SANCHEZ-YAMAGISHI, BEN HUNT, PABLO JARILLO-HERRERO, RAY C. ASHOORI, MIT, TAKASHI TANIGUCHI, KENJI WATANABE, NIMS — Shortly after the experimental discovery of graphene, it was predicted that Zeeman splitting of the graphene zero energy Landau level results in a quantum spin Hall phase, characterized by counterpropagating spin-filtered edge states. However, experimental realization of this state has been obscured by the existence of competing Coulomb interaction-driven insulating phases. We address this problem by fabricating monolayer graphene devices in which the Coulomb interaction is heavily screened by a proximal graphite gate. Despite the reduction in the strength of intralayer interactions, the resulting high mobility graphene on h-BN encapsulated bilayer graphene devices where one of hBN substrates provides a weak modulation of lattice potential. Under a strong magnetic field, interplay between periodic electric potential and quantizing magnetic field lead to fractal energy spectrum. In graphene, while spin and layer symmetry breakings are expected in dual gated devices under large magnetic fields, valley symmetry breaking in the Hofstadter regime is not so easily understood. We will present the observance of these measured gaps along with a discussion of symmetry breaking at these gaps. Through careful modulation of temperature and electron density, we have extracted a range of activation energies associated with symmetry breakings.

10:36AM A8.00014 Quantum spin Hall effect in the graphene zero energy Landau level - Part II, JAVIER D. SANCHEZ-YAMAGISHI, ANDREA F. YOUNG, BENJAMIN HUNT, MASSACHUSETTS INSTITUTE OF TECHNOLOGY, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, RAY C. ASHOORI, PABLO JARILLO-HERRERO, MASSACHUSETTS INSTITUTE OF TECHNOLOGY — Zeeman splitting of graphene’s zeroth Landau level has been predicted to lead to a quantum spin Hall effect, but a competing interaction-driven insulating state has hampered previous attempts to drive the graphene into this regime. By using a proximal graphite gate to screen Coulomb interactions in the graphene, we are able to reduce the strength of the competing insulating state and observe a continuous transition to a conductive state as a function of in-plane field. We study this transition simultaneously in capacitance and transport, and find that despite conduction increasing by many orders of magnitude with in-plane field the bulk remains gapped throughout the transition. These observations indicate the continuous closing of transport gap along the edge of the sample, with resulting counter-propagating edge states that are characteristic of the quantum spin Hall effect. We discuss the behavior of this transition across multiple samples with various levels of Coulomb screening, and present nonlinear multitemporal transport measurements designed to probe the nature of backscattering within the edge states. We also comment on the implications of our work for the rest of the graphene phase diagram at high magnetic fields.
10:48AM A8.00015 Role of the charge inhomogeneity on the breakdown of the quantum Hall effect in narrow single layer graphene devices\textsuperscript{1} . CENK YANIK, ISMET KAYA, Sabanci University, QUANTUM TRANSPORT AND NANOELECTRONICS LABORATORY TEAM — The breakdown of the quantum Hall effect, which is observed as an abrupt escalation in the longitudinal resistance with an associated loss in the quantization of Hall voltage is the major obstacle against improving the resistance standard which is currently based on this effect. Graphene is inherently a 2D material and has an unusual band structure that allows the quantization of the Hall resistance even at room temperature. These unique properties of graphene make it a good candidate as a high precision metrological characterization tool for the quantum Hall resistance. The uncertainty in the quantum Hall resistance in graphene has been rapidly improving recently and graphene samples have already been shown to reach the precision of the current best 2DEG samples. In this talk, experimental results on the breakdown of the quantum Hall effect in graphene on SiOx is presented. In narrow graphene samples of 1 micrometer width, the charge inhomogeneity is quite prominent and strongly affects the non dissipative transport in the quantum Hall regime. It is observed that in such samples the quantization of the Hall resistance can retain at high current densities in the excess of 1 A/m even in the presence of dissipative potential along the longitudinal probes.

\textsuperscript{1}This work is supported by Tubitak under the grant number 107T855

Monday, March 18, 2013 8:00AM - 10:48AM –
Session A29 DCMP: Three Dimensional Topological Insulators: Chalcogenides

8:00AM A29.00001 Superconductivity in a topological insulator Sb\textsubscript{2}Te\textsubscript{3} . LUKAS ZHAO, HAIMING DENG, MILAN BEGLIARBEKOV, INNA KORZHOVSKA, ZHIYI CHEN, JEFFREY SECOR, LIA KRUSIN-ELBAUM, CCNY — We report an observation of superconductivity in a topological material Sb\textsubscript{2}Te\textsubscript{3} synthesized under modest pressure (\textasciitilde 5.5 MPA ) that has the zero-field superconducting transition temperature $Tc \sim 5.3$ K. High resolution TEM and XRDI refinement analysis of the superconducting crystals show that while there is a 0.2\% elongation of the lattice parameter in the c-direction, the rhombohedral van der Waals unit cell structure is preserved. The upper critical field $Hc2$ anisotropy is surprisingly small, only \textasciitilde 1.5, much smaller than the crystalline anisotropy of \textasciitilde 8. This anisotropy appears consistent with the paramagnetically limited critical field, given the reported large value (\textasciitilde 10) of the g-factor. The diamagnetic state of this new superconductor is also unusual, since even in the normal state the system supports large orbital currents. We will discuss our observations in the context of topological superconductivity and Dirac energy-momentum dispersion of the surface states.

8:12AM A29.00002 Bi\textsubscript{1-x}Sb\textsubscript{x}(110): A non-closed packed surface of a topological insulator . LUCAS BARRETO, WENDELL SIMOES E SILVA, MALTIE STENSGAARD, SOREN ULLSTRUP, MARCO BIANCHI, XIE-GANG ZHU, MATTEO MICHIAIRD, MACIEJ DENDZIK, PHILIP HOFMANN, Department of Physics and Astronomy, Aarhus University, Denmark — Topological insulators are characterised by an insulating bulk band structure, but topological considerations require their surfaces to support gap-less, metallic states. Meanwhile, many examples of such materials have been predicted and found experimentally, but experimental effort has concentrated on the closed-packed (111) surface of these materials. Thus, the theoretical picture of an insulating bulk embedded in a metallic substrate from all sides of a crystal still needs to be confirmed. Here we present angle-resolved photoemission spectroscopy results from the (110) surface of the topological insulator Bi\textsubscript{1-x}Sb\textsubscript{x} (x = 0.15). The observed band structure and Fermi contour are in excellent agreement with theoretical predictions and slightly different from the electronic structure of the parent surface Bi(110), in particular around the X\textsubscript{1} time-reversal invariant momentum. We argue that the preparation of surfaces different from (111) opens the possibility to tailor the detailed electronic structure and properties of the topological surface states.

8:24AM A29.00003 Mass acquisition of Dirac fermions in the presence of magnetic doping in the topological insulator Sb\textsubscript{2}Te\textsubscript{3} . YEPING JIANG, CNAM, University of Maryland, ZHI LI, CANLI SONG, KE HE, LILI WANG, Institute of Physics, CAS, XI CHEN, Department of Physics, Tsinghua University, XUCUN MA, Institute of Physics, CAS, QIKUN XUE, Department of Physics, Tsinghua University — The nontrivial bulk band topology and time reversal symmetry yield gapless surface states in three dimensional topological insulators. The gapless nature of surface states in strong topological insulator is protected by the nontrivial bulk band topology, which is expected to be violated by time-reversal-symmetry breaking perturbations, which opens back-scattering channels between Kramers pairs and induces a massive gap near the Dirac point of surface states. Such a massive Dirac fermion system gives rise to an unconventional magnetoelectric response relating to many exotic phenomena such as half-quantized anomalous Hall effect, topological quantized magnetoelectric effect and even the magnetic monopole. Here we introduce time-reversal symmetry breaking by doping Cr atoms into the topmost quintuple layer and into the bulk of Sb\textsubscript{2}Te\textsubscript{3} thin films. We demonstrate for the first time by Landau level spectroscopy the deviation of zero modes, which indicates the acquisition of a mass term in the presence of surface or bulk magnetic doping. We also show that the magnitude of the mass term in the surface states depends on both the Cr doping level and the magnetic field, offering a new way of measuring the doping- and field-dependence of local magnetization of dopants. Our observation suggests Cr-doped Sb\textsubscript{2}Te\textsubscript{3} is a promising candidate for realization of proposed novel magnetoelectric effects.

8:36AM A29.00004 ABSTRACT WITHDRAWN –

8:48AM A29.00005 Possible topological insulating state in bismuth doped with arsenic: magneto-optical study . G.M. FOSTER, S.V. DORDEVIC, The University of Akron, N. STOJILJCOVIC, University of Wisconsin Oshkosh, M.V. NIKOLIC, Institute for Multidisciplinary Research, University of Belgrade, S.S. VUJATOVIC, Z.Z. DJURIC, P.M. NIKOLIC, Serbian Academy of Sciences and Arts, Z. CHEN, Z.Q. LI, National High Magnetic Field Laboratory, Tallahassee — Bismuth and its alloys with antimony have attracted attention in recent years due to their potential for novel electronic and magnetic properties. In particular, bismuth doped with arsenic is a promising candidate for realization of proposed novel magnetoelectric effects. In this study we have used infrared and magneto-optical spectroscopies to probe the photoresponse of bismuth doped with 1.0 \% of arsenic. The spectra will be presented for temperatures down to 5 K, and in magnetic fields as high as 18 Tesla. These results reveal strong magneto-optical activity, especially around the plasma minimum in reflectance. These findings will be compared and contrasted with magneto-optical results on topological insulator Bi\textsubscript{1-x}Sb\textsubscript{x}.

9:00AM A29.00006 Exotic magnetic properties of diluted magnetic binary chalcogenides . MAIA G. VERNGINI, Max Planck Institute of Microstructure Physics, XABIER ZUBIZARRETA, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany, MIKHAIL M. OTROOKOV, Tomsk State University, 634050 Tomsk, Russia, IGOR V. MAZNICHENKO, JURGEN HENK, Institut f黵 Physik, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany, EVGUENI V. CHULKOV, Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain, ARTHUR ERNST, Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — Using first-principles Green function approach we studied electronic and magnetic properties of diluted magnetic binary chalcogenides A\textsubscript{2}B\textsubscript{2-x}S\textsubscript{x}, doped with transition metals substituting the A element. The electronic structure of the impurities in the chalcogenides is mainly featured by the crystal field splitting. We found that two main mechanisms are responsible for long-range magnetic order in these materials: hole mediated magnetism within the layer of A atoms and indirect interaction between magnetic moments via a B atom. We also estimated Curie temperature of these systems, which was found in good agreement with the available experimental data. Our results shed light on the understanding of magnetic interaction and control in topological insulators.
Magneto-transport properties of the ternary topological insulator (Bi$_{0.5}$Sb$_{0.5}$)$_2$Te$_3$ in the presence of electrostatic gating and magnetic impurity, LIUQI YU, JORGE BARREDA, LONGQIAN HU, P. XIONG, Department of Physics, Florida State University, USA, TONG GUAN, XIAOYUE HE, K. WU, Y. LI, Institute of Physics, Chinese Academy of Sciences, China — A three-dimensional topological insulator, (Bi$_{0.5}$Sb$_{0.5}$)$_2$Te$_3$, is used to characterize the electronic properties of the spin helical conducting surface state. Epitaxial films are grown via MBE on (111) SrTiO$_3$ substrate, which serves as the gate dielectric. Magnetoresistance (MR) and Hall effect measurements have been performed at various back gate voltages. Ambipolar field effect has been observed, enabling effective tuning of the Fermi level across the band gap. Weak antilocalization effect is identified and used to differentiate the surface state. The Hikami-Larkin-Nagaoka (HLN) equation is used to analyze the MR data and the results show the top and bottom surfaces become decoupled when the Fermi level is in the bulk band gap. We also examine the effects of paramagnetic impurity (MI), which introduces time reversal symmetry breaking scattering, on the TI surface states. Taking advantage of the unique capability of in situ deposition in a customized dilution refrigerator, paramagnetic Cr atoms were incrementally quench-condensed onto the sample surface and transport measurements were performed at each MI density. The procedure eliminates any sample-to-sample variation and complications from air exposure. Pronounced changes in the weak antilocalization effect and the sample carrier density with increasing MI concentration were observed. Possible origins of these observations will be discussed.

Observations will be discussed.

Visualizing Landau levels of Dirac electrons in Bi$_2$Te$_3$ in a one dimensional potential, DANIEL WALKUP, YOSHINORI OKADA, WENWEN ZHOU, CHETAN DHITAL, YING RAN, ZIQIANG WANG, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — When a magnetic field is applied to a solid, the electrons fall into discrete, highly degenerate Landau levels. In each Landau level the wavefunction has a certain characteristic spread, which increases with the energy (index) of the level. This has important physical consequences especially in the presence of spatial inhomogeneity. Using scanning tunneling spectroscopy, we have examined the Dirac electrons on Bi$_2$Te$_3$ under a magnetic field and subject to a smooth one-dimensional periodic potential. We find that the lowest Landau levels track the potential variation, but the higher levels are more homogeneous. Through a calculation of the Landau level wavefunctions, we form a coherent picture of how their spread interacts with the potential landscape, explain the experimental data. Our findings have important implications for transport and magneto-resistance measurements in Dirac materials with engineered potential landscapes.

Topological States Ruled by Stacking Faults in Bi$_2$Se$_3$ and Bi$_2$Te$_3$, LEANDRO SEIXAS, LEONARDO ABDALLA, Universidade de Sao Paulo, TOME SCHMIDT, Universidade Federal de Uberlandia, ADALBERTO FAZZIO, Universidade de Sao Paulo, ROBERTO MIWA, Universidade Federal de Uberlandia — Extended defects like stacking faults (SF) can originate topologically protected metallic states in bulk topological insulators (TIs). These induced topological states are a response to the weakening of the inter-layer van der Waals interactions due to the SF defect. In TI thin films the degeneracy of Dirac bands of opposite surfaces can be lifted upon the formation of SF defects. Such slab asymmetry can promote a net spin current, absent of backscattering processes, in thin film made of TIs. These results have been obtained by fully relativistic first principles calculations.

Proximity effect in MBE grown bismuth chalcogenide thin films, BRIAN MULCAHY, MAO ZHENG, CAN ZHANG, ALLISON DOVE, ZACHARY R. YOSCOVITS, GUSTAF OLSON, JAMES N. ECKSTEIN, University of Illinois at Urbana-Champaign — Topological insulators (TIs) comprise a new state of matter which provides access to novel physics. Of the set of materials that have exhibited spectroscopic evidence of topologically protected surface states, bismuth chalcogenide systems have garnered particular interest due to their relatively large nominal bulk band gap and a single Dirac cone near the Fermi surface. We are studying the superconducting proximity effect in MBE grown thin films of Bi$_2$Se$_3$, Bi$_2$Te$_3$, and related compounds. After in situ deposition of a low temperature superconductor, the films are patterned into devices containing a matrix of superconducting islands of tunable size and density on top of the TI layer. We discuss growth optimization, device processing, the role of the superconductor-TI interface, and proximity effect transport results.

Topological phase transition induced by atomic displacements in PbS and PbTe, JINWOOONG KIM, Dept. of Physics, POSTECH, SEUNG-HOON JHI, Dept. of Physics and Division of Advanced Materials Science, POSTECH — Discovery of 3D topological insulator initiates exploration of finding new materials having topological insulating phase or mechanisms for topological phase transitions. Introducing interactions or strains into non-interacting electron systems, for example, can produce non-trivial topological phases in them otherwise having trivial band insulating phase at equilibrium conditions. Using first-principles methods, we study emerging topological phases in band insulating PbS and PbTe, which are induced by selective atomic displacements. Phonon modes corresponding to the displacements are identified and conditions of inducing the topological phase transition are suggested. We show that surface states develop flickering Dirac cones at band-inversion k-points upon dynamic atomic displacements with sufficient amplitude. Our results demonstrate that elementary excitation modes like phonon can induce topological phases in trivial band insulators.

Optical selection rules for electron-hole pair excitation in 3D topological insulators, HARI PAUDEL, MICHAEL LEUENBERGER, University of Central Florida — Experiments using ARPES, which is based on the photoelectric displacements with sufficient amplitude. Our results demonstrate that elementary excitation modes like phonon can induce topological phases in trivial band insulators.

Disorder tuned anomalous Hall effect in thin films of Cr doped topological insulators, ZHIYI CHEN, LUKAS ZHAO, INNA KORZHOVSKA, HAIMING DENG, The City College of New York - CUNY, SIMONE ROAUX. JEAN JORDAN, IBM Research - Yorktown, LIA KRUSIN, The City College of New York - CUNY — The anomalous Hall effect (AHE) — an appearance of a voltage transverse to the electric current in the absence of an external magnetic field — is a process that arises from the spin-orbit coupling between current and magnetic moments that has been fundamentally linked to the topological nature of the Hall current. Recent first-principle calculations predict that when topological insulators (TIs) are doped with transition metal ions, such as Cr or Fe, a novel magnetically ordered insulating state will form — a state that in thin samples may support a quantized anomalous Hall conductance. Here we report an observation of AHE in rf sputtered thin Cr doped films of Bi$_2$Te$_3$. The anomalous Hall resistivity $\rho_{xy}$ scales with the longitudinal resistivity squared, $\rho_{xx}^2$, and a distinct ferromagnetic hysteresis response (loops) at temperatures below 10 K with coercive fields of the order of 0.5 T is observed. In as-deposited films the resistivity is below the resistivity quantum $h/e^2$. Using 2.5 MeV electron beam irradiation with varying fluence we can tune the resistivity upward by orders of magnitude. A large effect of controlled quenched point disorder on the quantization of AHE in Bi$_2$Te$_3$ will be discussed.
8:00AM A30.00001 Long range transport of colloids in aqueous solutions, DANIEL FLOREA, SAMI MUSA, JACQUES M.R.J. HUYGHE, HANS M. WYSS, Eindhoven University of Technology — Colloids in aqueous suspensions can experience strong, extremely long range repulsive forces near interfaces such as biological tissues, gels, ion exchange resins or metals. As a result exclusion zones extending over several millimeters can be formed. While this phenomenon has been previously described, a physical understanding of this process is still lacking. This exclusion zone formation is puzzling because forces acting over such long distances are not expected. In this paper we will present results of a systematic study of the influence of various parameters on the formation of these exclusion zones. We present a simple model that accounts for our experimental data and directly links the exclusion zone formation to an already known physical transport phenomenon. We show that the effect can be tuned by changing the zeta potential of the particles or by varying the species present in the aqueous solution. We thus provide a direct physical explanation for the intriguing exclusion zone formation and we illustrate how this effect can be exploited in a range of industrial applications.

8:12AM A30.00002 Transport of charged colloidal particles in a nonpolar solvent in response to an electric field, TINA LIN, THOMAS KODGER, DAVID WEITZ, Harvard University — In nonpolar solvents, particle charging is often controlled through the addition of suitable surfactants, which form charge-stabilizing reverse micelles. By combining microfluidics and confocal microscopy, we directly visualize the dynamics of charged colloidal particles in a nonpolar solvent with reverse micelles in response to an external electric field; this enables us to probe the internal electric field as well as the charging properties of the particle solution. We discover some surprising particle behavior: despite a constant applied electric field, particle transport through the fluid is nonlinear and the apparent particle mobility decays in time; subsequently, the charged particles appear to diffuse freely within the bulk solution. We characterize this behavior and find that the charged reverse micelles play a significant role.

8:24AM A30.00003 Revisiting Taylor Dispersion: Differential enhancement of rotational and translational diffusion under oscillatory shear, BRIAN LEAHY, Department of Physics, Cornell University, DESMOND ONG, Cornell University, XIANG CHENG, ITAI COHEN, Department of Physics, Cornell University — The idea of Taylor dispersion - enhancement of translational diffusion under shear - has found applications in fields from pharmacology to chemical engineering. Here, in a combination of experiment and simulations, we study the translational and rotational diffusion of colloid dimers under triangle-wave oscillatory shear. We find that the rotational diffusion is enhanced, in addition to the enhanced translational diffusion. This “rotational Taylor dispersion” depends strongly on the strain rate (Peclet number), aspect ratio, and the shear strain, in contrast to the translational Taylor dispersion in a shear flow, which depends only weakly on strain rate and aspect ratio. This separate tunability of translations and orientations promises important applications in mixing and self-assembly of solutions of anisometric colloids. We discuss the corresponding effects on the structure and rheology of denser suspensions of rod-like particles.

8:36AM A30.00004 Hydrodynamic Behavior of Colloidal Nanorods and Characterization of Length Distributions, CARLOS SILVERA BATISTA, CONSTANTINE KHIRPIN, XIAOMIN TU, MING ZHENG, JEFFREY FAGAN, National Institute of Standards and Technology — Single-walled carbon nanotubes (SWCNTs) are 1D, cylindrical, structures of carbon with long persistence lengths and consistent diameters. In this talk, I will discuss the use of doubly sorted SWCNTs (by buoyancy and length), which are effectively colloidal rods, to explore experimentally the effectiveness of theoretical approximations for the hydrodynamic drag of a freely rotating rod. The objective of this work is to establish and validate the use of Analytical Ultracentrifugation (AUC) as a technique to measure the length distribution of rodlike colloidal particles including SWCNT dispersions. This is particularly necessary for applications of nanotube dispersions, as the transport, optical, and thermal properties, as well as the toxicity of SWCNTs have all been demonstrated to depend on the length. Contrary to AFM, the technique most commonly used to measure length distributions, AUC is able to measure the whole population of particles as they exist in liquid phase. I will present measurements and analysis of SWCNT samples with narrow distributions in length, diameter and buoyancy as measured through AUC and compare them against independent measurements conducted with AFM. Using this data, the validity of hydrodynamic theory for this application is verified.

8:48AM A30.00005 Clustering of Attractive Colloids in Flow, MING HAN, Northwestern University, JONATHAN K. WHITMER, University of Wisconsin-Madison, ERIK LUIJTEN, Northwestern University — The behavior of colloidal suspensions under flow is important for numerous applications, including direct-write techniques employing “colloidal ink.” Here we investigate the behavior of colloids flowing through narrow channels. When colloidal particles experience sufficiently strong attractive interactions, cluster formation and ultimately gelation may result. We employ computer simulations to investigate how the size and structure of these clusters, as well as their distribution in the flow, is influenced by various experimental variables, including flow velocity, attraction strength, fluid viscosity, and channel diameter. These simulations incorporate explicit hydrodynamics through the multiparticle collision dynamics (MPC) algorithm. Particular attention is paid to the role of channel boundaries and to the dimensionless parameters characterizing the suspension.
Gcracking behavior. By adding emulsion droplets into colloidal suspensions, we systematically decrease the storage modulus, G".

Department of Physics, The Chinese University of Hong Kong, Hong Kong — When colloidal suspensions dry, stresses build up and cracks often occur — a phenomenon undesired for important industries such as paint and ceramics. We demonstrate that the two viscoelastic moduli, G" and G'"', determine the cracking behavior. By adding emulsion droplets into colloidal suspensions, we systematically decrease the storage modulus, G" and effectively decrease the amount of cracks. At a critical droplet concentration, cracking disappears completely. Furthermore, adding droplets also varies the speed of air invasion and provides a powerful method to adjust drying rate. With the effective control over cracking and drying rate, our experiment may find important applications in many drying and cracking related industrial processes.

9:12AM A30.00007 Determination of the hydrodynamic friction matrix for various anisotropic particles

1 Financial support through a Rubicon grant by the Netherlands Organisation for Scientific Research.

9:24AM A30.0008 Enhanced Diffusion in Quasi-Two-Dimensional Suspensions

9:36AM A30.00009 Vibrational properties of dense colloidal suspensions with short-range interparticle attraction

1 Project supported by jointed scholarship of Chinese Academy of Sciences and Max-Planck Society

10:00AM A30.00011 Order Preservation Between Brownian Particles Modeled By Langevin Dynamics

1 This work was supported by NIH grant 1R21HG005100-01.

10:12AM A30.00012 Eliminating cracking during drying

9:00AM A30.00006 Measurements of anisotropic Brownian motion of colloidal clusters

10:00AM A30.00011 Order Preservation Between Brownian Particles Modeled By Langevin Dynamics

1 This work was supported by NIH grant 1R21HG005100-01.
10:24AM A30.00013 Aging in Colloidal Glasses: a comparison between micro and macro rheology1 , XIAOJUN DI, XIAOGUANG PENG, GREGORY MCKENNA, Texas Tech University, TEXAS TECH UNIVERSITY TEAM — The analogy between colloidal dynamics and the dynamics of molecular glasses remains an important area of study. Of particular interest to our team is the aging responses of the two systems. We have been investigating the dynamics of colloidal systems composed of thermosensitive particles that change diameter upon change of temperature and comparing the behavior to what is expected in molecular glass-formers. In particular, we have found that concentration jumps in these systems mimic three important behaviors of molecular glasses: the intrinsic isotherm, the asymmetry of approach, and memory effect. In our early work, we were able to show, using multiscale diffusing wave spectroscopy, that although the three signatures are observed in the concentration jump conditions, they are not identical to the observations in molecular glasses. In the present work, in order to get better resolution for the temperature dependent properties, we are employing PNIPAAM/PS particles with core-shell structure to lessen the temperature sensitivity of the system. A series of different particles with different PNIPAAM fractions (different thermal sensitivity) is being investigated and a comparison of the aging between the microrheology and the macro rheology will be made.

1 NSF CBET-1133279

10:36AM A30.00014 When Colloids Can Deform, JIE ZHANG, CHANGQIAN YU, SUNG CHUL BAE, STEVE GRANICK, UIUC — Most colloidal systems that have been explored so far are hard-spheres, which limits their phase behavior and other physical properties to be not so rich as atomic and molecular systems. Here we present a new class of soft and deformable microgel colloidal particles with thermo-sensitivity and ability to display autonomous oscillation when driven by special fuels. The deformability, size changes and structure formation of micron-sized poly(NIPAM) particles and dumbbells of polystyrene-poly(NIPAM) interpenetrating networks can be imaged in situ and analyzed. Other mechanical and other physical properties attributable to deformability can be measured.

Monday, March 18, 2013 8:00AM - 10:48AM
Session A35 DCMP: Superconductivity: Tunneling Phenomena 343 - John Zasadzinski, Illinois Institute of Technology

8:00AM A35.00001 Scanning Tunneling Microscopy of Fe Impurities in Bi2Sr2CaCu2O8+d , MICHAEL BOYER, BRIAN KOOPMAN, LING FU, Clark University, W.D. WISE, KAMALESH CHATTERJEE, MIT, GENDA GU, Brookhaven National Laboratory, E.W. HUDSON, Penn State University — We utilize scanning tunneling microscopy measurements to probe the effects of intentionally doped magnetic Fe impurities in the high-temperature superconductor Bi2Sr2CaCu2O8+d. Our spectroscopy measurements indicate an absence of particle-hole symmetry in impurity affected regions. In addition, we find evidence that the Fe impurities which substitute for Cu atoms in the CuO2 plane are shifted from their expected locations. Both of these findings are in contrast to previous STM measurements on magnetic Ni impurities in Bi2Sr2CaCu2O8+d which find spectra which are overall particle-hole symmetric and centered at Cu sites.[1] Interpretations of our measurements may help us understand on a local scale why introduced Fe impurities are more detrimental to superconductivity than Ni impurities as determined by bulk measurements.[2] [1] E.W. Hudson et al., Nature 411, 920 – 924 (2001). [2] T.D. Hien et al., J. Magn. Magn. Mater. 262, 506 – 513 (2003).

8:12AM A35.00002 Can STM detect nematic ordering in underdoped Bi2Sr2CaCu2O8+x or other correlated systems?1 , EDUARDO DA SILVA NETO, PEGOR AYNAJIAN, Princeton University, SHIMPEI ONO, CRIEPI, Japan, RYAN BAUMBACH, ERIC BAUER, Los Alamos National Laboratory, JOHN MYDOSH, Kamerling Onnes Laboratory, Leiden University, ALI YAZDANI, Princeton University — Electronic nematic phases, where, for example, the electronic states undergo a spontaneous four-fold (C4) to two-fold (C2) symmetry breaking, have recently gained vast interest as a possible candidate for various hidden order states in several correlated electron systems such as cuprates, pnictides, and heavy-fermions. Such states are difficult to detect using non-local probes because of possible twin domain structures in macroscopic samples. STM spectroscopy has been proposed as a possible approach to detect such nematic orders, with several recent experiments reporting signals in the cuprates and iron-based superconductors. We specifically investigate the situation in which STM topographic data shows C4 symmetry while energy-resolved spectroscopic maps signal C2 symmetry. We find that such behavior can in fact occur for asymmetric tip geometries and discuss both model calculations and experimental results that provide evidence for this false nematic signature. We discuss possible future STM experiments that could unambiguously detect electronic nematic order.

1Work supported by the Office of Basic Energy Science of the DOE and NSF-DMR.

8:24AM A35.00003 STM investigation of incipient order in Bi2Sr2CaCu2O8+d , PEGOR AYNAJIAN, EDUARDO H. DA SILVA NETO, Princeton University, SHIMPEI ONO, Komae, Tokyo, JINSHENG WEN, ZHIJUN XU, GENDA GU, Brookhaven National Laboratory, ALI YAZDANI, Princeton University — We investigate the spatial and momentum structure of electronic excitations in underdoped samples of the high-temperature superconductor Bi2Sr2CaCu2O8+d using spectroscopic mapping with the scanning tunneling microscope. A defining feature of the electronic states in these samples is a strong Cu-O bond oriented modulation of the local density of states (Q*). Characterizing Q* as a function of temperature and doping we have established that it appears at the onset of the pseudogap phase at T*, above the regime attributed to fluctuating superconductivity [1]. Model calculations that include both the effects of impurity-induced quasiparticle scattering and incipient order reproduce the energy-dispersion of the measured Q* below and above Tc near optimal doping — where incipient order effects are weak [2]. To extend our understanding to the underdoped samples, we have carried out new high-resolution spectroscopic mapping measurements as a function of doping which more clearly identify the low-energy signatures of the incipient order.

8:36AM A35.00004 Studies of Magnetic Impurities in Bi2Sr2CaCu2O8+d, EDUARDO CALLEJA, JIXIA DAI, University of Colorado at Boulder, GENDA GU, Brookhaven National Laboratory, KYLE MCELROY, University of Colorado at Boulder — Impurities in high temperatures superconductors, studied with spectroscopic imaging tunneling spectroscopy (SI-STS) have served as a valuable tool to investigate the electronic structure of these materials (E.W. Hudson et al., Nature 411, 920 (2001); S.H.Pan et al., Nature 403,746 (2000)). These experiments revealed the appearance of a quasi-localized bound state near the impurity site whose structure is sensitive to the superconducting gap symmetry and the band structure and originates from the charge scattering nature of these impurities. We studied the effects of Fe impurities in Bi2Sr2CaCu2O8+d and discovered that the impurities have a different behavior than those previously observed. In particular the quasi bound state near the impurity seems to be behaving as that predicted for a magnetic impurity. The superconducting gap and local electronic density of states was studied in the vicinity of the impurities using SI-STS and will be presented.
8:48AM A35.00005 Persistent electrical doping of Bi2Sr2CaCu2O8+x mesa structures, HOLGER MOTZKAU, THORSTEN JACOBS, SVEN-OLOF KATTERWE, ANDREAS RYDH, VLADIMIR M. KRASNOV, Stockholm University, 106 91 Stockholm, Sweden — We study resistive switching phenomena in small Bi2Sr2CaCu2O8+x (Bi-2212) mesa structures. Applying a significantly large bias voltage or short current pulses, we are able to controllably and reversibly manipulate the normal state resistance and doping state of the same single crystal from an underdoped to the overdoped state without changing its chemical composition. We employ this effect for an analysis of the doping dependence of the electronic spectra of Bi-2212 single crystals by means of intrinsic tunneling spectroscopy. It is observed that such a physical doping is affecting superconductivity in Bi-2212 similar to chemical doping by oxygen impurities: with overdoping the superconducting gap decreases, indicating the presence of the critical doping point. We distinguish two main mechanisms of persistent electric doping: (i) even in voltage contribution, attributed to a charge transfer effect, and (ii) odd in voltage contribution, attributed to reordering of oxygen impurities.

9:00AM A35.00006 Tunneling Spectroscopy of Heavily Underdoped Bi2212 Films, NICKOLAS GROLL, Argonne National Laboratory, CHAOYUE CAO, IIT Chicago and Argonne National Laboratory, MIKE HINTON, THOMAS LEMBERGER, Ohio State University, THOMAS PROSLIER, Argonne National Laboratory, JOHN ZASADZINSKI, IIT Chicago and Argonne National Laboratory — SIS break junctions and the pseudogap decrease, indicating the presence of the critical doping point. We distinguish two main mechanisms of persistent electric doping: (i) even in chemical doping by oxygen impurities: with overdoping the c-axis critical current rapidly increases, while the critical temperature, the superconducting gap and the pseudogap decrease, indicating the presence of the critical doping point. We distinguish two main mechanisms of persistent electric doping: (i) even in voltage contribution, attributed to a charge transfer effect, and (ii) odd in voltage contribution, attributed to reordering of oxygen impurities.

9:12AM A35.00007 Imaging chemical disorder in cuprates using scanning tunneling microscopy1, ILIJA ZELJKOVIC, DENNIS HUANG, CAN-LI SONG, Harvard University, TAY-RONG CHANG, National Tsing Hua University, Taiwan, HONGLONG JENG, Institute of Physics, Academia Sinica, Taipei, ZHIJUN XU, JINSHENG WEN, GENDA GU, Brookhaven National Laboratory, JOUKO NIEMINEN, Tampere University of Technology, Finland, ARUN BANSIL, ROBERT MARKIEWICZ, Northeastern University, JENNIFER HOFFMAN, Harvard University — High-Tc superconductors are chemically, electronically and structurally inhomogeneous at the nanoscale. Although a body of theoretical work has predicted that local and global superconductivity may be dramatically impacted by particular dopant configurations, the exact positions of dopants introduced into cuprates to induce superconductivity are generally unknown. Here we use scanning tunneling microscopy to reveal the intra-unit-cell location of two different types of oxygen dopants in Bi2212 and Sr1+yCa2-xCu3O7+x. Furthermore, we show the relationship between these interstitial oxygen dopants, oxygen vacancies, and a global structural buckling known as the supermodulation. We compare our findings to theoretical simulations.

9:24AM A35.00008 Cryomagnetic STM spectroscopy study of multiband pairing in layered superconductors1, IGOR FRIDMAN, University of Toronto, VLADIMIR LUKIC, Stevens Institute of Technology, CHRISTIAN KLOC, Nanyang Technological University, Singapore, CEDORIM PETROVIC, Brookhaven National Laboratory, PENGCHENG DAI, University of Tennessee in Knoxville, J.Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Cooper pairing in layered superconductors can involve multiple bands and give rise to complex gap structures in momentum space. Using scanning tunneling microscopy (STM) with a magnetic field applied parallel to the in-plane, we investigate multiband pairing under diamagnetically-induced superfluid momentum. STM spectroscopy and conductance imaging were performed down to 300 mK and up to 10 T, on single-crystals of the Nb-chalcogenide 2H-NbSe2 and the Fe-pnictides LiFeAs and electron-doped BaFe2As2. Spectroscopy data taken on 2H-NbSe2 at 300 mK showed a distinctly two-sloped field evolution of the zero-bias conductance, consistent with Doppler-induced depairing on parts of the Fermi surface [1]. Spatial conductance maps revealed stripe patterns that originate from in-plane vortices whose cores are buried in the bulk [2] and which undergo a transition as pairing on one of the bands is suppressed. Our results demonstrate a general method for probing multiband superconductors, especially ones whose band structures host coexisting orders and also play a direct role in the pairing mechanism.

1This research was supported by NSF Career grant DMR-0847433 and the New York Community Trust—George Merck Fund.

9:36AM A35.00009 Doping-dependent vortex-state scanning tunneling spectroscopic (STS) studies of cuprate superconductors, C.-C. CHEN, M. L. TEAGUE, Z.-J. FENG, R.T.-P. WU, N.-C. YEH, Dept. of Physics, Caltech, Pasadena, CA 91125 — We report STS studies of YBa2Cu3O7−δ(Y-123) and Ca-doped Y-123 superconductors as a function of magnetic field (H) and hole doping level (p). Our studies suggest that the origin of the pseudogap (PG) is associated with competing orders (COs), and that the occurrence (absence) of PG above the superconducting (SC) transition Tc is associated with a CO energy ΔCO larger (smaller) than the SC gap ΔSC. We derive ΔSC and ΔCO by two approaches. For zero-field STS we apply Green function techniques to fit the “peak” features for ΔSC and the “kink” features for ΔTf ≡ [(ΔSC)2 + (ΔCO)2]1/2. For H > 0 we analyze the PG features in the intra-vortex STS for ΔCO and the peak features in the inter-vortex STS for ΔSC. Both approaches yield consistent results. For optimally and underdoped Y-123, we find that ΔSC < ΔCO with dominant d2−s* pairing wave, and that ΔSC decreases with decreasing p while ΔCO increases. Both ΔSC and ΔCO exhibit long-range spatial homogeneity. For Ca-doped Y-123, the substitution of Y by Ca contributes to excess holes and disorder. For p > 0.16, both ΔSC and ΔCO decrease with increasing p, ΔCO < ΔSC for p > 0.23, and the pairing symmetry becomes (d2−s* + s) with increasing s-wave component, implying the diminishing Mott nature in overdoped cuprates. This work was supported by NSF through IOM at Caltech.

9:48AM A35.00010 Spatial Complexity Due to Locally Oriented Charge Modulations in a Cuprate Superconductor, ERICA CARLSON, Purdue University, ELIZABETH MAIN, Harvard University, BENJAMIN PHILLABAUM, Purdue University, HIROSHI IKUTA, Nagaoka University, KARIN DAHMEN, University of Illinois, Urbana-Champaign, ERIC HUDSON, Penn State University, JENNIFER HOFFMAN, Harvard University — Surface probes such as scanning tunneling microscopy (STM) have detected complex electronic patterns at the nanoscale in many high temperature superconductors. We use scanning tunneling microscopy to image the local orientation of the static charge modulations in Bi2-yPb2+ySr2-yLa2CuO8+x, for samples spanning a wide range of doping. For each sample, we compute the universal cluster properties arising from the locally x-oriented and locally y-oriented clusters in order to identify the fundamental physics controlling the complex pattern formation. By comparing these quantitative measures to known universality classes for rotational symmetry breaking, we find that the charge modulations are not confined only to the surface, but they also extend throughout the bulk of the material.
10:00 AM A35.00011 Tunneling Spectroscopy of SRF Cavity Grade Niobium. CHAOYUE CAO, Illinois Institute of Technology, Argonne National Laboratory, NICK GROLL, THOMAS PROSLIER, Argonne National Laboratory, JOHN ZASADZINSKI, Illinois Institute of Technology, Argonne National Laboratory. — Mechanical contact tunneling measurements are presented on high purity Nb pieces from the starting plate for superconducting radio frequency (SRF) cavity construction as well as from hot spot and cold spot regions of a tested cavity. A varying scattering rate, gamma, is found which broadens the BCS density of states. Detailed fits using Shiba theory indicate that this scattering may be due to magnetic pairbreaking. Hot spot samples reveal a zero bias conductance peak that splits in magnetic field and can be fit using Appelbaum-Anderson theory of spin flip scattering. Together these measurements indicate that the native oxide of Nb can contain varying amounts of localized magnetic moment defects, possibly due to oxygen vacancies in niobium pentoxide.

10:12 AM A35.00012 Andreev Reflection Spectra of d-wave Superconductors. CHARLES SNIDER, JESSICA GIFFORD, JONNY MARTINEZ, TINGYONG CHEN, Arizona State University. — At a normal metal/superconductor interface Andreev reflection occurs, which can be utilized to measure spin polarization of the normal metal and also the superconducting gap of the superconductor. An s-wave superconductor has an isotropic gap and for an unpolarized current the Andreev reflection spectrum within the gap is twice that of outside the gap. A fully spin polarized current suppresses the Andreev reflection therefore causes zero conductance within the gap. The scenario is quite different in a d-wave superconductor because the order parameter has anisotropy and phase. In this work, we calculate Andreev Reflection spectra of an interface between a normal metal and a d-wave superconductor for a current with any polarization, based on the recent Chen-Tesanovic-Chien (CTC) model. It is shown that the point angle of the interface can drastically change the Andreev spectra and a zero bias anomaly (ZBA) is observed in the tunneling regime only if the point angle is large. The spin polarization can also drastically affect the spectra and can completely suppress the ZBA. Our calculation shows that one can use both the spin polarization and the point angle to verify the ZBA in unconventional superconductors.

10:24 AM A35.00013 Direct Probe of IntermEDIATE between Local Structure and Superconductivity in FeTe0.55Se0.45. WENZHI LIN, QING LI, BRIAN SALES, STEPHEN JESSE, ATHENA SAFA-SEFAT, SERGEI KALININ, MINGHUA PAN, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA. — We explore the interplay between local crystallographic structure, composition and local electronic and superconducting properties. Direct structural analysis of scanning tunneling microscopy (STM) data allows local lattice distortions and structural defects across a FeTe0.55Se0.45 surface to be explored on a single unit-cell level. Concurrent superconducting gap (SG) mapping reveals suppression of the SG at well-defined structural defects, identified as a local structural distortion (Guinier-Preston zone). The strong structural distortion is related to the vanishing of the superconducting state. This study provides insight into the origins of superconductivity in iron chalcogenides by providing an example of atomic-level studies of the structure-property relationship. Research was supported (WL, BCS, AS, SVK) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division. This research was conducted (MP, QL) at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy. (Wenzi Lin and Qing Li, these authors contributed equally to this work)

10:36 AM A35.00014 ABSTRACT WITHDRAWN

Monday, March 18, 2013 11:15 AM - 2:15 PM

Session B1 DCMP: Invited Session: Logical Spin Qubits for Quantum Computation

Ballroom I

11:15 AM B1.00001 Entanglement of Singlet-Triplet Qubits. MICHAEL SHULMAN, Harvard University. — Spins in semiconductor quantum dots are promising candidates for the building blocks of a quantum information processor due to their potential for miniaturization and scalability. Singlet-triplet (S-T0) qubits, a certain type of spin qubit, store information in the joint spin state of two electrons. However, these qubits’ weak interaction with the environment, which leads to their long coherence times, makes two-qubit operations challenging. We perform the first two-qubit operation between two S-T0qubits, exploiting the capacitive coupling between two adjacent qubits to generate a CPHASE gate. In order to combat low frequency noise we use a dynamically decoupled sequence that maintains the two-qubit coupling while decoupling each qubit from its fluctuating environment. Using state tomography we show that the two-qubit operation has the intended effect on the state of the qubits, and we provide definitive proof of entanglement by demonstrating that the state switch to coherent oscillations originating from alternative potentially useful qubit states and how to distinguish them.


11:51 AM B1.00002 The exchange-only spin qubit. CHARLES MARCUS, Niels Bohr Institute, University of Copenhagen. — No abstract available.

12:27 PM B1.00003 Exchange-based CNOT gates for singlet-triplet qubits with spin orbit interaction. JELENA KLINSOVAJA, Department of Physics, University of Basel. — We propose a scheme for implementing the CNOT gate over qubits encoded in a pair of electron spins in a double quantum dot [1]. The scheme is based on exchange and spin-orbit interactions and on local gradients in Zeeman fields. We find that the optimal device geometry for this implementation involves effective magnetic fields that are parallel to the symmetry axis of the spin-orbit interaction. We show that the switching times for the CNOT gate can be as fast as a few nanoseconds for realistic parameter values in GaAs semiconductors. In particular we will describe measurements where the Landau-Zener–Stückelberg approach previously demonstrated in double dots is extended to three- interacting spin states permitting us to demonstrate phenomena such as pairwise exchange control. We will also demonstrate how by tuning the experimental parameters one can controllably switch to coherent oscillations originating from alternative potentially useful qubit states and how to distinguish them.


This work was funded by NRC, NSERC and CIFAR.
Cu sites are the main, although not the only, actors in the play. Inelastic and elastic scattering of x rays, when performed at the Cu L3 is the short and mid range ordering of spin and charge degrees of freedom when doping disrupts the long range antiferromagnetic order of parent compounds.

We have used angle-resolved resonant inelastic soft x-ray scattering (RIXS) and resonant elastic soft x-ray scattering (REXS) to identify two-dimensional charge fluctuations with an incommensurate periodicity of $\sim 3.2$ lattice units in the copper oxide planes of the superconductors (Y,Nd)Ba$_2$Cu$_3$O$_{6+x}$ with hole concentrations $0.00 < p < 0.13$ per planar Cu ion [G. Ghiringhelli et al, Science 337, 821 (2012)]. The intensity and correlation length of the fluctuation signal increase strongly upon cooling down to the superconducting transition temperature, $T_c$; further cooling below $T_c$ abruptly reverses the divergence of the charge correlations. In combination with prior observations of a large gap in the spin excitation spectrum, these data indicate an incipient charge-density-wave instability that competes with superconductivity. Further measurements on an Ortho III sample have confirmed that the charge fluctuations are independent of the chain ordering [A. J. Achkar et al, Phys. Rev. Lett. 109, 167001 (2012)]. Put into perspective, these results show that often elastic and inelastic x-ray scattering experiments should be ideally performed jointly, to explore with the greatest sensitivity charge and spin fluctuations [L. Braicovich et al, Phys. Rev. Lett. 104, 077002, (2010)].

11:51AM B2.00002 Charge and spin correlations in high temperature superconductors

STEPHEN HAYDEN, University of Bristol — The cuprate high temperatures superconductors are characterised by numerous competing, and in some cases, co-existing broken symmetries. A important question is to what extent such additional ordered states exist for compositions with high superconducting transition temperatures. I will discuss high-energy X-ray diffraction measurements which show that a charge density wave state (CDW) develops at zero field in the normal state of superconducting YBa$_2$Cu$_3$O$_{6.67}$ ($T_c = 67$ K). This material has a hole doping of 0.12 per copper and a well-ordered oxygen chain superstructure. Below $T_c$, the application of a magnetic field suppresses superconductivity and enhances the CDW. We find that the CDW and superconductivity are competing orders with similar energy scales, and the high-$T_c$ superconductivity forms from a pre-existing CDW environment. Our results provide a mechanism for the formation of small Fermi surface pockets which can explain the negative Hall and Seebeck effects and the $T_c$ plateau in this material.


11:15AM B2.00001 Incommensurate charge density fluctuations in underdoped YBCO detected by resonant x-ray scattering

GIACOMO GHIRINGHELLI, Politecnico di Milano - Italy — A key issue in high $T_c$ superconductivity is the short and mid range ordering of spin and charge degrees of freedom when doping disrupts the long range antiferromagnetic order of parent compounds. Cu sites are the main, although not the only, actors in the play. Inelastic and elastic scattering of x rays, when performed at the Cu L3 absorption resonance, can be used to map the spin and charge excitation spectra and, simultaneously, to unveil the presence of spatial modulations in the charge or spin densities. We have used angle-resolved resonant inelastic soft x-ray scattering (RIXS) and resonant elastic soft x-ray scattering (REXS) to identify two-dimensional charge fluctuations with an incommensurate periodicity of $\sim 3.2$ lattice units in the copper oxide planes of the superconductors (Y,Nd)Ba$_2$Cu$_3$O$_{6+x}$ with hole concentrations $0.00 < p < 0.13$ per planar Cu ion [G. Ghiringhelli et al, Science 337, 821 (2012)]. The intensity and correlation length of the fluctuation signal increase strongly upon cooling down to the superconducting transition temperature, $T_c$; further cooling below $T_c$ abruptly reverses the divergence of the charge correlations. In combination with prior observations of a large gap in the spin excitation spectrum, these data indicate an incipient charge-density-wave instability that competes with superconductivity. Further measurements on an Ortho III sample have confirmed that the charge fluctuations are independent of the chain ordering [A. J. Achkar et al, Phys. Rev. Lett. 109, 167001 (2012)]. Put into perspective, these results show that often elastic and inelastic x-ray scattering experiments should be ideally performed jointly, to explore with the greatest sensitivity charge and spin fluctuations [L. Braicovich et al, Phys. Rev. Lett. 104, 077002, (2010)].

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11:15AM B3.00001 Superconductivity Near Quantum Critical Points, GILBERT G. LONZARICH, Shoenberg Laboratory for Quantum Matter, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — The study of itinerant-electron systems on the border of charge and spin density wave transitions at low temperatures is leading to an increasing number of discoveries of unusual forms of superconductivity and other types of quantum order. Examples will be reviewed of electron-electron pair instabilities in particular on the border of ferromagnetic, antiferromagnetic, ferroelectric and structural quantum phase transitions. The superconducting transition temperature in a number of nearly magnetic metals from heavy fermion compounds to the copper oxide superconductors appears to scale with the characteristic spin fluctuation temperature. These best known materials will be compared and contrasted with examples from other classes of materials in which the spin fluctuation temperature far exceeds the peak of the superconducting transition temperature in the temperature-pressure phase diagram near a magnetic quantum critical point.

11:51AM B3.00002 Quantum spin liquid in organics with quasi-triangular lattices, KAZUSHI KANDODA, University of Tokyo — No abstract available.

12:27PM B3.00003 A Topological Spin Glass State of a Frustrated Magnet, SEUNG-HUN LEE, University of Virginia — We will present a simple way of understanding the physics of the kagome-triangular-kagome trilayer antiferromagnet by mapping the magnetic interactions onto a problem of an ordered tricolor and a disordered binary spin degree of freedom. By doing so, we will show a systematic way of constructing different classical ground states, and will identify possible zero-energy excitations that involve “partial but extended” numbers of spins in the system. Given the unique properties of the ground state, we argue that a topological spin glass is the ground state for the quasi-two-dimensional frustrated magnet.

1:03PM B3.00004 On Short Ranged Resonating Valence Bond Liquids, SHIVAJI SONDHI, Princeton University — Over 40 years ago, P W Anderson proposed the short ranged resonating valence bond state as an alternative to Neel order in antiferromagnets with strong fluctuations—in hindsight, the first proposal for a topologically ordered Z2 spin liquid. In the last year, convincing numerical evidence has accumulated for the existence of such Z2 spin liquids in short ranged Hamiltonians on simple lattices in two dimensions. I will sketch the intellectually productive historical route between these two developments and survey what we now know about the physics of the short ranged RVB and allied states of matter.

1:39PM B3.00005 Critical Behavior of a Strongly-Interacting 2D Electron System, MYRIAM P. SARACHIK, City College of New York - CUNY, New York, NY 10031, USA — Two-dimensional (2D) electron systems that obey Fermi liquid theory at high electron densities are expected to undergo one or more transitions to spatially and/or spin-ordered phases as the density is decreased, ultimately forming a Wigner crystal in the dilute, strongly-interacting limit. Interesting, unexpected behavior is observed with decreasing electron density as the electrons’ interactions become increasingly important relative to their kinetic energy. The resistivity undergoes a transition from metallic to insulating temperature dependence; the resistance increases sharply and then saturates abruptly with increasing in-plane magnetic field; a number of experiments indicate that the electrons’ effective mass exhibits a substantial increase approaching a finite “critical” density. There has been a great deal of debate concerning the underlying physics in these systems, and many have questioned whether a change of the resistivity from metallic to insulating signals a phase transition or a crossover. In this talk, I will report measurements [1] that show that with decreasing density na, the thermopower S of a low-disorder 2D electron system in silicon exhibits a sharp increase by more than an order of magnitude, tending to a divergence at a finite, disorder-independent density na. This recent behavior has been directly linked to the formation of a phase transition at the pseudogap boundary in underdoped YBCO. In this talk, I will present a quantum oscillation study of underdoped YBa2Cu3O6+x. This work was performed in collaboration with G. Lonzarich (University of Cambridge), N. Harrison, M. Altarawneh, F. Balakirev (Los Alamos National Laboratory), and R. Liang, W. Hardy, D. Bonn (University of British Columbia)

[1] Work done with S. Li and B. Wen (City College of NY), A. Mokashi and S. V. Kravchenko (Northeastern U.), A. A. Shashkin and V. T. Dolgopolov (ISSP, St. Petersburg), K. Kanoda (University of Tokyo).


Monday, March 18, 2013 11:15AM - 2:15PM –

Session B4 DAMOP DCMP: Invited Session: Cold Atoms on Higher Orbital Bands –

Ballroom IV - Erhai Zhao, George Mason University
11:15 AM B4.00001 Unconventional superfluidity in higher bands of an optical lattice, ANDREAS HEMMERICH, Institut für Laser-Physik, Hamburg University — Atoms trapped in optical lattices have been used successfully to study many-body phenomena. However, the shape that bosonic ground-state wavefunctions can take is limited, apparently compromising the usefulness of this approach. Such limitations, however, do not apply to excited states of bosons. The study of atomic superfluids realized in higher Bloch bands, where orbital degrees of freedom are essential, can bring the world of optical lattices closer to relevant condensed matter systems. I will discuss our observations of long coherence times, chiral superfluid order and topological features in higher bands in a square optical lattice.

11:51 AM B4.00002 Beyond Standard Fermi Hubbard Models, MACIEJ LEWENSTEIN, ICFO - Institut of Photonic Sciences — In my talk I will focus on novel physics and novel quantum phases that are expected in a system of ultracold fermionic atoms with long range interactions, such dipolar ones. I will discuss various terms in the Hubbard model that, normally neglected, have to be included in the theory. These terms involve both lowest band physics, as well as higher bands. I will describe several exemplary effects that new terms may lead to: spontaneous breaking of symmetries, such as time-reversal, smectic-like metal phases, spontaneous formation of exotic lattices and 3D textures.

12:27 PM B4.00003 Higher orbital physics and artificial gauge fields with ultracold quantum gases, KLAUS SENGSTOCK, Universitaet Hamburg, ILP, Luruper Chaussee 149, 22761 Hamburg — Recently the physics of quantum gases in higher orbitals attracted a lot of attention, theoretically and experimentally. We report on studies of a new type of superfluid described by a complex order parameter, resulting from an interaction-induced hybridization of the two lowest orbitals for a binary spin-mixture. As a main result we observe a quantum phase transition between the normal superfluid and this unconventional superfluid phase, where the local phase angle of the complex order parameter is continuously twisted between neighboring lattice sites [1]. In addition we discuss new experimental work on the creation of artificial gauge potentials for neutral atoms in 1D and 2D, which do not rely on the internal structure of the atoms. Via a time-dependent driving of the optical lattice we have full control over amplitude and phase of the complex valued hopping parameters. In a 2D triangular lattice, we demonstrate the realization of gauge invariant staggered fluxes [2]. Our system consists of an array of tubes filled with bosonic atoms having a well-defined local phase. The phase distribution obtained in presence of large amplitude staggered fluxes — where frustration plays a key role — obeys two fundamental symmetries, the discrete Ising symmetry (Z2) and a continuous global phase symmetry (U(1)). Via the full control of the staggered gauge fields [3], we are able to break the Ising symmetry on purpose which means lifting the degeneracy of the two possible Ising states, in analogy to a longitudinal homogenous magnetic field in the standard Ising-Spin model. The measurements reveal “textbook like” magnetization curves with the well known dependence on both, the external magnetic field and the temperature. We observe a thermally driven phase transition from an ordered Ising (ferromagnetic) to an unordered (paramagnetic) state. Future directions to combine orbital physics and gauge fields will be discussed.

1:03 PM B4.00004 Orbital physics in one dimensional optical lattices, XIAOPENG LI, University of Pittsburgh — We explore orbital physics of fermions and bosons in one dimensional optical lattices. In a system of one dimensional p-orbital bosons, various phases, including anti-ferro-orbital Mott, anti-ferro-orbital superfluid and para-orbital superfluid, have been found. Signatures of phase transitions, in particular time-reversal symmetry breaking, in time-of-flight image are predicted. A fermionic ladder system composed of s and p orbitals is proposed, and we find a topological state featuring fractional defects. An equivalent of spin-orbit coupling naturally arises, not requiring artificial gauge field, in this quantum orbital ladder when the s and p orbital states are identified as a pseudo-spin 1/2. Extending this ladder system to two dimensions we find a flat-band protected by parity. The flat-band makes it plausible to study strongly correlated physics in this system. We also discuss the connection of this fermionic ladder to frustrated π flux models and spin-orbital coupled fermions.

11:39 AM B4.00005 Generation and exploration of the Spin-Orbit coupled Bose gas, JIAN-WEI PAN, Hefei National Lab for Physical Sciences a Microscale and Department of Modern Physics, University of Science and Technology of China, Hefei, 230026 — To generate an artificial gauge field with ultracold quantum gas becomes a very hot topic in last few years and will continue to be attractive for ultracold atomic physics. By using non-linear optical lattice, we generate artificial gauge fields by manipulating the polarization of the incident laser. In this context, we have generated an artificial gauge field in both one and two dimensions with cold atomic Fermi gas and in both one and two dimension with cold atomic Bose gas. The key step to generate an artificial gauge field is to control the polarization of the incident laser, which can be done in linear optical lattice. The artificial gauge field can be used to study many-body phenomena in ultracold atomic physics, such as fractional order and topological features in higher bands in a square optical lattice.

Monday, March 18, 2013 11:15AM - 2:15PM –
Session B19 DCMP: Metal Insulator transitions in Vanadates: exp/theory 321 - Mumtaz Qazilbash, College of William and Mary

11:15 AM B19.00001 Nanoscale Thermal Mapping of VO₂, ADAM PIVONKA, MAGDALENA HUEFNER, CHANGHYUN KO, ALEX FRENZEL, KEVIN O’CONNOR, SHRIRAM RAMANATHAN, Harvard University, ERIC HUDSON, The Pennsylvania State University, JENNIFER HOFFMAN, Harvard University — We present a method for nanoscale thermal imaging of insulating thin films. We image the local temperature of the metal-insulator transition in a VO₂ film, and investigate the role of Joule heating in two-terminal geometry. By sweeping the voltage applied to a conducting atomic force microscope tip in contact mode, we locally trigger and detect the transition to the metallic phase. By fitting the Poole-Frenkel conduction regime immediately preceding the transition, we extract the local temperature. Finally, we find grains displaying two electronic transitions, consistent with a locally stable intermediate insulating phase.

We acknowledge financial support from Harvard’s Nanoscale Science and Engineering Center, funded by NSF grant PHY 01-17795 and the Sloan Fellowship. Adam Pivonka acknowledges the support of the New York Community Trust—George Merck Fund. Magdalena Huefner acknowledges the support of the Deutsche Forschungsgemeinschaft (HU 1960/11).
11:27AM B19.00002 Strain-dependent Metal-Insulator Transition in VO\(_2\) single-crystalline thin films, NAGA PHANI AETUKURI, Stanford University/IBM Almaden Research Center, ALEXANDER GRAY, SLAC National Accelerator Laboratory, MATTEO COSSALE, MARC DROUARD, LI GAO, IBM Almaden Research Center — Vanadium dioxide (VO\(_2\)) has a near room temperature metal insulator transition (T\(_{\text{MIT}}\) 340 K) accompanied by a structural transition making the origin of this transition controversial. In this work, we have continuously changed T\(_{\text{MIT}}\) by as much as 60 K in VO\(_2\) (001) single crystal thin films by using RuO\(_2\) buffer layers. We observe a decrease in the T\(_{\text{MIT}}\) as a function of decreasing c-axis length in the rutile phase which is unexpected from a one-dimensional Peierls model. By performing complementary bulk-sensitive spectroscopic measurements, namely, \(\pi\)-ray absorption spectroscopy (XAS) and \(\pi\)-ray photoelectron spectroscopy (XPS), we identify changes in orbital occupation and electron-electron correlations as a function of strain in the metallic state that explain the observed T\(_{\text{MIT}}\) dependence on strain.

11:39AM B19.00003 Broadband Infrared Spectroscopy of Vanadium Dioxide Films Under the Influence of Strain\(^1\), T.J. HUFFMAN, PENG XI, A.J. HOLLINGSHEAD, N.E. PENTHORN, D.J. BROOKER, M.M. QAZILBASH, LEI WANG, R.A. LUKASZEW, Department of Physics, College of William and Mary, R.D. PIKE, Department of Chemistry, College of William and Mary, B.-J. KIM, H.-T. KIM, Center of Metal-Insulator Transition, ETRI — Vanadium dioxide (VO\(_2\)) undergoes a phase transition between an insulating monoclinic phase and a conducting rutile phase. Even in this simple, stoichiometric material, a complete explanation of the phase transition has proved elusive. This transition, like phase transitions in other correlated electron systems, involves interacting electronic, lattice, and orbital degrees of freedom. This leads to physical properties that are particularly sensitive to small changes in external parameters such as T and \(\pi\)-ray incidence. By probing in situ the structural and electronic properties of thin films grown on different substrates subject to differing strain effects that often affect the shift in the transition temperature. Broadband infrared (IR) and optical spectroscopy allows us to examine the electronic structure and dynamics as well as IR-active, zone-center phonons of strained films grown on sapphire and quartz. Comparing and contrasting the IR and optical properties of these films, and those of bulk crystals, will provide insight into the influence of strain on the electronic and lattice degrees of freedom.

\(^1\)MMOQ gratefully acknowledges support from the Jeffress Memorial Trust

11:51AM B19.00004 In-situ studies on the Martensitic-type transition in VO\(_2\) thin films, VISWANATH BALAKRISHNAN, SHIRiram Ramanathan, School of Engineering and Applied Sciences, Harvard University — We present in-situ kinetic studies across metal-insulator transition in epitaxial and polycrystalline VO\(_2\) thin films through electrical resistance and stress measurements along with TEM investigations. Variable temperature wafer curvature experiments enable the probing of in situ stress relaxation kinetics associated with the structural component of the metal insulator transition. Primarily, no time or drive rate dependence is observed in the stress relaxation trend offering insight into the athermal nature of the phase transition kinetics. However, proximate to the phase transition boundary, minor fraction of isothermal component that show time dependence in both stress relaxation and electrical measurement is captured. In situ electron diffraction and micro structural observations across the metal insulator transition probe the evidence of the martensitic type transition in polycrystalline VO\(_2\) thin films. The studied aspects of time independent, Martensitic type, athermal transition kinetics along with negligible fraction of isothermal kinetics have significance in understanding the dynamics of structural phase transitions that accompany electronic property changes.

12:03PM B19.00005 T\(_c\) anisotropy and phase separation in strained Vanadium Dioxide films, MENGKUN LIU, MARTIN WAGNER, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA, ELSA ABREU, Department of Physics, Boston University, Boston, Massachusetts 02215, USA, SALINPORN KITTIWATANAKUL, Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA, ALEXANDER MCELOD, MICHAEL GOLDFLAM, ZHE FEI, SIYUAN DAI, MICHAEL FOCLER, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA, JIWEI CHEN, Department of Materials Science and Engineering, University of Virginia, Charlottesville, Virginia 22904, USA, STUART WOLF, Department of Materials Science and Engineering & Department of Physics, University of Virginia, Charlottesville, Virginia 22904, USA, RICHARD AVERITT, Department of Physics, Boston University, Boston, Massachusetts 02215, USA, D.N. BASOV, Department of Physics, The University of California at San Diego, La Jolla, California 92093, USA — We report infrared near field study on strain induced transition temperature (T\(_c\)) anisotropy in vanadium dioxide (VO\(_2\)) films via direct visualization of a spontaneous structural and electronic phase separation. The films are epitaxially grown on [110], or [100] TiO\(_2\) substrates and exhibit large uniaxial strain. By mapping the film topography with AFM and electronic percolation with Infrared scattering scanning near-field optical microscopy, a temperature dependent electron-lattice correlation can be clearly observed. Our work sheds a new light onto the nature of the T\(_c\) anomaly in metal-insulator transition and leads to the possibility of controlling the material’s properties through strain induced phase separation.

12:15PM B19.00006 Hydrogen doping and the metal-insulator transition in vanadium dioxide, TALIP SERKAN KASIRGA, CHUNMING HUANG, JAE H. PARK, JIM M. COY, ZAIYAO FEI, AARON M. JONES, XIAODONG XU, DAVID H. COBDEN, University of Washington Department of Physics — Vanadium dioxide has a first-order metal-insulator transition (MIT) at 67 \(^\circ\)C. It has recently been shown [1] that hydrogen doping of VO\(_2\) by spillover from a metal catalyst in hydrogen gas gradually reduces the gap in the insulating phase to zero, and eventually eliminates the MIT. The dependence on hydrogen concentration enables optical and electrical detection of the local hydrogen density. We exploit this to study the diffusion of hydrogen and its dependence on temperature, direction, strain, and phase in single-domain nanobeam and platelets of VO\(_2\). For example, we find that diffusion is faster along the rutile c-axis, and can be significant even at the transition temperature. We also study the effects of hydrogen doping on the phase diagram, on the low temperature conductivity, and on the continuous-wave and ultrafast optical response.


12:27PM B19.00007 Comparative studies of electrically driven metal insulator transition in VO\(_2\) single crystal and thin film, HONGYOUNG JU, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, BONGJIN MUN, Dept. of Applied Physics, Hanyang University, Ansan, Republic of Korea, JOONSEOK YOON, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, SUNG-KWAN MO, ALS, LBNL, Berkeley, USA, KAI CHEN, ALS, LBNL, Berkeley, USA, CAMP-Nano State Key Laboratory for Mechanical Behavior of Materials,Xi’an Jiaotong University, Xi’an, China, NOBUMICHI TAMURA, CATHERINE DEJOIE, MARTIN KUNZ, ZHI LIU, ALS, LBNL, Berkeley, USA, YVETTE LEE, KYUNG-SUN MOON, Dept. of Phys., Yonsei Univ., Seoul, Republic of Korea, CHANGWOO PARK, Division of applied Chemistry and Biotechnology, Hanbat National University, Daejon and Advanced Nano Products, Chungwon, Republic of Korea — Electrically driven metal-insulator transition (MIT) characteristics of VO\(_2\) single domain crystal and thin-film were investigated by temperature and external bias voltage dependent electrical transport, optical microscopy, and synchrotron-based polychromatic \(\pi\)-ray micro-diffraction measurements. Our results suggest that electrically driven metallic state of VO\(_2\) is similar to that of temperature driven metallic state. However, after the electrically driven MIT, VO\(_2\) single crystal exhibits metallic and insulating colors on the surface of the crystals simultaneously. In addition, the origin of electrically driven MIT of crystals seems different from that of electrically driven MIT films. In this talk, we will present comparative studies of electrically driven MIT of VO\(_2\) single crystal and thin-film, and discuss the origins of electrically driven MIT and its implications.
12:39PM B19.00008 VO₂ and V₂O₃: different pathways for the same phase transition?¹, E. ABREU, J. ZHANG, Physics Dpt, BU, Boston MA, S. WANG, Dpt of Physics and Center for Advanced Nanoscience, UCSD; Materials Science and Eng Pgm, UCSD, La Jolla CA, K. GENG, L. CAO, Physics Dpt, BU, Boston MA, S. KITTIWATANAKUL, J. LU, Dpt of Materials Science and Eng, UVA, Charlottesville VA, M. LIU, Dpt of Physics, UCSD, La Jolla CA, J.G. RAMIREZ, Dpt of Physics and Center for Advanced Nanoscience, UCSD, La Jolla CA, S.A. WOLF, Dpt of Materials Science and Engineering, UVA, Charlottesville VA, I.K. SCHULLER, Dpt of Physics and Center for Advanced Nanoscience, UCSD; Materials Science and Eng, UVA — Vanadium dioxide (VO₂) is a well-known correlated material that exhibits a metal-semiconductor transition at 340K, with several orders of magnitude change in the resistivity. In this study, we report the effect of Mn-doping and Al-doping, with different doping recipes; the films were deposited by Reactive Bias Target Ion Beam Deposition, and their single phase was confirmed by X-ray diffraclometry. The different doping recipes had a very dramatic impact on the crystallinity of the vanadium dioxide films. It was found that using a lower frequency for the pulsed dc target bias was desirable for the improvement of the film quality. Both Al and Mn doping can enhance the transition; while the Al doped VO₂ also raises the transition temperature.

1:03PM B19.00010 Benchmark study of the application of density functional theory to correlated t₂g vanadates, DANilo PUGGIONI, JAMES RONDINELLI, Drexel University — SrVO₃ and CaVO₃ are strongly correlated perovskite-structured metals belonging to the class of transition-metal oxides with a 3d¹ electronic configuration. Both cubic SrVO₃ and orthorhombically distorted CaVO₃ are classified as Pauli paramagnets, yet their magnetic states at low temperature remain controversial. Here, we present and discuss the results of systematic density functional theory (DFT) calculations on the magnetic and magnetic structures of both SrVO₃ and CaVO₃ to shed light on this issue. We use standard and “beyond-DFT” exchange magnetic states. We conclude by discussing both the accuracy of these methods for reproducing the atomic structures of the t₂g vanadates and their implications on artificially structured oxide superlattices.

1:15PM B19.00011 Ab initio study of metal-insulator transition in VO₂¹, HUIHUO ZHENG, LUCAS K. WAGNER, Department of Physics, University of Illinois at Urbana-Champaign — The structure distortion accompanied metal-insulator transition (MIT) of vanadium dioxide (VO₂) at 340K has been a matter of ongoing controversy for near decades. It is still unclear whether the nature of this transition is due to a Peierls instability, a Mott-Hubbard transition, or other physics. Most density functional theory based methods fail to describe the nature of the electronic state in this system, further complicating theoretical description of VO₂. We will report on progress in applying the first principles diffusion quantum Monte Carlo method to the electronic structure of VO₂ in the metallic and insulator phases. By examining the energetic properties, one particle reduced density matrix, as well as other static correlations in the two phases of the system, we will comment on which of the two common descriptions is a closer representation of the physical reality of VO₂.

¹This work was supported by the Strategic Research Initiatives project at Illinois(HZ) and NSF DMR 12-06242 (LKW).

1:27PM B19.00012 Phonon Softenings and the Mott-spin-Peierls Transition in VO₂, SOORAN KIM, KYOO KIM, CHANG-JONG KANG, B.I. POSTECH — To explore the driving mechanisms of the metal-insulator transition (MIT) and the structural transition in VO₂, we have investigated phonon dispersions of rutile VO₂ (R-VO₂) in the DFT and the DFT+U (U: Coulomb correlation) band calculations. We have found that the phonon softening instabilities occur in both cases, but the softened phonon mode only in the DFT+U describes properly both the MIT and the structural transition from R-VO₂ to monoclinic VO₂ (M-VO₂). The present ab-initio phonon dispersion calculations clearly demonstrate that the Coulomb correlation effect plays an essential role of assisting the Peierls transition in R-VO₂ and producing the spin-Peierls ground state in M-VO₂.

1:39PM B19.00013 Examining the density functional theory description of VO₂ above and below the metal-insulator transition¹, RICARDO GRAU-CRESPO, THOMAS A. MELLAN, Department of Chemistry, University College London, UK, HAO WANG, UDO SCHWINGENSCHLÖGL, KAUST, PSE Division, Saudi Arabia — Vanadium oxide (VO₂) exhibits a metal-insulator transition at 341 K, which is accompanied by a change from a tetragonal to a monoclinic structure. In both the metallic and insulator phases, we have investigated phonon dispersions of rutile VO₂ (R-VO₂) in the DFT and the DFT+U (U: Coulomb correlation) band calculations. We have found that the phonon softening instabilities occur in both cases, but the softened phonon mode only in the DFT+U describes properly both the MIT and the structural transition from R-VO₂ to monoclinic VO₂ (M-VO₂). The present ab-initio phonon dispersion calculations clearly demonstrate that the Coulomb correlation effect plays an essential role of assisting the Peierls transition in R-VO₂ and producing the spin-Peierls ground state in M-VO₂.

¹Support from EPSRC grant EP/J001775/1 is gratefully acknowledged.

1:51PM B19.00014 Spatial complexity due to strong correlations in vanadium dioxide, SHUO LIU, BENJAMIN PHILLABAUM, ERICA CARLSON, Purdue University, KARIN DAHMEN, University of Illinois at Urbana-Champaign, MUMTAZ QAZILBASH, College of William and Mary, DMITRI BASOV, University of California, San Diego, VIDHYADHIRAJA SUDHINDRA, JNCAWR — Near-field scanning infrared microscopy on the Mott-metal-insulator system vanadium dioxide (VO₂) has revealed complex nanoscale pattern formation in the form of insulating and metallic puddles near the insulator-to-metal transition [1]. We use and extend recently developed cluster techniques [2] in order to understand the fundamental physics driving this multiscale pattern formation. We map the observed metallic and insulating clusters to Ising variables by a rigorous choice of threshold amplitude, and quantify the statistics of the sizes and shapes of the geometric clusters. These in turn yield critical exponents including the cluster size distribution exponent ν, and the fractal dimensions associated with the cluster formation. These quantitative measures show power-law behavior over multiple decades, revealing a delicate interplay between interactions and disorder in the material. The cluster techniques employed here can be readily applied to 2D image data in the context of other materials and measurement techniques.


2:03PM B19.00015 Structural and vibrational properties of VO2 from DFT and DFT+U calculations\textsuperscript{1}, ERIC J. WALTER, HENRY KRAKAUER, TYLER J. HUFFMAN, PENG XU, M. M. QAZILBASH, College of William and Mary — Vanadium dioxide (VO\textsubscript{2}) undergoes a metal-insulator transition (MIT) at 340 K from a metallic, high-temperature rutile phase to an insulating, low-temperature monoclinic phase. In thin films, the extremely fast switching times (\approx 100 femtoseconds) of the MIT have led to many suggested device applications. Understanding the MIT driving mechanism and the long-debated importance of electronic correlation is important to these developments. We have computed the relaxed geometry and phonon frequencies using DFT and DFT+U for both phases of VO\textsubscript{2}. The dependence of vibrational mode frequencies and oscillator strengths on the Hubbard $U$ parameter and their sensitivity to the Born effective charges in the insulating monoclinic phase will be reported. The calculated frequencies for $U = 5$ eV are in good agreement with recent experimental infrared micro-spectroscopy measurements on single crystal platelets of VO\textsubscript{2}\textsuperscript{2}. Our results indicate that strong electron-electron correlation must be included to describe the vibrational properties.

\textsuperscript{1}Supported by ONR

\textsuperscript{2}T. J. Huffman et al., PRB, submitted.

Monday, March 18, 2013 11:15AM - 2:03PM
Session B22 DCMP: Nano Particles, Wires, and Cavities 324 - Sergio Ulloa, Ohio University

11:15AM B22.00001 Optical properties and circular dichroism of chiral metal nanoparticles\textsuperscript{1}, ZHIYUAN FAN, ALEXANDER GOGOVOROV, Department of Physics and Astronomy, Ohio University. Athens, Ohio 45701, OU TEAM — In nature, biological systems are built up by homochiral building blocks, such as a sugar and protein. Circular dichroism (CD) is an effective tool of resolving molecular conformations. It utilizes circularly polarized light to detect differential absorption of chiral molecules. In medicine, it will help us to develop new drugs and therapies, if we understand the connection between the physical or chemical properties of drug molecules and their conformations. With the rapid development of nanotechnologies, chiral nanomaterials attract lots of attentions nowadays. CD signals of chiral molecules can be enhanced or shifted to the visible band in the presence of plasmonic nanocrystals. Here we present a plasmonic CD mechanism from a single chiral metal nanocrystal\textsuperscript{[1]}. The mechanism is essentially different from the dipolar plasmon-plasmon interaction in a chiral NP assembly\textsuperscript{[2]}, which mimics the CD mechanism of chiral molecules. Chiral metal nanocrystals are expected to have promising applications in biosensing. Recently a few experimental papers reported successful realizations of chiral nanocrystals in a macroscopic ensemble in solution. Particularly the paper\textsuperscript{[3]} described silver nanoparticles grown on chiral template molecules and demonstrating characteristic CD signals at a plasmonic wavelength. The plasmonic CD signals in Ref [3] can come from a dipolar plasmon-molecule interaction or from a chiral shape of nanocrystals. \textsuperscript{[1]}Z.Fan, et al. Nano Lett., 12, 3283 (2012). \textsuperscript{[2]}S.Kuzyk, et al., Nature 483, 311 (2012). \textsuperscript{[3]}B.Maaz, et al. J. Am. Chem. Soc. 134, 17807 (2012).

\textsuperscript{1}This work was supported by the NSF (project: CBET- 0933782) and by the Volkswagen Foundation.

11:27AM B22.00002 Transport measurements across single nanoparticles, QIAN YU, LIMIN CUI, Laboratoire de Physique et d’Etude des Matériaux, UMR 8213, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, 75231, Paris, France, CHRISTIAN ULYSSE, Laboratoire de Photonique et de Nanosciences, CNRS, Marcoussis, France, ALIREZA MOTTAGHIZADEH, ALEXANDRE ZIMMERS, HERVÉ AUBIN, Laboratoire de Physique et d’Etude des Matériaux, UMR 8213, ESPCI-ParisTech-CNRS-UPMC, 10 rue Vauquelin, 75231 Paris, France — During this last decade, numerous progresses have been obtained in the chemical synthesis of nanoparticle. Various materials (oxides, chalcogenides) known for their peculiar electronic or magnetic properties – superconductivity, Mott localization, topological protection – can now be obtained as nanoparticles through chemical synthesis. These new nanomaterials are offering a unique opportunity to study the effect of quantum confinement on unconventional electronic orders. To improve the preparation of samples with single nanoparticles trapped within a nanogap, we developed a new method where nanoparticles are projected in-vacuum on chip circuits covered by nanogap spaced electrodes. Continuous current measurements during the projection allow identifying the trapping of a single nanoparticle within the nanogap. We apply the method for trapping single gold nanoparticles, which led to the observation of Coulomb blockade. We also applied the method to magnetite (Fe\textsubscript{3}O\textsubscript{4}) nanoparticles, which allows to describe the electric field induced insulator to metal transition in only a few nanoparticles.

11:39AM B22.00003 Characterization of TbAs nanoparticles embedded in GaAs using pump-probe measurements of carrier relaxation dynamics, LAURA R. VANDERHOEF, University of Delaware, ABUL K. AZAD, DIBAKAR R. CHOWDHURY, Los Alamos National Laboratory, CORY BOMBERGER, JOSHUA M. O. ZIDE, MATTHEW F. DOTY, University of Delaware — Rare-earth-monopnictide nanoparticles epitaxially deposited within III-V semiconductors have been shown to improve the performance of devices for applications ranging from thermoelectrics to THz pulse generation. However, the electronic structure of small (approximately 1.5 nm diameter) TbAs nanoparticles remains poorly understood. We use ultrafast pump-probe spectroscopy to investigate the electronic structure of the TbAs nanoparticles. The samples studied were grown by co-deposition of Tb, Ga, and As on a GaAs substrate, resulting in TbAs nanoparticles embedded within a GaAs host. We study the dynamics of carrier relaxation into the TbAs states, which essentially acts as traps, using both optical-pump terahertz-probe and optical-pump optical-probe techniques. By analyzing how the carrier relaxation rates depend on both pump fluence and sample temperature we conclude that the TbAs states are saturable, which suggests the existence of a bandgap for TbAs nanoparticles.

11:51AM B22.00004 Optical and electronic properties of self-assembled nanoparticle-ligand metasurfaces\textsuperscript{1}, JAKE FONTANA, Naval Research Laboratory, JOHN LIVENERE, Norfolk State University, JOSHUA CALDWELL, CHRISTOPHER SPILLMANN, JAWAD NACIRI, RONALD RENDELL, BANAHALLI RATNA, Naval Research Laboratory — The optical and electronic properties of inorganic nanoparticles organized into two-dimensional lattices are highly sensitive to the properties of the organic ligand shell coating the nanoparticles. We study the optical and electronic properties of these two-dimensional metasurfaces consisting of gold nanoparticles functionalized with ligands and self-assembled into macroscopic monolayers on non-templated substrates. Using these metasurfaces we demonstrate an average surface-enhanced Raman scattering (SERS) enhancement factor on the order of 10\textsuperscript{6} for benzenethiol ligands and study the mechanisms that influence the enhancement. These metasurfaces may provide a platform for the development of low-power, low-cost next-generation chem/bio-sensors and new insights into the organic-inorganic interface at the nanoscale.

\textsuperscript{1}This work was supported with funding provided from the Office of Naval Research.

12:03PM B22.00005 Two photon excitation fluorescence from Ag nanotriangles and nanohexagons, CHI-YU JAO, Virginia Tech, BRENDEST MAGILL, Institute for Critical Technology and Applied Science at Virginia Tech, HANS ROBINSON, Virginia Tech — We report on measurements of two photon excitation fluorescence (TPEF) from arrays of silver nanotriangles and nanohexagons fabricated by nanosphere lithography. The silver nanoparticles exhibit localized surface plasmon resonances (LSPRs) that depend on the size, shape and aspect ratio of the particles. When the particles are excited by femtosecond pulsed laser light resonant with the LSPRs, they emit TPEF with significantly higher intensity than when excited off resonance. Moreover, if the light intensity is turned up sufficiently to cause some of the particles to melt into spherical particles, we observed an increase in the TPEF from the spheres by as much as an order of magnitude, even though their LSPRs are no longer resonant with the laser. Finally, we note that the silver particles also generate light at the second harmonic of the laser frequency, although the efficiency of this process depends strongly on the dielectric environment of the silver particles, which is not the case for the TPEF.
12:15PM B22.00006 Investigation of the electronic transport in polarization-induced nanowires using conductive atomic force microscopy (AFM), CAMELIA SELCU, SANTINO C. CARNEVALE, THOMAS F. KENT, FATH AKYOL, PATRICK J. PHILLIPS, MICHAEL J. MILLS, SIDDEHAR H. HOJAN, JONATHAN P. PELZ, ROBERTO C. MYERS, The Ohio State University — In the search to improve short wavelength light emitting diodes (LED’s), where the dislocations limit their performance and hole doping (Mg) is a fundamental challenge, the III-Nitride polarization-induced nanowire LED provides a promising system to address these problems. The new type of pn diode, polarization-induced nanowire LED (PINLED), was developed by linearly grading AlGaN composition of the nanowires (from GaN to AlN and back to GaN) from 0% to 100% and back to 0% Al (Carnevale et al, Nano Lett., 12, 915 (2012)). In III-Nitrides (Ga,Al/N), the effects of polarization are commonly observed at the surfaces and interfaces. Thus, in the case of the polarization-induced nanowire LEDs, taking advantage of the bound polarization charge, due to the grading of the AlGaN, the pn diodes are formed. The polarity of the nanowires determines the carrier type in each graded region, and therefore the diode orientation (n/p vs p/n). We used conductive AFM to investigate polarity of the PINLED’s as well as hole conductivity in PINLED’s made of AlGaN with and without acceptor doping. The results reveal that most of the wires are n-top/p-bottom (N-face), but some are p-top/n-bottom (Ga-face). Also, we found that the current density is 3 orders of magnitude larger in the case of the doped nanowires than the nanowires with no impurity doping.

12:27PM B22.00007 Critical Role of Modal Spatial Overlap in Nanoscale Nonlinear Optics, JIMIN ZHAO, RUI WANG, BEN-LI WANG, R.J. LIU, X.H. LU, ZHI-YUAN LI, Institute of Physics, Chinese Academy of Sciences — We unambiguously demonstrate the critical role of modal spatial overlap in nonlinear optics for nanoscale structures. Our experimental and theoretical investigations show that, within a sub-wavelength metallic hole, spatial overlap between the linear and nonlinear modes strongly correlates to the conversion efficiency. Our results provide an accurate explanation for the long-embattled but elusive shape effect. Moreover, our investigation stimulates new angles for and deeper insights into general nonlinear optics at nanoscale.

12:39PM B22.00008 Nanocluster effects on magneto-resistance and optical second-harmonic generation in Au-Co composite films, KAIDA YANG, Department of Applied Science, College of William and Mary, TATIANA MURZINA, Quantum Electronics division, Department of Physics, Moscow State University, ALE LUKASZEW, Department of Physics, College of William and Mary — Magnetic nanomaterials typically exhibit significant differences in their magnetic and magnetic-optical properties compared to bulk. A viable nanoscale platform to investigate the magnetic and magneto-optical properties of magnetic nanomaterials is in composite thin films to have magnetic clusters embedded on a different matrix material which size can be tailored. The Au-Co binary system is a typical phase-separation system in bulk phase diagram. The nanocomposite geometry allows tailoring the actual composition and microstructure of the composite by exploiting different temperature during deposition. In our previous studies, Au/Co/Au trilayers as well as Au-Co nanocomposite thin films exhibit strong enhancement of the magneto-optical activities due to surface plasmon polariton excitation in the noble metal. In this study, we investigate other non-linear optical properties such as second harmonic generation (SHG) in Au-Co nanocomposite thin films and understand its correlation with the magneto-transport properties of the composite. Optical SHG is a sensitive probe of surface and buried interfaces due to inversion symmetry breaking at the interfaces of centrosymmetric materials which allows probing of the structural and morphological properties near interfaces.

12:51PM B22.00009 Far-infrared transmission through periodic arrays of cross-shaped holes, LUYI YAN, CHANG LONG, DAVID TANNER, University of Florida, N. BRADMAN, N. MCFARLAND, J.B. MARBRUGER, Advanced Plasmonics Inc. — The far-infrared transmission of light incident on a free-standing metal film perforated with periodic cross-shaped holes is investigated. These metal-mesh filters show enhanced “extraordinary” infrared transmission at particular wavelengths. A number of filter samples having different periodicities and geometries have been measured over frequencies from 20-650 cm^{-1}/0.6-19.5 THz. The results will be compared with calculations from surface plasmon polarization (SPP) theory. It is shown that for certain periodicity and geometry, the SPP mode and the localized surface plasmon (LSP) mode may have their resonance peaks nearly superimposed on each other. The bandwidth of this transmission peak is related to the ratio of the width and length of the cross-shaped holes. The correlation between transmission properties and the incident angle of the far-infrared light has also been measured for both polarization conditions. As the incident angle is increased, the transmission peak shows a blue shift when illuminated by s-polarized light, while for p-polarized light it splits into two parts which shift in opposite directions.

1:03PM B22.00010 ABSTRACT WITHDRAWN

1:15PM B22.00011 Time-resolved nonlinear dynamics of quantum dots coupled to a photonic crystal cavity in the Purcell regime, JEIEUN LEE, TIMOTHY SAUCER, Department of Physics, University of Michigan, ANDREW MARTIN, JOANNA MILLUNCHICK, Department of Materials Science and Engineering, University of Michigan, VANESSA SIH, Department of Physics, University of Michigan — Recently, there has been great interest in studying the optical nonlinearities of light confined in a solid-state nano-cavity interacting with a quantum emitter for on-chip applications. The nonlinearity in the strong coupling regime has enabled ultrafast all-optical switching at low incident power using exciton-photon coupled systems. In this report, we show that nonlinear optical properties can also be observed in the Purcell regime using a cavity with a moderate quality factor (Q), which arises from the saturation of a single quantum dot and describes the time-resolved dynamics of two transitions (exciton and biexciton) exhibiting different nonlinearities. In order to conduct these investigations, we used the luminescence intensity autocorrelation method and measured the variation of nonlinear emission dynamics while varying the incident power over nearly three orders of magnitude and found excellent agreement with a numerical simulation. We expect the method and the theoretical model will be applicable for understanding other nonlinear effects such as lasing and cavity-QED.

1:27PM B22.00012 Entangled photons from the polariton vacuum in a switchable optical cavity, ADRIAN AUER, GUIDO BURKARD, Department of Physics, University of Konstanz, Germany — We study theoretically the entanglement of two-photon states in the ground state of the intersubband (ISB) cavity system, called polariton vacuum. The system is formed by a sequence of quantum wells (QWs) located inside a microcavity and the interaction of cavity photons with ISB excitations inside the QWs leads to the formation of polariton states. In the ultrastrong coupling regime, the polariton vacuum already contains a finite number of photons, of which pairs with opposite in-plane wave vectors are correlated. In an explicit solution for the polariton vacuum, we only consider certain two-photon states by post-selection and analyze them for mode entanglement, i.e. in the momentum degree of freedom. We find an analytical expression for the entanglement using the concurrence [1], which depends on the absolute values of the in-plane wave vectors of the photons. In the limit of large cavities and for photon energies around the ISB resonance in the mid infrared regime, the photons are almost maximally entangled, which is fundamentally important for their possible use in quantum information processing. Furthermore, there exists a continuous set of mode pairs, for which the photons are maximally entangled.

This work is support by National Science Foundation under grant DMR-1104383, Gordon and Betty Moore Foundation as well as the National Science Foundation MRSEC Program through the Princeton Center for Complex Materials (DMR-0819860).

11:15AM B30.00001 Coarsening of firefighting foams containing fluorinated hydrocarbon surfactants, MATTHEW J. KENNEDY, JOHN A. DOUGHERTY, NICHOLAS OTTO, MICHAEL W. CONROY, BRADLEY A. WILLIAMS, RAMAGOPAL ANANTH, JAMES W. FLEMING, Naval Research Laboratory — Diffusion of gas between bubbles in foam causes growth of large bubbles at the expense of small bubbles and leads to increasing mean bubble size with time thereby affecting drainage. Experimental data shows that the effective diffusivity of nitrogen gas in aqueous film forming foam (AFFF), which is widely used in firefighting against burning liquids, is several times smaller than in 1% sodium dodecyl sulfate (SDS) foam based on time-series photographs of bubble size and weighing scale recordings of liquid drainage. Differences in foam structure arising from foam production might contribute to the apparent difference in the rates of coarsening. AFFF solution produces wetter foam with initially smaller bubbles than SDS solution due in part to the lower gas-liquid surface tension provided by the fluorosurfactants present in AFFF. Present method of foam production generates microbubble foam by high-speed co-injection of surfactant solution and gas into a tube of 3-mm diameter. These results contribute to our growing understanding of the coupling between foam liquid fraction, bubble size, surfactant chemistry, and coarsening.

11:27AM B30.00002 Competition between phase separation and crystallization in attractive colloids, BARBARA FRISKEN, ARTHUR BAILEY, JUAN SABIN, GABRIEL ESPINOSA, Simon Fraser University, Canada — We will present results from recent experiments on Earth and on the International Space Station investigating the interplay between phase separation and crystallization in samples prepared in the three-phase region (gas-liquid-crystal) of the phase diagram of a colloid-polymer mixture. On Earth, our samples first separate into a colloid-rich phase and a colloid-poor phase, with crystals forming in the colloid-rich phase. The denser phases sediment as expected. In microgravity, photographic images obtained in the BCAT-5 experiment reveal phase separation with crystal formation in the denser phase, where the phase separation continues normally until the dominant length scale is about 25% of the cell thickness, at which point both phase separation and crystal growth are arrested before macroscopic phase separation can occur. We propose that this arrest occurs because a crystalline network forms in the liquid phase and that the gas-liquid surface tension is not sufficient to overcome the stiffness of this network.

11:39AM B30.00003 Colloidal Wigner Crystals Near the Melting Transition, EMILY RUSSELL, DAVID WEITZ, Harvard University — We demonstrate the formation of colloidal “Wigner” crystals at low particle volume fraction. Particles are suspended in a nonpolar solvent and charged by the addition of a small amount of surfactant, generating a long-range interparticle repulsion which induces crystalization above a critical volume fraction of order 10%. Confocal microscopy allows us to study in detail the three-dimensional structure and dynamics of these colloidal crystals as we vary the volume fraction, and we find a growing population of especially mobile particles with large local Lindemann parameter as we approach the critical volume fraction. We discuss our results and the implications of our findings to competing ideas of the mechanism of bulk crystal melting.

11:51AM B30.00004 Visualization of colloidal liquid nucleation induced by Critical Casimir forces, DUC NGUYEN, PhD, PETER SCHALL, Dr — We show that with precise temperature control of critical Casimir forces we achieve reversible control of colloidal gas-liquid. The exquisite temperature control of the potential allows us to even tune the degree of supersaturation of the liquid phase. We use a confocal microscopy to elucidate the particle potential or the particle size distribution. We estimate the interfacial tension of the aggregates at different degree of supersaturation directly from the particle potential and pair correlation function using Kirkwood and Buff theory. A good agreement between the two methods provides new insight into the gas-liquid transition.
for the formation of polymer microspheres with narrow size distribution (CV ≈ 1.9%). We obtain the microspheres with diameter ranging from 20 to 300 μm by modulating mold dimensions. We provide a synthesis method to produce microspheres in micromolds for various reaction schemes: UV-polymerization, sol-gel reactions and colloidal assemblies.

12:15PM B30.00006 Domain, Stripe, and Pattern Formation for Colloids on Optical Trap Arrays. DANIELLE MCDERMOTT, University of Notre Dame. JEFFERY AMELANG, California Institute of Technology. LENA LOPATINA, CYNTHIA REICHARDT, CHARLES REICHARDT, Los Alamos National Laboratory — We examine pattern formation of colloids atop a square periodic substrate using large scale numerical simulations. The pins forming the substrate are modeled with a muffin-tin potential which is flat with localized traps. We show that with 4 colloids per pinning site the system has triangular ordering and with 5 colloids per site it has square ordering. We study intermediate fillings and identify a rich variety of distinct ordering regimes including disordered grain boundaries, crystalline stripe structures, superlattice orderings, and disordered patches of multiple phases. These different regimes are characterized with a Voronoi analysis, energy dispersion plots, and ordination of domains. We extend our studies to a wide range of other fillings which feature similar boundary formation patterns. Our results show that periodic substrates of muffin-tin potentials can be used to tailor grain boundary formation.

12:27PM B30.00007 Anisotropic colloids for building complex molecular structures using critical Casimir effect. TRUC ANH NGUYEN, University of Amsterdam, DANIELA KRAFT, New York University, SANDRA VEE, PETER SCHALL, University of Amsterdam — Here, we present a new way to build complex colloidal scale structures using critical Casimir forces on anisotropic colloids. These forces arise from the confinement of critical solvent fluctuations between the particle surfaces and allow temperature-control over the particle interactions. We use doublet particles made of polymethyl-methacrylate (PMMA) and exhibiting anisotropic surface charge densities, suspended in a binary liquid mixture. By controlling the applied temperatures of the system, we can tune the particle interactions of the two ends of the particles to observe different superstructures formed in time and space: at low temperature, the particles are randomly distributed and represent a gas phase; however, at higher temperatures, the particles form long chain-like structures and cubic crystal structures depending on the temperature difference to the solvent phase separation. This opens new opportunities to assemble complex building blocks for nano- and micro-devices.

12:39PM B30.00008 Direct observation of the nucleation in colloidal solid-solid transitions1. YI PENG, FENG WANG, ZIREN WANG, YILONG HAN, Department of Physics, Hong Kong University of Science and Technology. Clear Water Bay, Hong Kong, China — Solid-solid phase transitions are ubiquitous in nature, but their microscopic mechanisms remain poorly understood. We employed thermally sensitive microlbeads to study the solid-solid transitions between square and triangular lattices in colloidal thin films. Two types of nucleation processes were directly observed by video microscopy and studied at the single-particle level. Under low flow rates, the nucleation is a two-step process: square lattice → liquid nucleus → triangle nucleus and its precursor is a local particle-exchange loop, whereas under high flow rates the nucleus of the triangle lattice forms directly from a dislocation pair by a martensitic mechanism. We measured the critical nucleus size, the energy barrier height and the hysteresis loop of the solid-solid transitions. Our results cast new light to solid-solid transitions in carbon systems, nano-crystals and geophysics.

1Hong Kong GRC grants 601208 and 601911

12:51PM B30.00009 Frustrated Ordering of Colloidal Crystals in Spatially Varying Potentials. VISHAL SONI, WILLIAM T.M. IRVINE, University of Chicago — Frustrated ordering processes are of wide interest in condensed matter systems. Experiments on interfacial colloidal systems have resulted in several recent insights into the two dimensional ordering of crystalline lattices frustrated by Gaussian curvature. We study the ordering of two-dimensional lattices of colloids frustrated by spatially varying dielectrophoretic forces. In particular, we investigate the role of topological defects in organizing the conformal-crystal like ground state and the defect dynamics that lead to equilibration as the applied dielectrophoretic force is increased.

1:03PM B30.00010 Preparation of monodisperse microspheres from the Laplace pressure induced droplet formation in micromolds. CHANG-HYUNG CHOI, JONGMIN KIM, SUNG-MIN KANG, Chungnam National University, JIN KEE LEE, Sungkyunkwan University, CHANG-DOO LEE. Chungnam National University — Monodispense microspheres play critical roles in many applications such as micro-electromechanical systems (MEMS), chemical release systems, optical materials and various biological applications. Although microfluidic systems have been developed for producing monodisperse microspheres, it still definitively requires pressure driven flow for continuous fluid injection as well as use of surfactant to achieve their uniformity. Here, we present a novel molding method that generates monodisperse microspheres through surface-tension-induced flow. Two immiscible fluids that consist of photocurable monomer and hydrophobic oil are sequentially applied onto the mold. The mold geometry results in Laplace pressure induced droplet formation, and these droplets formed are individually localized into each micromold. Photopolymerization of the droplets allows for the formation of polymer microspheres with narrow size distribution (CV = 1.9%). We obtain the microspheres with diameter ranging from 20 to 300 μm by modulating mold dimensions. We provide a synthesis method to produce microspheres in micromolds for various reaction schemes: UV-polymerization, sol-gel reactions and colloidal assemblies.

1:15PM B30.00011 Formation of Uniform Hollow Silica microcapsules. HUAN YAN, CHANJOONG KIM, Liquid Crystal Institute, Kent State University — Microcapsules are small containers with diameters in the range of 0.1 – 100 μm. Mesoporous microcapsules with hollow morphologies possess unique properties such as low-density and high encapsulation capacity, while allowing controlled release by permeating substances with a specific size and chemistry. Our process is a one-step fabrication of monodisperse hollow silica capsules with a hierarchical pore structure and high size uniformity using double emulsion templates obtained by the glass-capillary microfluidic technique to encapsulate various active ingredients. These hollow silica microcapsules can be used as biomedical applications such as drug delivery and controlled release.
1:27PM B30.00012 Interstitials in 2D colloidal crystals. LICHAO YU, SUNGCHOEK KIM, Brown University, ALEXANDROS PERTSINIDIS, Sloan-Kettering Institute, XINSHENG LING, Brown University — Point defects in crystalline solids are important in many areas of condensed matter physics, ranging from the mechanical properties of metals, to superconductivity in quantum solids, and most recently the magnetic properties of graphene. A key question to point defects is how they diffuse in the crystalline lattice. Colloidal crystals provide a perfect model system for studying the dynamics of point defects, since the kinetic pathways of diffusion can be identified in direct real-time video imaging experiments. Here we report an experimental study of another type of point defects: interstitials. We found that interstitial diffusion in a 2D colloidal crystal is also dominated by a dislocation pair unbinding-binding process. Similar to vacancies, interstitial diffusion exhibits strong memory effects. However, the contrast lies in the observation that the interstitials, as quasi-particles, diffuse faster than vacancies. We propose that higher diffusion constant of the interstitials is a result of the suppression of the Peierls barrier for the edge dislocations by the excess strain created by the extra particle(s). This work was supported by NSF-DMR.

1:39PM B30.00013 Effects of Particle Shape on Growth Dynamics at Edges of Evaporating Drops of Colloidal Suspensions1, PETER J. YUNKER, Harvard University, MATTHEW A. LOHR, TIM STILL, University of Pennsylvania, ALEXEI BORODIN, Massachusetts Institute of Technology, D.J. DURIAN, A.G. YODH, University of Pennsylvania — We study the influence of particle shape on growth processes at the edges of evaporating drops. Aqueous suspensions of colloidal particles evaporate on glass slides, and convective flows during evaporation carry particles from drop center to drop edge, where they accumulate. The resulting particle deposits grow homogeneously from the edge on the air-water interface in two-dimensions. The deposition front, or growth line, varies in space and time. Measurements of the fluctuations of the deposition front during evaporation enable us to identify distinct growth processes. Interestingly, three distinct growth processes were discovered in the evaporating colloidal suspensions by tuning particle shape-dependent capillary interactions and thus varying the microscopic rules of deposition. Sphere deposition exhibits a classic Peierls barrier for the edge dislocations by the excess strain created by the extra particle(s). This work was supported by NSF-DMR.

5:10PM B30.00014 Non-equilibrium Ionic Assemblies of Oppositely Charged Colloids. RUI ZHANG, PRATEEK JHA, MONICA OLVERA DE LA CRUZ, Northwestern University — The structure and evolution kinetics of non-equilibrium clusters formed in a solution of oppositely charged colloids are analyzed by a kinetic Monte Carlo simulation scheme. A wide range of dynamic cluster configurations are obtained by varying the various external parameters controlling the interaction strength between colloids, screening length, and packing density of colloids. At low-salt concentrations, clusters with structures ranging from NaCl-type cubic aggregates to fibril-like chains are observed, while at high-salt concentrations, disordered compact clusters are observed. A chain-folding barrier model is proposed to explain the kinetically trapped fibril-like assemblies. In higher-density solutions, ionic clusters of bigger size and percolated gel structures are observed. Our work demonstrates the structural richness of non-equilibrium ionic assemblies of oppositely charged colloids and elucidates the effect of ionic correlations, not captured by mean field models such as the modified Poisson-Boltzmann approaches, in determining the structure of assemblies of oppositely charged colloids. These “ionic composites” hold great promise in a variety of emerging applications such as templated polymerization of charged molecules and assembly of charged particles.

2:03PM B30.00015 Directional Entropic Forces in Hard Colloids. GREG VAN ANDERS, KHALID AHMED, ROSS SMITH, MICHAEL ENGEL, SHARON GLOTZER, University of Michigan. — Based on known results from the literature of hard particles we introduce the concept of entropically patchy particles — particles that bind with angular specificity entirely due to their geometry via directional entropic forces or “bonds”. Unlike ordinary patchy particles, in which “valence” vis-a-vis angular specificity is dictated by microscopic energetic considerations (sticky patches), entropic forces causing the binding of particles at entropic patch sites are emergent. Using basic examples we show both theoretically and computationally that we can alter the geometry of a particle to create an entropic patch and tune the resulting effective pair potential in such a way that it can lead to angularly specific binding, even in the absence of depletants.

Monday, March 18, 2013 11:15AM – 2:15PM –
Session B35 DCMP: Superconductor: Spin Properties

11:15AM B35.00001 Magnetic excitations in the high-Tc superconductor HgBa2CuO4+d at low doping1, CHELSEY DOROW, M.K. CHAN, Y. TANG, G. YU, University of Minnesota, YUAN LI, Max Planck Institute for Solid State Research, Germany, N. BARISIC, University of Minnesota, J. PARK, P. SOBOLEV, A. TEICHERT, Forschungsnuernenonqueille Heinz Maier-Leibnitz, Germany, Y. SIDIS, Laboratoire Leon Brillouin, France, P. STEFFENS, Institut Laue Langevin, France, D. ABERNATHY, Oak Ridge National Lab, X. ZHAO, University of Minnesota, Jilin University, China, P. BOURGES, Laboratoire Laure Brilloin, France, M. GREVEN, University of Minnesota — We report on the observation of magnetic excitations in the very underdoped regime of the high-Tc superconductor HgBa2CuO4+d (Hg1201). Our previous inelastic neutron scattering measurements of optimally doped (Tc ≈ 95 K) and moderately underdoped (Tc ≈ 65 K) samples revealed two novel, weakly-dispersive magnetic excitation branches below the pseudogap temperature T* [Y. Li et al., Nature 468, 283 (2010); Y. Li et al., Nature Phys. 8, 404 (2012)]. These excitations are associated with the translational symmetry preserving magnetic order previously established to be a universal property of the pseudogap phase [B. Fauqué et al., Phys. Rev. Lett. 96, 197001 (2006); Y. Li et al., Nature 455, 372 (2008); Y. Li et al. Phys. Rev. B 84, 224508 (2011)]. In HgBa2CuO4+d, the strength of this order was found to decrease in very underdoped samples [V. Balédent et al. Phys. Rev. B 83, 104504 (2011)]. Indeed, we find no evidence of pseudogap excitations in very underdoped Hg1201 (Tc ≈ 45 K), and instead we observe strong antiferromagnetic fluctuations over a large energy range (10 – 150 meV).

1Work supported by DOE-BES.

11:27AM B35.00002 Unusual form factor of the novel pseudogap excitations in HgBa2CuO4+d, MUN CHAN. C. DOROW, Y. TANG, G. YU, M. GREVEN, University of Minnesota, N. BARISIC, CEA Saclay, Y. LI, Peking University, K. HRADIL, R. MOLE, Forschungsnuernenonqueille Heinz Maier-Leibnitz, Germany, P. STEFFENS, Institut Laue Langevin, France, X. ZHAO, Jilin University, Y. SIDIS, P. BOURGES, Laboratoire Leon Brillouin, France — Following the discovery of a universal novel magnetic order in the pseudogap phase of the cuprates [B. Fauqué et al. PRL 96, 197001 (2006); Y. Li et al., Nature 455, 372 (2008)], we have performed inelastic neutron scattering measurements of HgBa2CuO4+d (Hg1201) revealed two weakly-dispersive excitation branches associated with this ordered state [Y. Li et al., Nature 468, 283 (2010); Y. Li et al., Nature Phys. 8, 404 (2012)]. The dependences of the mode intensities on the momentum transfer Q = (HKL) (r.l.u.) are inconsistent with traditional magnetic or structural form factors. The intensity of the high-energy mode is zero when Q is parallel to the copper-oxygen planes (i.e., for L = 0), peaks at L = 8 (r.l.u.), and decreases again at large L. We observe the opposite behaviour for the low-energy mode, which is strongest when L = 0. In combination with polarized inelastic neutron scattering results, this indicates possible dual magnetic and structural characteristics of the novel excitations. Work supported by DOE-BES.
of electrons and an odd, PEETS, H. TAKATSU, Y. MAENO, Kyoto University, Japan — Multiple experimental and theoretical studies provide compelling support for triplet pairing that the spin block order verges on a noncollinear in-plane-spin phase observed in Tl$_2$O$_6$ superconducting state. However, we find no evidence of this type of excitation in YBa$_2$Cu$_3$O$_{6.9}$.

Cu$_2$O$_{6.9}$, CHRISTOPHER LESTER, STEPHEN HAYDEN, University of Bristol, JIRI KULDA, Institut Laue-Langevin, DAVID CARDWELL, NADENDLA HARI BABU, University of Cambridge — On cooling through $T_c$, the spin excitation spectra of cuprate superconductors becomes dominated by the neutron spin resonance (NSR), a collective mode centred at $Q_{NR}$. We have used polarized inelastic neutron scattering to measure the spin excitations of YBa$_2$Cu$_3$O$_{6.9}$ ($T_c = 93$ K), unequivocally confirming the magnetic character of the NSR in both the odd and even channels. In the odd channel, the NSR is anisotropic in spin space, that is, the out of plane ($c$) component of $x^0(Q,\omega)$ is approximately 1.4 times larger than the in-plane ($a/b$) component. Conversely, the much weaker even channel resonance is isotropic to within experimental error, and the low energy response maintains a large gap ($\sim 30$ meV) in the normal state. While it is generally accepted that the NSR is ubiquitous in at least the hole-doped cuprates, recently two further collective modes have been observed in HgBa$_2$CuO$_{4+y}$. If these weakly-dispersive ‘ising-like’ modes were also universally present, then they might radically alter our view of the cuprate superconducting state. However, we report bulk measurements of the susceptibility of UPt$_3$, and we find no evidence of this type of excitation in YBa$_2$Cu$_3$O$_{6.9}$, suggesting that these modes may in fact be unique to certain systems.

11:51AM B35.00004 Effective $J_1$-$J_2$ model for the spin wave in the superconducting (Tl,Rb)$_2$Fe$_2$Se$_5$, SONGXUE CHI, FENG YE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, WEI BAO, Department of Physics, Renmin University of China, Beijing, 100872, China, ANDREI T. SAVICI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, MATTHEW B. STONE, Quantum Condensed Matter Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, RANDY S. FISHMAN, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, H. D. WANG, C. H. DONG, MINGHUI FANG, Department of Physics, Zhejiang University, Hangzhou 310027, China — Spin wave excitations in the superconducting state of (Tl,Rb)$_2$Fe$_2$Se$_5$ were determined by inelastic neutron scattering measurements. Four doubly degenerate spin wave branches, one gapped acoustic and 3 optical, span an energy range of about 210 meV. The spin wave spectra were successfully described by a $J_1$-$J_2$ Heisenberg model which includes the in-plane nearest ($J_1$ and $J_1'$), next nearest neighbor ($J_2$ and $J_2'$) interactions within and between the 4-spin blocks, inter-plane interaction ($J_3$) and a single-ion anisotropy. The exchange coupling constants obtained indicate that the spin block order verges on a noncollinear in-plane-spin phase observed in Tl$_2$Fe$_2$Se$_5$.

12:03PM B35.00005 Anisotropy of the Superconducting State in Sr$_2$RuO$_4$$^1$, M.R. ESKILDSEN, C. RASTOVSKI, University of Notre Dame, IN, USA, W.J. GANNON, Northwestern University, IL, USA, C.D. DEWHURST, Institut Laue-Langevin, France, D. PEETS, H. TAKATSU, Y. MAENO, Kyoto University, Japan — Multiple experimental and theoretical studies provide compelling support for triplet pairing of electrons and an odd, $\Psi$-wave order parameter symmetry in superconducting Sr$_2$RuO$_4$. However, seemingly contradictory experimental results have left important questions concerning the detailed structure and coupling of the orbital and spin parts of the order parameter in this compound unresolved. We have used small-angle neutron scattering to study the vortex lattice in Sr$_2$RuO$_4$ in order to measure the intrinsic anisotropy ($\Gamma_{ac}$) of the superconducting state between the the c axis and the RuO$_2$ basal plane. Up to fields of 1.2 T and temperature of 800 mK, we found no variation of $\Gamma_{ac}$ $\approx$ 60. This is consistent with the Fermi velocity anisotropy on the $\beta$ Fermi-surface sheet, but greatly exceeds the critical field anisotropy $H_{c2}^{\alpha}/H_{c2}^{\beta}$ $\approx$ 20. This result poses significant constraints on the possible order parameter symmetry in Sr$_2$RuO$_4$.

$^1$This work is supported by the U.S. Department of Energy, Office of Basic Energy Sciences under Award DE-FG02-10ER46783.

12:15PM B35.00006 Bulk Magnetization in the Superconducting State of UPt$_3$$^1$, WILLIAM GANNON, WILLIAM HALPERIN, Northwestern University, Department of Physics and Astronomy, USA, CATHERINE RASTOVSKI, MORTEN ESKILDSEN, University of Notre Dame, Department of Physics, USA, PENGCHENG DAI, University of Tennessee, Department of Physics and Astronomy, USA, ANNE STUNAULT, William Halperin, Northwestern University, Department of Physics and Astronomy, USA, WEI BAO, Department of Physics, Renmin University of China, Beijing, 100872, China, ANDREI T. SAVICI, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA — The unconventional superconductor UPt$_3$ has long been thought to have an odd parity orbital, and triplet spin state. An important signature of such a state is the temperature independence of the spin susceptibility across the superconducting transition temperature. Here, we report bulk measurements of the susceptibility of UPt$_3$ for magnetic fields along the crystal a-axis performed with polarized neutron diffraction. Temperature independence at all magnetic fields is observed, suggesting a spin triplet superconducting state for the entirety of the phase diagram, with equal spin pairs in the crystal basal plane. These results will be discussed in the context of existing theories for the superconducting state of this paradigm heavy fermion material [Graf et. al., PRB 62, 14393; Tsutsumi et. al., JPSJ 81, 074717 (2012)].

$^1$Support from US Department of Energy, Basic Energy Science, Division of Materials Science and Engineering awards DE-FG02-05ER46248, DE-FG02-10ER46783, and DE-FG02-05ER46202

12:27PM B35.00007 Kerr effect studies of the heavy fermion superconductor URu$_2$Si$_2$$^1$, ELIZABETH SCHEMM, Department of Physics, Stanford University, HOVNANAT KARAPETYAN, Department of Applied Physics, Stanford University, ERIC BAUER, Los Alamos National Laboratory, AHIRAN KAPITULNIK, Department of Physics and Department of Applied Physics, Stanford University — In the heavy fermion metal URu$_2$Si$_2$, the very large entropy carried by the 5f electrons is released at a $\sim 17.5$ K via a second-order phase transition to a “hidden order” state. Below $\sim 1.5$ K superconductivity emerges with an as-yet unknown gap structure, adding to the mystery associated with this material. In this talk we present polar Kerr effect (KPE) measurements of URu$_2$Si$_2$ crystals using a Sagnac interferometer. PKE is sensitive to time-reversal symmetry (TRS) breaking since it measures the existence of an antisymmetric contribution to the real and imaginary parts of the frequency-dependent dielectric tensor. Such a contribution is necessarily absent if TRS is not broken in the material. We find a weak magnetic signal in the hidden order phase that seems to not influence superconductivity. The presence of a finite Kerr signal below $T_c$ provides strong evidence that time reversal symmetry is broken in the superconducting state. The relationship between the magnetic response in the hidden order phase and superconductivity is also studied. We further compare our results to other unconventional superconductors.

$^1$This work was supported by the U.S. DOE, Office of Basic Energy Sciences, under contract DEAC02-76SF00515.

12:39PM B35.00008 High resolution $^{17}$O Knight shift measurements of HgBa$_2$CuO$_{4+y}$ single crystals$^1$, ANDREW M. MOUNCE, SANGWON OH, JONGSEOP A. LEE, W.P. HALPERIN, Northwestern University, A.P. REYES, P.L. KUHNS, National High Magnetic Field Lab, M. CHAN, L. LI, University of Minnesota, D. XIA, X. ZHAO, University of Minnesota, Jilin University, M. GREVEN, University of Minnesota — The high superconducting transition temperature and also the simple tetragonal structure of HgBa$_2$CuO$_{4+y}$ (Hg1201) makes this material an ideal candidate to study unconventional superconductivity in the cuprates$^1$. Nuclear magnetic resonance has been performed on Hg1201 single crystals which have been annealed in an $^{17}$O atmosphere to achieve superconducting transition temperatures of underdoped 72 K and overdoped 76 K. Oxygen spectra are sufficiently narrow to resolve planar, apical, and dopant oxygen sites in addition to all satellite transitions of the planar and apical sites. The deconvoolution of oxygen spin shifts into isotropic and axial shifts, for the underdoped crystal, shows temperature dependence in both the isotropic and axial components of the planar oxygen while the apical oxygen only has temperature dependence in the axial component. The rotational dependence of the apical oxygen shift does not indicate a predicted static local field component due to circulating orbital currents$^2$ which have been observed by neutron scattering$^3$.


$^1$This work is done by DOE/BES: DE-FG02-05ER42428, DE-SC0006858 and the NHMFL by NSF and the State of Florida.
12:51PM B35.00009 NMR study of spin fluctuations and superconductivity in LaFeAsO\(_1\_x\)H\(_x\).\(^1\) — NOAKI FUJIWARA, RYOSUKE SAKURAI, Graduate School of Human & Environmental Studies, Kyoto University, SOUSHI IMURA, SATORU MATSUISHI, HIDEO HOSONO, Material and structures laboratory (MSL), Tokyo Institute of Technology, YOICHI YAMAKA, HIROSHI KONTANI, Department of Physics, Nagoya University and JST, TRIP — We have performed NMR measurements in LaFeAsO\(_1\_x\)H\(_x\), an isomorphic compound of LaFeAsO\(_1\_x\)F\(_x\). LaFeAsO\(_1\_x\)H\(_x\) is most recently known for having double superconducting (SC) domes on H doping. LaFeAsO\(_1\_x\)H\(_x\) is an electron- doped system, and protons act as \(H^+\) as well as \(\delta^+\). The first SC dome is very similar between F and H doping, suggesting that H doping supplies the same amount of electrons as F doping. Interestingly, an excess amount of H up to \(x=0.5\) can be replaced with \(O^{2-}\). In the H-overdoped regime (\(x>0.2\)), LaFeAsO\(_1\_x\)H\(_x\) undergoes the second superconducting state \([1]\). We measured the relaxation rate of LaFeAsO\(_1\_x\)H\(_x\) for \(x=0.2\) and 0.4, and found an anomalous electronic state; spin fluctuations measured from \(1/T_1\) is enhanced with increasing the doping level from \(x=0.2\) to 0.4. The enhancement of spin fluctuations with increasing carrier doping is a new phenomenon that has not observed in LaFeAsO\(_1\_x\)F\(_x\) in which the upper limit of the doping level is at most \(x=0.2\). We will discuss the phenomenon in relation to superconductivity.

\[^1\] S. imura, \textit{et al.}, Nature Communications (2012)

\[\text{Grant (KAKENHI 23340101) from the Ministry of Education, Sports and Science, Japan}\]

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1:03PM B35.00010 Electronic and Magnetic Properties of Ba\(_1\_x\)K\(_x\)Mn\(_2\)As\(_2\) Studied by \(^{55}\)Mn and \(^{75}\)As-NMR. — S. YENINAS, A. PANDEY, D.C. JOHNSTON, Y. FURUKAWA, The Ames Laboratory — BaMn\(_2\)As\(_2\) (Mn\(^{2+}\); \(S=5/2\)) is a G-type antiferromagnetic (AF) semiconductor with Neél temperature \(T_N \approx 625\) K and a small band gap of \(\approx 27\) meV. Hole doping by substitution of Ba with K drives BaMn\(_2\)As\(_2\) into a metallic state while maintaining the same AF spin structure with similar high \(T_N\). In order to investigate hole doping effects on electronic and magnetic properties in Ba\(_1\_x\)K\(_x\)Mn\(_2\)As\(_2\)from a microscopic point of view, we have conducted \(^{55}\)Mn and \(^{75}\)As-NMR spectra and spin-lattice relaxation measurements on single crystals of Ba\(_1\_x\)K\(_x\)Mn\(_2\)As\(_2\) \((x=0, 0.04, 0.4)\). The temperature \((T)\) dependence of \(1/T_1\) for \(^{55}\)Mn and \(^{75}\)As for the \(x=0\) compound shows \(1/T_1\sim T^2\) dependence for both nuclei, suggesting that \(1/T_1\) of the nuclei arises from interactions with magnon excitations in the local-moment AF state. On the other hand, the \(1/T_1\) of both nuclei is found to be proportional to \(T\) (Korringa relation) in K-doped materials below \(T_N\), which corresponds to the AF metallic state in Ba\(_1\_x\)K\(_x\)Mn\(_2\)As\(_2\).

1:15PM B35.00011 ABSTRACT WITHDRAWN —

1:27PM B35.00012 High Energy Magnetic Excitations in overdoped high temperature Superconductors. — M. LE TACON, MPI FKF, G. GHIRINGHELLI, Politecnico di Milano, D.C. PEETS, MPI FKF, M. MORETTI-SALA, ESRF, S. BLANCO-CANOSA, MPI FKF, M. MINOLA, Politecnico di Milano, V. HINKOV, MPI-UBC center for Quantum Materials, R. LIANG, D. BONN, W. HARDY, UBC, C.T. LIN, MPI FKF, T. SCHMITT, SLS - PSI, L. BRAICOVICH, Politecnico di Milano, B. KEIMER, MPI FKF — Motivated by the search for the mechanism of high-energy spin-phonon and spin-electron excitations in high temperature superconducting (HTS) materials, we have recently observed a variety of magnetic excitations up to \(\approx 200\) meV in \(\alpha\beta\)-plane. Taking advantage of the recent developments of RIXS, we have shown that high energy magnetic excitations with dispersions and spectral weights similar to those of magnons in AF cuprates exist up to optimal doping. In the overdoped region, the normal state appears in many aspects similar to a Fermi liquid, and the available data on the magnetic excitations is rather limited. Inelastic neutron scattering work by Lipscombe et al. revealed the persistence of magnetic excitations up to \(160\) meV in an overdoped LSCO. This surprising result motivates us to investigate further the high energy magnetic excitations using RIXS in \(\alpha\beta\) and Ti2201 compounds. We show that the high energy part of the excitation spectrum is essentially unaffected with hole doping, and that excitations up to \(300\) meV survive even at doping levels at which SC vanishes.

1:39PM B35.00013 Two Dimensional Incommensurate Spin Excitations and Lattice Fluctuations in \(La_{1-x}Ba_xCuO_4\). — J.J. WAGMAN, McMaster University, J.P. CARLO, Villanova University, G. VAN GASTEL, McMaster University, Y. ZHAO, National Institute of Standards and Technology, A.B. KALLIN, E. MAZUREK, H.A. DABKOWSKA, Brockhouse Institute for Materials Research, A. SAVICII, G.E. GRANROTH, Oak Ridge National Laboratory, Z. YAMANI, Z. TUN, National Research Council, Canadian Neutron Beam Centre, Chalk River Laboratories, B.D. GAULIN, McMaster University — ‘Hour-glass’ shaped dispersions of antiferromagnetic (AF) spin fluctuations are a robust feature common to many high temperature superconductors. In 214 cuprates, these phenomena are well known to display a strong dependence on the concentration of holes that are introduced into the copper oxide planes by doping. The incommensurability (IC) of the two dimensional magnetic order in this system is sensitive to hole concentration. Here, we present a series of neutron scattering measurements on single crystals of \(La_{1-x}Ba_xCuO_4\) (LBCO), with \(0.035 \leq x \leq 0.055\), a doping range that spans the transition from diagonal to parallel IC ordering wavevectors, and from non-superconducting to superconducting ground states. Our measurements map out the evolution of the spin excitations for energies below \(\approx 50\) meV, and focus on the enhancement in the scattered intensity centered in the \(17-20\) meV at the AF IC positions. This regime corresponds to the approximate crossing of very dispersive spin excitations and weakly dispersive low lying optic phonons in LBCO.

\[^1\] NSERC, Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy

1:51PM B35.00014 ABSTRACT WITHDRAWN —

2:03PM B35.00015 Spin Susceptibility Enhancement in Superconductors\(^1\) — BEN ROSEMEYER, ANTON VORONTSOV, Montana State University — We calculate electronic vector-dependent spin susceptibility tensor, \(\chi(q)\), in the superconducting state, for a 2D Fermi surface. We investigate dependence of \(\chi(q)\) on: a) magnetic ordering wave vector \(q\); b) symmetry of the order parameter, \(\Delta(k)\); c) temperature; and d) effects of external Zeeman field. We find that under certain conditions longitudinal and transverse components of the susceptibility in the superconducting state can be enhanced compared to the normal state value, indicating effective attraction between magnetically ordered and superconducting phases. In particular, \(d\)-wave superconductors at low temperatures in strong magnetic field show increase of \(\chi\) for \(q=2k_F - \delta q\). We show that such enhancement or lack thereof to behavior of low-energy excitations in the system. These findings may be relevant to materials where magnetic and superconducting phases are close neighbors, such as heavy fermion CeCoIn\(_5\), or Fe-based superconductors.

\[^1\] Supported by NSF Grant DMR-0954342

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Monday, March 18, 2013 11:15AM - 2:15PM —

Session B40 DCMP: Surfaces, Interfaces, and Thin Films: Electronic and Magnetic Properties

349 - Michael Horn von Hoegen, Universitaet Duisburg-Essen
11:15AM B40.00001 OAM and spin structure of Cu(111) and Au(111) surface state bands. BEOMYOUNG KIM, PANJIN KIM, WONSIC JUNG, YEONGKWAN KIM, YOONYOUNG KOH, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, MASASHI ARITA, KENYA SHIMADA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-0046, Japan, CHOONG H. KIM, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — We performed angle-resolved photoemission studies on Cu(111) and Au(111) surface states with circularly polarized light to investigate local orbital angular momentum (OAM) structures. Existence of OAM is confirmed, as predicted, to exist in systems with an inversion symmetry breaking. Cu(111) surface state bands are found to have chiral OAM in spite of very small spin-orbit coupling, consistent with the theoretical prediction. As for Au(111), we observe split bands for which OAM for the inner and outer bands are parallel, unlike the Bi2Se3 case. We also performed first-principles calculations and the results are found to be consistent with experimental results. Moreover, the majority of OAM is found to have orbital origin while a small contribution comes from orbitals. An effective Hamiltonian that incorporates the role of OAM is derived and is used to extract the spin and OAM structures. We discuss the evolution of angular momentum structures from a pure OAM system to a strongly spin-orbit-entangled state.

11:27AM B40.00002 Electronic properties of precious-metal coated W tips in STM: Role of spin-orbit coupling1, T. YAMASHITA, T. AKIKAYAMA, K. NAKAMURA, T. ITO, Mie U., S.H. RHIM, A.J. FREEMAN, Northwestern U. — Scanning tunneling microscopy (STM) has proved a versatile tool invigorating many physics at an atomic scale, where chemical identity and shape of the probe tip greatly affect resolution and sensitivity. There have been many efforts to functionalize STM tips: coating W tips with organic molecules and 3d transition metals, which facilitate the selective imaging with enhanced tunneling current. In this work, we model W(110) tips coated by precious metals such as Au, Ag, and Pt, in which large spin-orbit coupling significantly influences the electronic structure of the STM probe. Furthermore, we argue that this spin-orbit coupling can be used as a spin detecting STM probe without additional bias switching. The stability of the W(110) apex atom for each metal coating is also discussed.

1Supported at N. U. by the DOE (DE-FG02-05ER45372), and at Mie U. by the Young Researcher Overseas Visits Program for Vitalizing Brain Circulation (R2214) from the Japan Society for the Promotion of Science.

11:39AM B40.00003 Ion bombardment of Ni(110) studied with inverse photoemission, LEED, and simulations. BENJAMIN YOUNG, JIM WARNER, DAVID HESKETT, University of Rhode Island — Inverse Photoemission Spectroscopy (IPES) performed on clean Ni(110) reveals an unoccupied electronic surface state ∼2eV above the Fermi level at the Γ point of the surface Brillouin Zone. Ion bombardment (sputtering) of the sample creates vacancies and adatoms, which reduce the intensity of the representative state peak in IPES spectra. While the intensity of this IPES peak decreases with sputtering, well-defined diffraction spots in the surface LEED pattern give way to more diffuse spots with higher background intensity. Quantization of these permits analysis of their intensity profiles. Results of these techniques are presented for various sputtering conditions with 1keV Ne + and compared to previous results for 500eV Ar + on the same sample. Finally, we connect sputtering trends in the IPES and LEED data to Monte Carlo simulations of the sputtering process.

11:51AM B40.00004 Measurement of the Spectral Distribution of Low Energy Electrons Emitted as a Result of M2,3VV Auger Transitions in Cu(100) and the N2,3VV transition in Ag1, PRASAD JOGLEKAR, SUMAN SATYAL, KARTHIK SHAstry, Dept of Physics, University of Texas at Arlington, STEVEN HULBERT, NSLS, Brookhaven National Laboratory, ALEXANDER WEISS, Dept of Physics, University of Texas at Arlington — Auger Photoelectron Coincidence Spectroscopy (AP ECS) was used to investigate the physics of electron emission in the Low Energy Tail (LET) of the M2,3VV and N2,3VV Auger spectra obtained from Cu(100) and Ag(100) surfaces, respectively. A beam of 200eV photons (180 eV in the case of Ag) was used to probe the Cu (Ag) sample. Two Cylindrical Mirror Analyzers (CMAs) were used to select the energy of electrons emitted from the sample. Auger electrons were detected in coincidence with the 3p 3/2 photoemission peak in the case Cu and the 4p photoemission peak in the case of Ag. A set of coincidence measurements were made with the fixed analyser set at a series of energies between the core and the valence band in order to obtain an estimate of the background due to the inelastic scattering of the valence band electrons. This background was then subtracted yielding a spectrum consisting only of electrons emitted as a result of the Auger transition process.

1NSF, DOE, Welch Foundation

12:03PM B40.00005 Transient Exciton at Ag(111) Surface1, CONG WANG, XUEFENG CUI, ADAM JOHN ARGON-DIZZO, University of Pittsburgh, Department of Physics & Astronomy, SEAN GARRETT-ROE, University of Pittsburgh, Department of Chemistry, HROVJE PETEK, University of Pittsburgh, Department of Physics & Astronomy — We investigate the surface states on Ag(111) by means of multi-photon photoemission using ultrashort laser pulses. The angle-resolved photoemission spectra at the non-resonant range are consistent with the well-known structures of Shockley states and image potential states. But when we tune the wavelength to the resonant range by two photon, the spectra is dominated by a non-dispersive feature, which should correspond to a localized state, and we assign it to transient exciton. Then we do time-resolved measurements and take Fourier Transformation with respect to the delay-axis. The dominant response of the Ag(111) sample is the driving frequency, which is unexpected because there is no one-photon resonant transition in the excitation scheme.

1Department of Energy
2Corresponding Author

12:15PM B40.00006 Phonon spectra on ultrathin Pb films with scanning tunneling spectroscopy. HYOUNGDO NAM, CHIH-KANG SHIH, Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA — After Blatt and Thomson’s prediction [Phys. Rev. Lett. 10, 332 (1963)], several groups have reported the quantum size effect on transition temperature(Tc) as a function of thickness of atomically flat ultrathin Pb film. In those cases, Tc oscillation related to film thickness was attributed to oscillation of the density of states (DOS) near the Fermi energy. However, the Tc oscillation amplitude is much smaller than that derived from the DOS oscillation. One therefore would ask: What is the role of electron-phonon interaction? Also as reported by Qin, et. al. [Science 324, 1314 (2009)], when the film is only 2ML thick, the pseudo-morphically strained film has lower Tc than the unstrained one, suggesting that interfacial phonons may play a role. To answer to above question, we perform layer-dependent scanning tunneling spectroscopy of Pb films on Si(111) at 2.3 K to observe the phonon related features in the tunneling spectra. Detailed analysis of thickness dependence of photon spectra will be reported.
12:27PM B40.00007 An STM and STS study on Iridium modified Si(111) Surface

DYLAN NICHOLLS, University of North Dakota — The structure of Si(111) √7 × √7 R 19.10° I Ir reconstructed surface have been investigated with the help of scanning tunneling microscopy/spectroscopy and low energy electron diffraction. We propose a model based on the experimental data. The model defines a unit cell containing one surface substitutional iridium atom centered under six silicon ad-atoms. Once the sample is annealed at 1200 °C, a low density lattice gas of these ring clusters forms on top of an impurity stabilized ’1 × 1’ domains. These ring clusters and ’1 × 1’ domains co-exist with 7 × 7 domains of clean Si(111) surface. The local density of states graphs measured on Si(111) √7 × √7 R 19.10° I Ir reconstructed surface contains an asymmetric peak at the edge of the valence band suggesting that there is a surface state exhibiting a Rashba type spin-orbit coupling.

3This work was supported by the North Dakota EPSCoR office (NSF grant #EPS-814442) and the University of North Dakota.

12:39PM B40.00008 Surface Electronic Excitations of Quantum Confined Mg Films on Si(111) 1

AO TENG, The University of Tennessee and Oak Ridge National Laboratory, KRZYSZTOF KEMPKA, Boston College, XIAOGUANG LI, Fudan University, MUSTAFA OZER, The University of Tennessee and Oak Ridge National Laboratory, SABAN HUS, The University of Tennessee, PAUL SNIJders, Oak Ridge National Laboratory, GEUNSEOP LEE, Inha University, HANNO WEITERING, The University of Tennessee and Oak Ridge National Laboratory — We have investigated surface electronic excitations at atomically-smooth ultrathin Mg(0001) films on a Si(111)-7×7 substrate using high-resolution electron energy loss spectroscopy. The monopole and multipole surface plasmons of bulk Mg have their counterparts in the thin film regime. The dispersion of the monopole mode, as well as the relative intensity of the multipole mode, exhibit interesting thickness dependencies that are directly associated with quantum size effects in the Mg films. Additionally, we present the first clear observation of a photo-threshold excitation not seen at the surface of bulk Mg. Its intensity is also thickness dependent and anti-correlates with the multipole mode intensity. The results can be modeled with an effective jellium model in which the local Wigner-Seitz radius follows the thickness-dependent variation of the ground-state charge density at the surface. The results are a clear manifestation of quantum-size phenomena in the collective plasmon response of ultrathin metal films.

1Research supported in part (AT, MNO, PCS) by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

12:51PM B40.00009 Oscillation of conductivity in layer-by-layer growth of Bi thin film phase

YASUNORI FUJIKAWA, Institute for Materials Research, Tohoku Univ., EIJII SAITO, WPI-AIMR, Tohoku Univ. — Thin film growth of Bi and related compounds has been attracted much attention because of their exotic properties originating in the large spin-orbit interaction of Bi. Growth of its simple structure is known to result in the formation of a thin-film phase in the initial stage, which is taken over by the bulk growth when the coverage exceeds several monolayers (ML). [1] With typical growth conditions, this transition takes place before the completion of the thin-film layer, which tends to agglomerate to form 4-ML thick islands, making it difficult to measure the intrinsic property of the thin-film phase. In this work, Bi growth on Si(111)-7×7 has been performed in a multi-probe VT-STM system, which provides wide-ranging opportunity of kinetic control and in-situ transport measurement during the thin film growth. By tuning the kinetic condition of the growth, it becomes possible to grow the thin-film phase uniformly covering the substrate in layer-by-layer mode. In-situ transport measurement has been performed during the layer-by-layer growth of the Bi thin-film phase, distinguishing the conductivity of each growth unit. It oscillates with a period of 2 ML, which reflects the atomic structure of the thin-film phase. [1] Nagaoh et al., Phys. Rev. Lett. 93, 105501 (2004).

1:03PM B40.00010 ABSTRACT WITHDRAWN —


CHIH-PIN LU, GUOHONG LI, IVAN SKACHKO, EVA ANDREI, Department of Physics and Astronomy, Rutgers University, DEPARTMENT OF PHYSICS AND ASTRONOMY, RUTGERS UNIVERSITY TEAM — Molybdenum disulfide MoS2, a semiconductor in the layered transition-metal dichalcogenide family of materials which is composed of weakly interacting layers held together by van der Waals interactions, offers an attractive possibility as a field effect transistor in low-power switching devices. We studied ultrathin MoS2 samples, ranging from single to several layers in thickness, that were extracted by mechanical exfoliation from the bulk material. Using a device geometry which allows varying the carrier density by gating across a 300nm insulating layer of SiO2, together with low temperature Scanning Tunneling Microscopy and Spectroscopy, we investigated the bandgap and its dependence on doping and number of layers. For few layer samples we observe a well resolved atomic structure and a band gap of ~1.1eV which is a little smaller than bulk band gap of 1.2eV in agreement with photoluminescence measurements and can change by backgate voltage.

2DOE-FG02-99ER45742 and NSF DMR 1207108

1:27PM B40.00012 Probing the Effects of Interface Band Structure Using Ballistic Electron Emission Microscopy

ROBERT BALSANO, VINCENT LABELLA, College of Nanoscale Science and Engineering SUNY Albany — Ballistic electron emission microscopy (BEEM) is a scanning tunneling microscopy (STM) technique that can measure transport of hot electrons through materials and interfaces with high spatial and energetic resolution. Using this technique an attenuation length for electrons in the film can be extracted from the relationship between film thickness and the number of hot electrons transmitted through the film. The behavior of the attenuation lengths of carriers with energies just above the Schottky barrier height is indicative of the interface band structure. BEEM requires an additional contact to ground the metal base layer of a metal semiconductor junction. Performing BEEM in situ with the sample fabrication greatly increases the through put for these types of measurements. This presentation will detail our data on electron transport through metals and across different interfaces and also highlight our work to develop a special silicon substrate that has the extra contact and oxide hard mask built in to enable in situ BEEM without modifications to the STM.

1:39PM B40.00013 Interface States in the metal-CdSe interfaces

MICHELLE TOMASIK, JEFFREY GROSSMAN, MIT, VARADHARAJAN SRINIVASAN, Indian Institute of Science Education and Research — CdSe, a potential material for hybrid solar cells, has a well known reconstruction at the surface which removes the surface states. Using Density Functional Theory (DFT) we explore what happens to the now-removed surface states when CdSe is interfaced with two different metals, Al and Au. We compare and contrast this with the interfaces of a pristine unreconstructed CdSe surface with the two metals.
1:51PM B40.00014 Calculated Stability and Band Offsets for Compensated and Abrupt Polar Si/Zn(S,Se) (111) Interfaces
d, DAVID FOSTER, GUENTER SCHNEIDER, Oregon State University — Heterovalent semiconductor interfaces, particularly in the non-symmetrizable (111) and (0001) directions, present computational challenges that must be addressed in order to predict properties such as band offsets and interface energies. We perform first principles GGA+U calculations of interface energies and band offsets for the nominally polar interfaces Si/Zn(S,Se) (111). Such wide-gap/narrow-gap heterostructures have been proposed as a possible means for altering the relaxation channel branching ratios for the decay of high energy photoelectrons (blue to UV) in favor of impact ionization (two carrier pairs from one photon). Examining configurations with one and two substitutonal defect layers, we find the expected trend that compensated interfaces typically have lower energies than abrupt interfaces. The valence band offset (−0.8 ± 0.1 eV) for the lowest energy abrupt Si/ZnS interfaces agrees well with the experimentally determined value of −0.7 eV. We examine methods to address the ambiguities that arise from both finite size induced inter-interface charge transfer and the non-symmetrizability of (111) oriented supercells.

3:06PM C1.00002 Tuning the Spin-Orbit Coupled Ground State of Iridates with Pressure

This work is supported by National Science Foundation Award ID 1035513.

2:03PM B40.00015 Atom probe characterization of an AlN interlayer within HEMT structures grown by molecular beam epitaxy and metal-organic chemical vapor deposition, BAISHAKHI MAZUMDER, STEPHEN W. KAUN, Materials dept, University of California Santa Barbara, JING LU, STACIA KELLER, UMESH K. MISHRA, ECE dept, University of California Santa Barbara, MATERIALS DEPT, UCSB COLLABORATION, ECE DEPT, UCSB COLLABORATION — An AlN interlayer is introduced in a conventional AlGaN/GaN HEMT to enhance the density and mobility of the two dimensional electron gas (2DEG). MBE and MOCVD are two competitive and proven techniques to grow high quality AlN, but a chemical characterization technique is desired to investigate the purity of the AlN interlayer. Amongst nanoanalyzing techniques, atom probe tomography (APT) is unique for its spatial resolution and 3-D compositional images (< 0.2nm) with analytical sensitivity (10ppm). In this work, plasma assisted MBE(PAMBE) and MOCVD techniques were employed to grow AlGaN/AlN/GaN heterostructures. Detailed compositional data from atom probe shows that a pure AlN layer was grown by PAMBE. From Hall measurements, the carrier density (sheet resistance) was found to be 1.65 × 10^11 cm^-2 (425 Ω/sq). This work showed that MBE technique is more suitable than MOCVD for growing pure AlN interlayers and that APT can provide valuable nano scale information for further optimization of growth structures, thereby improving device performance.

Monday, March 18, 2013 2:30PM - 5:30PM –
Session C1 DCMP: Invited Session: Spin-Orbit-Controlled Ground States in Single-Crystal Iridates
Ballroom I - Lance De Long, University of Kentucky

2:30PM C1.00001 Pressure and Doping Effects in Layered Iridates, GANG CAO, University of Kentucky — No abstract available.

3:06PM C1.00002 Tuning the Spin-Orbit Coupled Ground State of Iridates with Pressure

DANIEL HASKEL, Argonne National Laboratory — The electronic ground state of the novel magnetic insulators BaIrO_3 and Sr_2IrO_4 can be described by a SU(2) invariant pseudospin-1/2 Hubbard model very similar to that of the cuprates, but with a "twisted" coupling to external magnetic field (a g-tensor with a non-integer value). This perspective naturally explains the magnetic properties of Sr_2IrO_4. We also derive several simple facts based on this mapping and the known results about the Hubbard model and the cuprates, which may be tested in future experiments on Sr_2IrO_4.

4:20PM C1.00003 Twisted Hubbard Model for Sr_2IrO_4: Magnetism and Possible High Temperature Superconductivity

T. SENTHIL, Massachusetts Institute of Technology — Sr_2IrO_4 has been suggested as a Mott insulator from a single J_{eff} = 1/2 band, similar to the cuprates. However, this picture is complicated by the measured large magnetic anisotropy and ferromagnetism. Based on a careful mapping to the J = 1/2 (pseudospin-1/2) space, we propose that the low energy electronic structure of Sr_2IrO_4 can indeed be described by a SU(2) invariant pseudospin-1/2 Hubbard model, which is very similar to that of the cuprates, but with a "twisted" coupling to external magnetic field (a g-tensor with a staggered antisymmetric component). This perspective naturally explains the magnetic properties of Sr_2IrO_4. We also derive several simple facts based on this mapping and the known results about the Hubbard model and the cuprates, which may be tested in future experiments on Sr_2IrO_4.

4:44PM C1.00004 Exotic Physics from Doping a Strongly Spin-Orbit Coupled Mott Insulator

YUE CAO, University of Colorado at Boulder — Doping a Mott insulator, as in the case of high T_c cuprates, has given rise to many exotic physics in the doping diagram, such as the pseudogap, Fermi arc and vortex phase. An important topic in these strongly correlated systems is to distinguish the properties that are intrinsic to the Mott physics from those that are materials specific. Recent studies of Sr_2IrO_4, whose Mottness requires strong spin orbit coupling, provide a new venue to look into the topic, where the spin, orbital, charge and lattice degrees of freedom interact. Using ARPES we studied the evolution of the electronic structure of Sr_2IrO_4 with both Rh and La doping. We show that the Rh substitution acts as immobile effective local holes, without a strong renormalization of the overall band structure, while La acts as an electron dopant. Particularly interesting is the lightly hole-doped regime, which showcases some of the same exotic physics as seen in the cuprates, including pseudogaps and Fermi arcs. By observing the scattering rate evolution as a function of energy and temperature, we confirm the non-Fermi liquid nature of the Fermi arc.
Magnetic and crystal structures of the honeycomb lattice Na$_2$IrO$_3$ and single layer Sr$_x$IrO$_3$.

FENG YE, Oak Ridge National Laboratory — 5$d$ based iridates have recently attracted great attention due to the large spin-orbit coupling (SOC). It is now recognized that the SOC that competes with other relevant energies, particularly the on-site Coulomb interaction $U$, and have driven novel electronic and magnetic phases [1-3]. Combining single crystal neutron and x-ray diffractions, we have investigated the magnetic and crystal structures of the honeycomb lattice Na$_2$IrO$_3$ [4]. The system orders magnetically below 18.1 K with Ir$^{4+}$ ions forming zigzag spin chains within the layered honeycomb network with ordered moment of 0.22 $\mu$B / Ir site. Such a configuration sharply contrasts the Neel or stripe states proposed in the Kitaev-Heisenberg model. The structure refinement reveals that the Ir atoms form nearly ideal 2D honeycomb lattice while the IrO$_6$ octahedra experience a trigonal distortion that is critical to the ground state. The results of this study provide much-needed experimental insights into the magnetic and crystal structure crucial to the understanding of the exotic magnetic order and possible topological characteristics in the 5$d$-electron based honeycomb lattice. Neutron diffraction experiments are also performed to investigate the magnetic and crystal structure of the single layer iridate Sr$_x$IrO$_3$, where new structural information and spin order are obtained that is not available from previous neutron powder diffraction measurement.


This work was supported in part by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

Monday, March 18, 2013 2:30PM - 5:30PM —
Session C2 DCMP: Invited Session: Coulomb Drag and Exciton Condensation in Semiconductor and Graphene Double Layers — Ballroom II - Michael Lilly, Sandia National Laboratories

2:30PM C2.00001 Exciton Transport and Perfect Coulomb Drag$^1$. DEBALEENA NANDI, California Institute of Technology — Exciton condensation is realized in closely-spaced bilayer quantum Hall systems at $\nu_T = 1$ when the total density in the two 2D electron layers matches the Landau level degeneracy. In this state, electrons in one layer become tightly bound to holes in the other layer, forming a condensate similar to the Cooper pairs in a superconductor. Being charge neutral, these excitons ought to be free to move throughout the bulk of the quantum Hall fluid. One therefore expects that electron current driven in one layer would spontaneously generate a “hole” current in the other layer, even in the otherwise insulating bulk of the 2D system. We demonstrate precisely this effect, using a Corbino geometry to defeat edge state transport. Our sample contains two essentially identical two-dimensional electron systems (2DES) in GaAs quantum wells separated by a thin AlGaAs barrier. It is patterned into an annulus with arms protruding from each rim that provide contact to each 2DES separately. A current drag geometry is realized by applying a drive voltage between the outer and inner rim on the 2D system. We demonstrate precisely this effect, using a Corbino geometry to defeat edge state transport. Our sample contains two essentially identical two-dimensional electron systems (2DES) in GaAs quantum wells separated by a thin AlGaAs barrier. It is patterned into an annulus with arms protruding from each rim that provide contact to each 2DES separately. A current drag geometry is realized by applying a drive voltage between the outer and inner rim on the 2DES layer while the two rims on the opposite layer are connected together in a closed loop. There is no direct electrical connection between the two layers. At $\nu_T = 1$ the bulk of the Corbino annulus becomes insulating owing to the quantum Hall gap and net charge transport across the bulk is suppressed. Nevertheless, we find that in the drag geometry appreciable currents do flow in each layer. These currents are almost exactly equal magnitude but, crucially, flow in opposite directions. This phenomenon reflects exciton transport within the $\nu_T = 1$ condensate, rather than its quasiparticle excitations. We find that quasiparticle transport competes with exciton transport at elevated temperatures, drive levels, and layer separations. This work represents a collaboration with A.D.K. Finck, J.P. Eisenstein, L.N. Pfeiffer and K.W. West.


This work is supported by the NSF under grant DMR-1003080.

3:06PM C2.00002 Coulomb Drag and Magnetotransport in Graphene Double Layers$^1$. EMANUEL TUTUC, The University of Texas at Austin — Graphene double layers, a set of two closely spaced graphene monolayers separated by an ultra-thin dielectric, represent an interesting electron system to explore correlated electron states. We discuss the fabrication of such samples using a layer-by-layer transfer approach, the electron transport in individual layers at zero and in a high magnetic field, and Coulomb drag measurements. Coulomb drag, probed by flowing a drive current in one layer, and measuring the voltage drop in the opposite layer provides a direct measurement of the electron-electron scattering between the two layers, and can be used to probe the electron system ground state. Coulomb drag in graphene, measured as a function of both layer densities and temperature reveals two distinct regimes: (i) diffusive drag at elevated temperatures, above 50 K, and (ii) mesoscopic fluctuations-dominated drag at low temperatures [1, 2]. A second topic discussed here is a technique that allows a direct measurement of the Fermi energy in an electron system with an accuracy independent of the sample size, using a graphene double layer heterostructure. The underlying principle of the technique is that an interlayer bias applied to bring the top layer to the charge neutrality point is equal to the Fermi energy of the bottom layer, which in effect renders the top graphene layer a resistively detected Kelvin probe [3]. We illustrate this method by measuring the Fermi energy, Landau level spacing, and Landau level broadening in monolayer graphene. Work done in collaboration with S. Kim, I. Jo, J. Nah, D. Dillen, K. Lee, B. Fallahazad, Z. Yao, and S. K. Banerjee.


We thank ONR, NRI, and NSF for support.

3:42PM C2.00003 Interaction phenomena and Coulomb drag in graphene-based heterostructures$^1$. ANDRE GEIM, University of Manchester — Double-layer graphene heterostructures with boron nitride as a thin insulating barrier allow us to achieve a strongly interacting regime such that the two Dirac liquids effectively nest within the same plane but can be tuned and measured independently. The experiment reveals many unexpected features that are related to strong excitonic effects and mutual polarization of the graphene layers, which will be discussed in this talk.

$^1$In collaboration with Dr. Leonid Ponomarenko and Dr. Roman Gorbachev.
The existence of long been considered in nuclear matter, quantum Hall systems, liquid crystals, superfluid $^3$He and ultracold atoms. As their defining property they support a topological winding number of 1. In magnetic materials spin configurations with a non-vanishing topological winding number, driven by the interplay of magnetic anisotropies, dipolar interactions and geometrical frustration, have been known for a long time. This is contrasted by the recent discovery of skyrmion lattices in chiral magnets, i.e., long-range magnetic order in which each magnetic unit cell contains a skyrmion and thus a non-zero winding number. As a practical consequence, the non-zero topological winding number implies that the conduction electrons in the presence of a skyrmion experience changes of Berry phase, that correspond precisely to one quantum of emergent magnetic flux. In transport measurements this leads directly to a topological Hall signal. Moreover, tiny electric current densities are already sufficient to generate a motion of the skyrmions first observed indirectly in neutron scattering. Since the skyrmion supports one quantum of emergent magnetic flux the motion of the skyrmions induces an emergent electric field consistent with Faradays law of induction that may also be observed experimentally. The excellent theoretical description of the skyrmion lattices observed so far in metals, doped semiconductors and insulators suggests that they represent a rather universal phenomenon to be expected in a wide range of systems supporting chiral spin interactions. Taken together with the first insights into their emergent electrodynamics, skyrmion lattices in chiral magnets develop into a new area of condensed matter magnetism offering insights relevant for applications.

This work was supported by Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST program).
4:18PM C10.00004 Beller Lectureship: Dynamics of skyrmions under electric current, NAI TO NAGAOSA, University of Tokyo — Current-driven motion of the skyrmions and skyrmion crystal is attracting intense attention because of the very small critical current density, but the microscopic mechanism of their motion is not yet explored. In this talk, I will present a numerical simulation of the Landau-Lifshitz-Gilbert (LLG) equation and an analytic theory, which reveals a remarkably robust and universal current-velocity relation of the skyrmion motion driven by the spin transfer torque unaffected by either impurities or nonadiabatic effect in sharp contrast to the case of domain wall or spin helix. This is due to the peculiar dynamics of skyrmions characterized by inherent absence of the intrinsic pinning and flexible shape-deformation of skyrmions so as to avoid pinning centers. The effect of the constructed geometry will be also discussed. This work has been done in collaboration with J. Iwasaki and M. Mochizuki.

4:54PM C10.00005 Spontaneous atomic-scale magnetic skyrmion lattice in two dimensions, STEFAN HEINZE, Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany — Skyrmions are topologically protected field configurations with particle-like properties that play an important role in various fields of science. They have been predicted to exist also in bulk magnets and in recent experiments it was shown that they can be induced by a magnetic field. A key ingredient for their occurrence is the Dzialoshinskii-Moriya interaction (DMI) which was found to be strong also for magnetic nanostructures on substrates with large spin-orbit coupling [1]. In these systems the DMI stabilizes spin-spirals with a unique rotational sense propagating along one direction of the surface as observed for ultrathin films [1-3] and atomic chains [4]. Here, we go a step beyond and present an atomic-scale skyrmion lattice as the magnetic ground state of a hexagonal Fe monolayer on Ir(111) [5]. We develop a spin-model based on density functional theory that explains the interplay of Heisenberg exchange, DMI and the four-spin exchange as the microscopic origin of this intriguing magnetic state. Experiments using spin-polarized scanning tunneling microscopy confirm the skyrmion lattice which is incommensurate with the underlying atomic lattice. This work is a collaboration with G. Bihlmayer, S. Blügel, K. von Bergmann, M. Menzel, A. Kubetzka, J. Brede, and R. Wiesendanger.

References:

Monday, March 18, 2013 2:30PM - 5:30PM — Session C22 DCMP: Metamaterials and THz Spectroscopy 324 - Matt Doty, University of Delaware

2:30PM C22.00001 Hyperbolic dispersion of graded anisotropic metamaterial with optical Kerr effect, KA SHING HUI, HON PING LEE, KIN WAH YU, The Chinese University of Hong Kong — We have investigated the tunable optical dispersion relation from an anisotropic graded material with optical Kerr effect under the influence of external electric field. The permittivity of the material depends on incident electric field $\epsilon = \epsilon + \chi |E|^2$. In particular, a graded metallic thin film which dielectric permittivity is anisotropic in the parallel and perpendicular directions is considered. The permittivity in parallel direction is described by the graded Drude model and the permittivity in the perpendicular direction is described by epsilon-near-zero (ENZ) metamaterial. For ENZ metamaterial, the local electric field is enhanced such that $\chi |E|^2 \sim \epsilon$. As a result, the permittivity of ENZ metamaterial can be tuned by the optical Kerr effect. The dispersion relation and the electric field distribution are also examined in the quasi-static condition. By varying the intensity of the incident electric field, the dispersion relation can be switched from elliptical to hyperbolic which allow us to control light propagation. Furthermore, the implication of the switching from the elliptical to hyperbolic dispersion on the Goos-Hänchen shift will be studied.

2:42PM C22.00002 ABSTRACT WITHDRAWN

2:54PM C22.00003 Nonlinear Propagation in Fishnet Metamaterials, HAIM SUCHOWSKI, KEVIN O'BRIEN, ZI JING WONG, XIAOBO YIN, XIANG ZHANG, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, California 94720, USA — We present experimental and theoretical investigations of four-wave mixing in negative index metamaterials at optical frequencies with the goal of demonstrating a phase matched backward wave. The nonlinear propagation in thick fishnet structures are examined, in order to show an experimental observation of backward nonlinear optical generation in negative refractive index materials. We have fabricated a fishnet metamaterial with a negative refractive index in the near infrared and have measured its index using spectrally and spatially resolved interferometry. An infrared four wave mixing process was chosen to ensure that the linear properties of the fishnet can be treated with effective medium theory. The signal and idler are obtained from two optical parametric oscillators driven by synchronized femtosecond lasers. We find that with a counter-propagating pump and signal one can obtain perfect phase matching for the backward propagating idler and a large enough phase mismatch to suppress the forward propagating idler. Our efforts towards an experimental demonstration of nonlinear phase matching in negative index optical metamaterials will be discussed.

3:06PM C22.00004 Metagratings for Diffraction Based, Compact, Holographic Imaging, SANDEEP INAMPUDI, VIKTOR A. PODOLSKIY, University of Massachusetts Lowell, MULTISCALE ELECTROMAGNETICS GROUP TEAM — Recent developments in semiconductor technology brought to life a new generation of highly-compact visible-frequency cameras. Unfortunately, straight forward extension of this progress to long and mid-infrared domains (e.g., as mid-IR imaging) is impossible since the pixel size at these frequencies is limited by free-space diffraction limit. Here, we present an approach to realize highly-compact imaging systems at lower frequencies. Our approach takes advantage of high refractive index of materials commonly utilized in semiconductor detectors of mid-IR radiation, accompanied by metagratings, structures with engineered diffraction properties, to achieve a 10-fold reduction in the pixel size. In contrast to conventional refraction-based imaging, the approach essentially produces a digital hologram — a 2D projection of the 3D optical field, enabling a post-imaging “refocusing” of the picture. The perspectives of numerical recovery of the optical field and the stability of such recovery are discussed.

3:18PM C22.00005 Multiple-band transmission in an acoustic metamaterial, RU-WEN PENG, DONG-XIANG QI, REN-HAO FAN, Nanjing University, XIAN-RONG HUANG, Argonne National Laboratory, MING-HUI LUI, XU NI, QING HU, MU WANG, Nanjing University, NATIONAL LABORATORY OF SOLID STATE MICROSTRUCTURES, NANJING UNIVERSITY COLLABORATION, ADVANCED PHOTON SOURCE, ARGONNE NATIONAL LABORATORY COLLABORATION — We demonstrate that acoustic waves can achieve extremely flat transmission through a metallic grating under oblique incidence within multiple frequency bands separated by Wood’s anomalies. At the low-frequency band, the transmission of acoustic wave is independent of the frequency and presents a flat curve with the transmission efficiency reaching about 100%; while at high-frequency bands, the transmission decreases to be lower flat curves due to the diffraction effect. The transmission efficiency is insensitive to the thickness of the grating. This phenomenon is verified by experiments, numerical simulations, and an analytical model. The broadband high transmission is attributed to the acoustic impedance matching between the air and the grating. This research may open up a field for various potential applications of acoustic gratings, including broadband sonic imaging and screening, grating interferometry, and anti-reflection cloaking. References: D. X. Qi, R. H. Fan, R. W. Peng et al., Appl. Phys. Lett. 101, 061912 (2012); and R. H. Fan, R. W. Peng, X. R. Huang et al., Adv. Mater. 24, 1800 (2012).
3:30PM C22.00006 Two-Dimensional Control over Gradient Index in a VO$_2$ Memory Metamaterial. MICHAEL GOLDFLAM, University of California San Diego, TOM DRISCOLL, UCSD and Duke University, DANIEL BARNAS, University of California San Diego, MATTHEW ROYAL, TALMAGE TYLER, NAM JOKERST, DAVID SMITH, Duke University, GIWAN SEO, University of Science and Technology, BONG-JUN KIM, ETRI, HYUN-TAK KIM, ETRI and UST, DIMITRI BASOV, University of California San Diego — We have demonstrated the creation of spatial gradients in the optical properties of a metamaterial device through tuning of a vanadium dioxide layer that interacts with an array of split ring resonators (SRR). Application of a transient electrical pulse across the metamaterial-VO$_2$ system leaves persistent changes in the properties of the metamaterial due to the hysteresis of the insulator-to-metal transition in VO$_2$. Through modification of contact geometry, pulse shape, and pulse duration, we have shown increased control over such devices allowing for independent tuning of individual sections of our hybrid VO$_2$-SRR device through the application of several transient voltage pulses. The characteristics of the gradients resulting from the voltage pulses were measured using infrared transmission spectroscopy. We observed a 15% variation in the magnitude of transmission with spatial scales on the order of one wavelength at the resonance frequency. Thus we have demonstrated the viability of similar tunable metamaterial devices for use in communications and beam steering.

3:42PM C22.00007 Beating diffraction limit in an absorptive superlens. MENG XIAO, CHE TING CHAN, the Hong Kong university of Science and Technology — It is well known that a slab with both permittivity and permeability equals -1+i can achieve super resolution and its mechanism has been understood with the idea of complementary material. In practice, most metamaterials have always absorptive and thus absorb some sets an upper limit for the image resolution. Here, we study the image formation of stratified complementary slabs, where A is a super lens and B is normal material. We show that the superlens stack can beat the diffraction limit even in the presence of loss if the source has a time-dependent intensity profile. We derived a general analytical expression for the group velocity of an arbitrary k component including evanescent waves near frequency where “complementary” is satisfied and the analytical results can explain the super solution in the presence of absorption. And our results shows that, with a Gaussian shaped pulse illumination, the image resolution can be improved by about 45% relative to harmonic illumination for the same system.

3:54PM C22.00008 Lamb Shift in the Near Field of Hyperbolic Metamaterial Half Space$^1$. NAI JING DENG, KIN WAH YU, The Chinese University of Hong Kong — Hyperbolic metamaterials give a large magnification of the density of states in a specific frequency range, and has motivated various applications in emission lifetime reduction, strong absorption, and extraordinary black body radiation, etc. The boost of vacuum energy, which is proportional to the density of states, is expected in hyperbolic metamaterial. We have studied the Lamb shift in vacuum-hyperbolic-metamterial half spaces and shown the non-trivial role of vacuum energy. In our calculation, the easy-fabricated multilayer structure is employed to generate a hyperbolic dispersion relation. The spectrum of hydrogen atoms is calculated with a perturbation method after quantizing the half spaces with a complete mode expansion. It appears that the shift of spectrum is mainly contributed by the terahertz response of materials, which has been well described and predicted in both theories and experiments.

$^1$Work supported by the General Research Fund of the Hong Kong SAR Government

4:06PM C22.00009 Complex Oxide Thin Film Metamaterial Structures for THz applications. D. SHREIBER, U.S. Army Research Laboratory, R. CRAVEY, NASA Langley Research Center, M.W. COLE, U.S. Army Research Laboratory — Metamaterials operating in the frequency range of 0.1-1.5 THz are of a special interest for multiple Army applications such as communications, NDE of materials, and detection of chemical/biological substances. Several recent efforts have considered the use of complex oxide thin films for the development of metamaterials. However, the physical dimensions of these structures are limited due to the thin film nature which creates a set of challenges. In this work, we explore the potential of complex oxide thin film metamaterial structures for low frequency applications such as communications and NDE of materials.

4:18PM C22.00010 Analysis of Cyclotron Resonance Spectroscopy in a Landau-quantized 2DEG using Characteristic Matrix Methods$^1$. DAVID HILTON, University of Alabama at Birmingham — We develop a new characteristic matrix-based method to analyze cyclotron resonance experiments in high mobility ($\mu = 3.7 \times 10^6 \text{cm}^2 \text{V}^{-1} \text{s}^{-1}$) two-dimensional electron gas samples where direct interference between primary and satellite reflections has previously limited the frequency resolution. We use terahertz time-domain spectroscopy to measure the cyclotron resonance and extract the dephasing lifetime where multiple pulses from the substrate with a separation of $\sim 15$ ps directly interfere in the time-domain. We find a cyclotron dephasing lifetime of $15.1 \pm 0.5$ ps at 1.5 K and $5.0 \pm 0.5$ ps at 75 K.

$^1$This work is supported by the National Science Foundation under Grant No. DMR-1056827. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0654118

4:30PM C22.00011 Tunable Plasmonic Crystals Induced from a Two Dimensional Electron Gas$^2$. GREGORY DYER, Sandia National Laboratories, GREGORY AIZIN, City University of New York, S. JAMES ALLEN, UC Santa Barbara, ALBERT GRINE, DON BETHKE, JOHN RENO, ERIC SHANER, Sandia National Laboratories — A two dimensional electron gas (2DEG) with periodic variation of its screening$^1$, geometry,$^2$ or carrier density$^3$ provides an electromagnetic medium for the formation of a broadly tunable plasmonic crystal (PC). By using a periodic gate to control the 2DEG density in GaAs/AlGaAs heterostructures, we have induced terahertz (THz) PCs consisting of several bipartite crystal units. The PC band structure, Tamm states, and magnetically induced transparency phenomena are observed utilizing a gate-controlled defect adjacent to the PC to generate a plasmonic mixing photovoltaic. These integrated PCs have potential applications in the areas of frequency selective THz detection, strong light-matter interaction, and planar metamaterials. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000. The work at Sandia National Laboratories was supported by the DOE Office of Basic Energy Sciences. $^1$U. Mackens, et. al., Phys. Rev. Lett. 53, 1485 (1984). $^2$V. M. Muravev, et. al., Phys. Rev. Lett. 101, 216801 (2008). $^3$G. C. Dyer, et. al., Phys. Rev. Lett. 109, 126803 (2012).

4:42PM C22.00012 Controlling Metamaterial Field Enhancement at Terahertz Frequencies. GEORGE KEISER, HUSEYN SEREN, XIN ZHANG, RICHARD AVERITT, Boston University — With the advent of metamaterials has come an unprecedented ability to manipulate and engineer the index of refraction, n, and impedance, Z of materials. Engineering these far field properties has led to exciting developments such as negative index materials, electromagnetic cloaks, and perfect lensing. However, metamaterials can also be used to engineer designer microscopic charge distributions, current distributions, and polarizabilities. For instance, the on-resonance charge distribution in the capacitive gap of a split ring resonator (SRR) creates a localized region of high electric field enhancement that has seen prominent application in recent work. Here, we present a method to tune the magnitude of this resonant electric field enhancement. Via structural manipulation of the coupling between the SRR and a non-resonant closed conducting ring, we are able to increase and decrease the oscillation strength of the SRR and thus the field enhancement in the SRR’s capacitive gap. We present numerical simulations and experimental measurements at terahertz frequencies to confirm this result.
behavior can be explained considering the arrays' geometrical frustration and the thermally activated reconfiguration of the vortex lattice between isoenergetic states. This effect strongly depends on the temperature. We argue that this is fabricated via masked ion irradiation. Surprisingly, we found that minimal changes in the distance between pinning sites lead to the suppression of some of the multivalent and non-unique vortex states. This is done with YBCO films in which the nanoscale vortex energy landscape is strongly influenced by the pinning gradient, but the preservation of the sixfold ordering in the conformally transformed hexagonal lattice plays a crucial role. Our results can be generalized to a wide class of gradient-driven interacting particle systems such as colloids on optical trap arrays.

Energy, Office of Science, Office of Basic Energy Sciences (MLL, ZLX, LEO, RD, UW, WKK), under Contract No. DE-AC02-06CH11357

Arrays of Nanoscale Holes and Magnetic Dots

We have designed and fabricated micromachined three dimensional (3-D) air-liquid monopole antenna arrays. The air-liquid antenna arrays have been fabricated using high-aspect-ratio epoxy structures defined by ultraviolet (UV) lithography and subsequent metallization by thin film metal sputtering. The uniqueness of this monopole antenna lies in its strong coupling to incident THz waves with E-field perpendicular to the substrate, which is not the case with most substrate-printed antennas. A Bruker 113v FTIR system has been used to characterize the fabricated antenna arrays for both σ- (E-field parallel to the plane of incidence) and π- (E-field parallel to the plane of incidence) polarized light over 30-600 cm−1/1-20 THz. We measured monopole antenna arrays with diameters of 5 µm and different heights from 20 µm to 60 µm. Measurement results are compared to resonant frequency calculations and simulations. The results are in good agreement with those of the simulations.

5:06PM C22.00014 Photo-imprinted diffraction gratings for controlling terahertz radiation

We use vortex dynamics on artificial nanoscale energy landscapes as a model to experimentally investigate a generalized to a wide class of gradient-driven interacting particle systems such as colloids on optical trap arrays.

5:18PM C22.00015 Nonlinear THz Plasmonic Disk Resonators

Recent numerical simulations by Ray et al. predict that a conformal pinning array can produce stronger vortex pinning effect than other pinning structures with an equivalent density of pinning sites [1]. Here we present experimental investigations on conformal pinning structures. Direct and conformal pinning arrays of triangular and square lattices were introduced into MoGe superconducting films using focused-ion-beam milling or electron-beam lithography. Transport measurements on critical currents and magnetoresistances were carried out on these samples to reveal the advantages of conformal pinnings. Effects of random pinnings with the same average density were also studied for comparison. Details on sample fabrications and effects of pinning types (holes versus magnetic dots) will be presented. Reference: [1] D. Ray, C. J. Olson Reichhardt, B. Janko, C. Reichhardt, arXiv:1210.1229 (2012) Work supported by the US DoE-BES funded Energy Frontier Research Center (YLF), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (Mll, ZLX, LEO, RD, UW, WKK), under Contract No. DE-AC02-06CH11357

5:45PM C24.000033 Vortex Pinning in Superconducting MoGe Films Containing Conformal Arrays of Nanoscale Holes and Magnetic Dots

We use vortex dynamics on artificial nanoscale energy landscapes as a model to experimentally investigate a generalized to a wide class of gradient-driven interacting particle systems such as colloids on optical trap arrays.
3:06PM C35.00004 Critical currents, magnetic relaxation and pinning in NdBa2Cu3O7-δ films with BaZrO3 column defects1. A.O. LAJADOLA, Department of Physics, North Georgia College and State University, S.H. WEE, A. GOYAL, P.M. MARTIN, J. LI, Oak Ridge National Laboratory, J.R. THOMPSON, Department of Physics, University of Tennessee, D.K. CHRISTEN, Oak Ridge National Laboratory — The critical current density \( J_c \), and the magnetic relaxation (creep) properties have been studied for a set of NdBa2Cu3O7-δ (NbCO) films doped with BaZrO3 (BZO) nanoparticles to form columnar defects. The dependence of \( J_c \) on the magnitude and orientation of the applied magnetic field \( H_{app} \) (0-6.5 T) and temperature \( T \) (5 K-300 K) was investigated. The normalized flux-creep rate \( S = -\frac{d\ln(J_c)}{d\ln(t)} \) was determined as a function of \( t \). The current dependence of the effective activation energy \( \Delta U_{eff} \) was derived using the formalism developed by Maley. The results are well described by an inverse power law type barrier of the form \( \Delta U_{eff}(J) \sim U_0(J_0/J)^\mu \) with fitted values for the pinning energy scale \( U_0 \) and the glassy exponent \( \mu \). When comparing values for these parameters in the BZO-doped samples with those for their undoped control counterparts, the most striking difference is the increase of current density \( J_0 \) in the doped samples (a factor of 2.4 higher), while the other pinning parameters do not differ strongly. In the BZO-doped materials, the pinning energy scale \( U_0 \) increases with vortex density and \( J_0 \) decreases, with both following simple power law dependences on the field.

1Support from Department of Energy (Office of Basic Energy Sciences-Materials Sciences and Engineering Division), Oak Ridge Associated Universities and Office of Electricity Delivery and Energy Reliability (Advanced Cables and Conductors).

3:18PM C35.00005 Polaronic pinning of vortex in magnetic superconductors and magnetic-superconducting multilayers1. SHI-ZENG LIN, LEV BULAEVSIIK, Los Alamos National Laboratory — We present a new type of vortex pinning by enhancing the viscosity of vortex in magnetic superconductors with long relaxation time of magnetization and large magnetic susceptibility. In the absence of current, vortices are dressed by nonuniform magnetic polarization and form vortex-polarons. Under a small current and consequently low Lorentz force, the magnetic polarization follows the vortex motion. However, at large magnetic relaxation time of magnetization, there is additional dragging force by the magnetization besides the Bardeen-Stephen one, thus the effective viscosity of vortex is significantly enhanced resulting in suppression of dissipation. For a large current, the magnetic polarization cannot follow the vortex motion and the vortex-polaron dissociates, i.e. the magnetization and vortex become decoupled. In the IV characteristic, the decoupling transition shows as a voltage jump and can be identified as a depinning transition. The polaronic pinning mechanism successfully explains the observed enhancement of critical current in the ErNiBC superconductor at low temperatures. The polaronic pinning can be optimized in magnetic-superconducting multilayers. We show also that vortex-polaron creep is suppressed at low temperatures.

1This publication was made possible by funding from the Los Alamos Laboratory Directed Research and Development Program, project number 20110138ER.

3:30PM C35.00006 ABSTRACT WITHDRAWN —

3:42PM C35.00007 Role of twin boundaries on the vortex dynamics in CSD YBCO nanocomposites1. V. ROUCO, A. PALAU, M. COLL, R. GUZMAN, J. GAZQUEZ, S. YE, A. LLORDES, J. ARBIOL, S. RICART, X. OBRADORS, T. PUIG, Institut de Ciencia de Materials de Barcelona - CSIC — Vortex pinning landscape engineering is foreseen as the route to high performance YBCO coated conductors at high fields. Solution-derived nanocomposites with randomly oriented nanoparticles were shown to be an excellent low cost option with large isotropic pinning forces associated to a highly dense defect structure. We find that the local strain ensuing from the partial dislocation associated to intergrowths breaks the vertical coherence of twin boundaries (TB) and reduce the TB spacing. The lack of TB coherence will affect their role as pinning centers or channels for easy vortex flow. Transport measurements at different temperatures and magnetic fields realized in tracks with different crystallographic orientations has enabled to determine the effect of TB in a quantitative manner and establish their contribution (pinning and/or channeling) in a H-T diagram. We show that the anisotropic pinning coming from TBs has a minor role compared with the large enhancement of isotropic pinning in nanocomposites. On the contrary, we demonstrate that the reduction of the TB vertical coherence has a relevant effect on precluding vortex channelling at low temperatures avoiding a \( J_c \) suppression for field parallel to the c-axis.

1Spanish MICINN (MAT2011-29874-C02-01, NANOSELECT CSD2007-00041), Generalitat de Catalunya (2009 SGR 770 and Xarxas), UE (EURO-TAPES FPT 280432-2)

3:54PM C35.00008 Vortex dynamics in YBCO films with engineered antidots and ferromagnetic Nanostructures , A. PALAU, V. ROUCO, J.C. GONZÁLEZ, C. MONTON, T. PUIG, X. OBRADORS, Institut de Ciencia de Materials de Barcelona CSIC, Bellaterra, Spain, R. CÓRDOBA, J.M. DE TERESA, Instituto de Nanociencia de Aragón, Univ. Zaragoza, E-50009, Spain — Understanding vortex pinning mechanisms and the interaction between vortices and defects is still one of the major goals to enhance properties of nanostuctured superconductors. We have used high resolution lithography techniques (FIB, EBL and C-AFM) to create artificial pinning sites in YBCO films. Model systems with antidots and blind antidots with different geometries, distribution and density have been generated. Moreover, with the aim to study interactions in hybrid superconductor-ferromagnetic systems we have filled the antidots with cobalt rods by focused electron beam induced deposition. In-field critical current measurements have been performed in the single vortex pinning regime (T) and magnetic field (H) range in order to study vortex dynamics in these novel systems. As far as YBCO films with blind antidots, collective guided vortex motion is observed when we generate spatial asymmetric (ratchet) pinning potentials. By tuning H and T, the vortices undertakes the single vortex pinning to vortex-vortex interaction transition which determines the region where the ratchet effect is activated. As far as YBCO films with ferromagnetic rods, we demonstrate a clear interaction between the magnetic field generated by the cobalt nano-rods and the superconducting matrix.

4:06PM C35.00009 Non-equilibrium relaxation of vortex lines in disordered type-II superconductors1. ULRICH DOBRAMYSYL, HIBA ASSI, MICHEL PLEIMLING, UWE C. TÄUBER, Department of Physics, Virginia Tech — Vortex motion in disordered type-II superconductors display a remarkable wealth of behavior, ranging from hexagonally arranged crystals and a vortex liquid to glassy phases. The type and strength of the disorder has a profound influence on the structural properties of the vortex matter: Randomly distributed weak point pinning sites lead to the destruction of long range order and a Bragg glass phase; correlated, columnar disorder can yield a Bose glass phase with infinite tilt modulus. We employ a three-dimensional elastic line model and apply a Langevin molecular dynamics algorithm to simulate the dynamics of vortex lines in a dissipative medium. We investigate the relaxation of a system of lines that were initially prepared in an out-of-equilibrium state and characterize the transient behavior via two-time quantities. We vary the disorder type and strength and compare our results for random and columnar disorder.

1Research supported by the U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering under Award DE-FG02-09ER46613.
4:30PM C35.00011 Flux-quantum-discretized dynamics of intermediate state flux structures in current-driven type-I superconductors. G.R. BERDIYOROV, Department Fysica, Universiteit Antwerpen; Department of Physics, Loughborough University, A.D. HERNANDEZ-NIEVES, Centro Atomico Bariloche, Argentina, M.V. MILOSEVIC, F.M. PEETERS, Departement Fysica, Universiteit Antwerpen, Belgium, D. DOMINGUEZ, Centro Atomico Bariloche, Argentina. — Nonlinear flux dynamics in a current-carrying type-I superconductor is studied using Ginzburg-Landau theory. The current induces the intermediate state, where nucleation of flux domains is discretized to a single fluxoid at a time, whereas their final shape (tubular or laminar) and size depend on applied current. The current induces opposite flux domains on opposite edges, and subsequently drives them to annihilation—which is also discretized, as a sequence of vortex-antivortex pairs. In the presence of pinning centers, both pinning and depinning processes occur in a single flux-discretized form regardless of the shape and size of the flux configurations. Repulsive centers (i.e., obstacles) can result in shrinking of tubular domains and branching of laminar structures or transformation of them into tubular patterns. The discretization of nucleation and annihilation, as well as pinning/depinning processes leaves measurable traces in the voltage across the sample and in locally probed magnetization. The reported dynamic phenomena thus provide an unambiguous proof of a flux quantum being the smallest building block of the intermediate state in type-I superconductors.

4:42PM C35.00012 Comparison of local electrodynamic responses of superconducting materials—from bulk Nb to MgB2 and Nb thin films. TAMIN TAI, BEHNOOD GHAMSARI, University of Maryland-College Park, TENG TAN, XIAOXING XI, Temple University, STEVEN ANLAGE, University of Maryland-College Park. — A near-field magnetic field microwave microscope that enables mapping of the local electrodynamic response in the GHz frequency regime at liquid helium cryogenic temperatures was successfully built using the combination of a magnetic writer and a near field-microwave microscope [1]. Many superconducting materials, especially the candidate materials for superconducting RF cavities, were tested at a fixed location to analyze the local electromagnetic response, including both the intrinsic and extrinsic nonlinearities. The bulk Nb materials only show extrinsic nonlinearities consistent with vortex generation and annihilation in the material. The measurements on Nb and MgB2 thin film materials show not only the extrinsic nonlinearity but also the intrinsic nonlinearity. The intrinsic nonlinearity comes from the modulation of the superconducting order parameter near Tc, but behaves differently for single band gap (Nb) and two-gap (MgB2) superconductors. Quantitatively analyzing the nonlinear mechanisms will enable the microscope to extract many material parameters and image the superconducting properties by raster scanning.

1 This work is supported by the US DOE/HEP through grant DESC0004950, and also by the ONR AppEl Center, Task D10, (Award No. N000140911190), and UMD-CNAM.

4:54PM C35.00013 Lower critical magnetic field for a 2-D superconductor in a non-uniform field. JOHN DRASKOVIC, THOMAS LEMBERGER, The Ohio State University. — Our exploration of nonlinear effects in two-coil measurements of superfluid density in thin superconducting films led us to calculate the lower critical field of infinite-radius, thin superconducting films in the non-uniform field of a nearby coil powered by an external current supply. We obtain an expression for the Helmholtz free-energy of vortices and antivortices added to the vortex-free superfluid density in thin superconducting films. The lower critical field of infinite-radius, thin superconducting films in the non-uniform field of a nearby coil powered by an external current supply is studied using Ginzburg-Landau theory. The current induces the intermediate state, where nucleation of flux domains is discretized to a single fluxoid at a time, whereas their final shape (tubular or laminar) and size depend on applied current. The current induces opposite flux domains on opposite edges, and subsequently drives them to annihilation—which is also discretized, as a sequence of vortex-antivortex pairs. In the presence of pinning centers, both pinning and depinning processes occur in a single flux-discretized form regardless of the shape and size of the flux configurations. Repulsive centers (i.e., obstacles) can result in shrinking of tubular domains and branching of laminar structures or transformation of them into tubular patterns. The discretization of nucleation and annihilation, as well as pinning/depinning processes leaves measurable traces in the voltage across the sample and in locally probed magnetization. The reported dynamic phenomena thus provide an unambiguous proof of a flux quantum being the smallest building block of the intermediate state in type-I superconductors.

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5:06PM C35.00014 Nature of the Cuprate Pseudogap State in the Presence of High Magnetic Fields. PETER SCHERPELZ, DAN WULIN, KATHRYN LEVIN, James Franck Institute and Department of Physics, University of Chicago, ATTIPAT RAJAGOPAL, Inspire Institute and Harish-Chandra Research Institute. — We address the important question of how to characterize the pseudogap state of superconductors under the influence of magnetic fields strong enough to lead to vortex lattices in the condensate. Here we adopt a preferred pair interpretation of the pseudogap in which non-condensed pairs (arising from a stronger-than-BCS attraction) are present above and below Tc. We use a simple extension of Gor’kov theory to arrive at a formalism for treating BCS-to-BEC crossover physics. We thereby demonstrate how these pairs organize above the transition Tc into precursors of a vortex configuration via small distortions of the superconducting vortex state. We believe this provides a possible scenario for a normal state “pseudo”-vortex state which has been the object of discussion in the literature. Because their dispersion is no longer effectively one-dimensional, this precursor vortex configuration appears to enable otherwise problematic “Bose condensation” in a field.

5:18PM C35.00015 ABSTRACT WITHDRAWN
2:30PM C36.00001 Pump-probe reflectivity study of competing orders in the electron doped cuprate superconductor Nd$_{2-x}$Ce$_x$CuO$_4$+δ, J.P. HINTON, UC Berkeley, LBNL, J.D. KORALEK, LBNL, G. YU, University of Minnesota, E.M. MOTOYAMA, Stanford University, Y.M. LU, A. VISHWANATH, UC Berkeley, LBNL, M. GREVEN, University of Minnesota, J. ORENSTEIN, UC Berkeley, LBNL — We study the electron doped cuprate superconductor Nd$_{2-x}$Ce$_x$CuO$_4$+δ using optical pump-probe spectroscopy over a range of dopings including both superconducting and underdoped antiferromagnetic samples. We focus on the pseudogap (PG) response, which is observed over the entire doping range, and its interaction with superconductivity (SC). The PG response onsets below values of $T^*$ consistent with other probes, and its time dependence exhibits scaling consistent with critical fluctuations in samples near optimal doping. Furthermore, we observe laser fluxence-dependent interaction between the PG and SC responses below $T_c$, indicative of a repulsive interaction between superconductivity and another fluctuating order.

3Optics work supported by DOE Contract No. DE-AC02-05CH11231. Crystal growth and characterization work supported by NSF DMR-1006617 and a seed grant through the NSF MRSEC program.

2:42PM C36.00002 Fluctuating charge density waves in a cuprate superconductor, FAHAD MAHOOD, DARIUS TORCHINSKY, Massachusetts Institute of Technology, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory, NUH GEDIK, Massachusetts Institute of Technology — Cuprate compounds that host high-temperature superconductivity also exhibit various forms of charge and/or spin ordering whose role in the complex cuprate phase diagram is not fully understood. Static charge-density wave (CDW) ordering has been detected so far by diffraction probes only for special doping or in an applied external field. However, dynamic (fluctuating) CDWs may also be present more broadly while being difficult to detect by conventional techniques. To observe and characterize fluctuating CDWs in cuprates, and determine whether they favor or compete with HTS, is thus an important open problem. Here, we present a new method, based on ultrafast spectroscopy, to detect the presence and measure the lifetime of CDW fluctuations in cuprates. In an underdoped La$_{1.9}$Sr$_1$CuO$_4$ film ($T_c = 26$ K), we observe collective excitations of CDW that persist up to 100 K. This CDW is dynamic; it fluctuates with a characteristic lifetime of 2 ps at $T = 5$ K which decreases to 0.5 ps at $T = 100$ K. In contrast, in an optimally doped La$_{1.84}$Sr$_{0.16}$CuO$_4$ film ($T_c = 38.5$ K), we see no signatures of fluctuating CDW at any temperature, favoring the competition scenario. This work opens a path towards a broad study of fluctuating order parameters in various superconductors and other materials.

2:54PM C36.00003 Modified electron-boson coupling in Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ nanocrystals, LUKE SANDILANDS, University of Toronto, Canada, ZHJUN XU, ALINA YANG, GENDA GU, Brookhaven National Lab, USA, TOR PEDERSEN, FERENC BORONDICS, Canadian Light Source, Canada, KENNETH BURCH, University of Toronto, Canada — The coupling between electrons and bosons is thought to underlie a variety of unusual behavior in the cuprates. Here we present optical evidence that the electron-boson coupling is strongly modified in mechanically-exfoliated Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ nanocrystals. Through an extended Drude analysis of the mid-infrared optical conductivity, we demonstrate that the electron-boson spectral function is blue-shifted and enhanced in thin Bi$_2$Sr$_2$CaCu$_2$O$_{8+δ}$ nanocrystals. Taken together with complementary Raman and Laue diffraction data, our results provide further evidence that the bosons relevant to the electronic structure of the normal state are magnetic.

3:06PM C36.00004 Effect of out-of-plane disorder on electronic Raman spectra of Bi2212 single crystals, TAKAHIKO MASUI, NAOKI MURAI, Department of Physics, Graduate School of Science, Osaka University, MOTOUKI ISHIKADO, Japan Atomic Energy Agency, SHIGEYUKI ISHIDA, Department of Physics, University of Tokyo, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology (AIST), SHIN-ICHI UCHIDA, Department of Physics, University of Tokyo, SETSUKO TAJIMA, Department of Physics, Graduate School of Science, Osaka University — Out-of-plane disorder in cuprate superconductor is known to suppress $T_c$ without serious increase of residual scattering of conduction carriers. This is quite advantageous for spectroscopic measurements. In this study we have measured electronic Raman spectra of optimally-doped Bi2212 single crystals with different degree of out-of-plane disorders. In the superconducting state, the Bi2g electronic Raman spectra, which detect maximum of d-wave superconducting gap, show coherence peaks. Interestingly, the peak energies are independent of $T_c$ for lower $T_c$ samples. On the other hand, the peak position for a higher $T_c$ sample shifts to higher energy. This is clear contrast with the Bi2g electronic Raman spectra, which detect nodal region of the superconducting gap. The strange polarization dependence of superconducting Raman spectra could be a clue to understand the doping dependence of the superconducting Raman spectra.

3:18PM C36.00005 Optical scattering rate and effective mass throughout the phase diagram of Bi$_2$Sr$_2$La$_x$CuO$_{6+δ}$, R.P.S.M. LOBO, Y.M. DAI, LPEM, ESPCI, CNRS, Paris, France, H.H. WEN, Nanjing University, Nanjing, China, P. CHENG, H.Q. LUO, B. XIU, X.G. QIU, Institute of Physics, Chinese Academy of Sciences, Beijing, China — We determined the optical conductivity of Bi$_2$Sr$_2$La$_x$CuO$_{6+δ}$ at dopings covering the phase diagram from the underdoped to the overdoped regimes. The frequency dependent scattering rate shows a pseudogap extending into the overdoped regime. We found that the effective mass enhancement calculated from the optical conductivity is constant throughout the phase diagram. Conversely, the effective optical charge density varies almost linearly with doping. Our results suggest that the low frequency electronic and optical conductivity of Bi$_2$Sr$_2$La$_x$CuO$_{6+δ}$ is not strongly affected by the long range Mott transition. [Y. M. Dai et al., Phys. Rev. B 85, 092504 (2012)].

3:30PM C36.00006 Microwave conductivity survey of YBa$_2$Cu$_3$O$_{6+2δ}$: from underdoped to overdoped, JORDAN BAGLO, JAMES DAY, PINDER DOSANJH, RUIXING LIANG, WALTER HARDY, DOUG BONN, University of British Columbia — Recent experimental results and theoretical proposals suggest significant changes in the electronic structure of the high-$T_c$ cuprate superconductors as one approaches optimal doping, including Fermi surface reconstruction associated with proposed electronic ordering transitions. As sensitive probes of the low-energy electronic and optical properties, microwave conductivity measurements provide useful information on the nature of the Fermi surface and penetration depth measurements from which the real and imaginary parts of the microwave conductivity may be extracted - are well-suited for investigating such changes in the electronic structure of the cuprates across their phase diagram. Here we present preliminary results of a detailed and systematic doping dependence study of the microwave conductivity of the cuprate superconductor YBa$_2$Cu$_3$O$_{6+2δ}$ from the underdoped to the overdoped regime. The implications of these results for various proposed scenarios will be discussed.

3:42PM C36.00007 Disentangling the in- and out-of-plane components of the microwave surface resistance in Tl-2201, S. MAHYAD AGHIGHI, JAMES DAY, JORDAN BAGLO, Department of Physics & Astronomy, University of British Columbia, Vancouver, V6T 1Z1, Canada, DARREN PEETS, Max Planck Institute Festkörperforschung, D-70569 Stuttgart, Germany, LUDVINE CHAUVIÈRE, PINDER DOSANJH, RUIXING LIANG, WALTER HARDY, DOUG BONN, Department of Physics & Astronomy, University of British Columbia, Vancouver, V6T 1Z1, Canada, UBC SUPERCONDUCTIVITY GROUP (MICROWAVE MEASUREMENT) TEAM, UBC SUPERCONDUCTIVITY GROUP (MATERIAL DEVELOPMENT) TEAM — Investigation of Tl$_2$Ba$_2$Cu$_4$O$_8$ (Tl-2201) properties is important as it provides access to the overdoped side of the superconducting dome. We are measuring the surface resistance of Tl-2201, $R_s(T,\omega)$, using a bolometric technique well established by our group. Experimentally separating the in- and out-of-plane components of $R_s$ for Tl-2201, however, is challenging due to demagnetization effects. To account for this complication, we are measuring $R_s$ of an isotropic replica sample of NbZr in two specific orientations where the field is parallel and perpendicular to the crystal plane. In this talk I will describe the modified bolometric technique, share the technical difficulties encountered in preparing the replica, and present the most up-to-date results.

1This project has been supported by Natural Sciences and Engineering Research Council of Canada (NSERC).
3:54PM C36.00008 Ion-size effects in HTS cuprates - superfluid density and energy gaps. BENJAMIN MALLET, MacDiarmid Institute, Victoria University of Wellington, CHRISTIAN BERNHARD, University of Fribourg, THOMAS WÖLF, Karlsruhe Institute of Technology, EDI GILIOLI, Istituto dei Materiali per l’Elettronica ed il Magnetismo (IMEM), JEFF TALLON, MacDiarmid Institute, Industrial Research Limited — The demonstrated central role that ion size plays in determining $T_c$ in the HTS cuprates needs to be further explored in order to determine whether the demonstrated systematic behaviour plays out in other superconducting properties. After all, $T_c$ can be diminished simply by disorder effects. What is the effect of systematic ion-size variation on the superfluid density and superconducting energy gap? And can these effects be used to infer details concerning the pairing mechanism? To address these issues we report the effect of changing ion size on muon spin relaxation measurements of the superfluid density and Raman measurements of the superconducting gap in the model system $RA_2Cu_3O_6$ (where $R = La,\ldots, Lu$ and $A = Ba_{2-x}Sr_x$). The electronic density of states is determined from the effect of Zn substitution in this system and we are able to discount disorder scattering as the source of the systematic changes in superconducting properties. Our results confirm a picture where the polarizability of the charge-reservoir layer plays a key role in setting the energy scale for pairing in this system.

4:06PM C36.00009 New insights into the phase diagram of the copper oxide superconductors from electronic Raman scattering. ALAIN SACUTO, SIHAN BENHABIB, YANN GAILLAS, MAXIMILIEN CAZAYOUS, MARIE-AUDE MEASSON, SEBASTIEN BLANC, Université Paris Diderot, Laboratoire Matériaux et Phénomènes Quantiques, Paris, France, GENDA GU, Brookhaven National Laboratory, Condensed Matter Physics & Materials Science Department, NY 11973, DOROTHEE COLSON, Service de Physique de l’Etat Condensé, CEA-Saclay, 91911 Gif-sur-Yvette, France — We explore the cuprate phase diagram by electronic Raman spectroscopy and shed light on the superconducting state in hole doped cuprates. Namely, how superconductivity is impacted by the pseudogap.

4:18PM C36.00010 Ion-size effects in HTS cuprates – dielectric versus magnetic pairing. JEFFERY TALLON, MacDiarmid Institute, Industrial Research Ltd, BEN MALLET, MacDiarmid Institute, Victoria University, NEIL ASHCROFT, LASSP, Cornell University — We have been exploring the systematic effects of changing ion size on superconducting and normal-state properties of the HTS cuprates. In the model system $RA_2Cu_3O_6$ (where $R = La,\ldots, Lu$ and $A = Ba_{2-x}Sr_x$) the maximum $T_c$ in the dome-shaped phase curve can be shifted from 70 to 110 K in the model system. Surprisingly $T_c$ correlates with the dielectric properties and not the magnetic properties. This highlights the fundamental importance of charge fluctuation and dielectric screening in the cuprates and may signal a novel pairing mechanism having its origin with quantized waves of electronic polarization.

4:30PM C36.00011 Berry phase mechanism for polarization rotation in chiral metals. JOSEPH ORENSTEIN, JOEL MOORE, UC Berkeley and LBNL — There is currently considerable interest in inversion symmetry breaking in unconventional metals, particularly in chiral stacking of atomic layers with stripe-like charge density modulation in systems such as TiSe2 and the cuprate superconductor LBCO. A signature of broken chiral symmetry is optical gyrotropy, that is, different indices of refraction for left and right circular polarized light. In this talk we show that intraband gyrotropic response is a consequence of the anomalous velocity associated with the non-zero Berry curvature and we derive its strength for a model band structure as a function of the chiral order parameter. This work demonstrates that optical gyrotropy in chiral metals is the linear response counterpart to the anomalous Hall effect in time-reversal breaking metals.

3Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

4:42PM C36.00012 Faraday and Kerr Effect Measurements of Cuprates in THz Regime. Y. LUBASHEVSKY, LIDONG PAN, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA, T. KIRZHNER, G. KOREN, Physics Department, Technion - Israel Institute of Technology Haifa, 32000, Israel, N.P. ARMITAGE, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA — Recent results using a laser-based zero-area loop Sagnac interferometer have found a small but significant spontaneous Kerr rotation [1] suggesting an emergent chiral or time-reversal broken character to the pseudogap regime in the cuprate superconductors. In this work, we have performed high resolution THz polarimetry to measure the low frequency Faraday and Kerr rotation in these compounds. The THz range gives an advantage for these studies as it presumably corresponds more closely to frequency scales relevant for the pseudogap (1 THz - 48 K). We have found that low frequencies enhance the signal into the tens of milliradians range. Moreover, time-domain THz spectroscopy reveals more information about this phenomena as frequency dependent and birefringent effects among others can be measured. Results from YBCO and LBCO will be presented.


4:54PM C36.00013 Elastic moduli across the superconducting and pseudogap phase boundaries in four cuprate compounds. BRAD RAMSHAW, ARKADY SHEKHTER, JON BETTS, ALBERT MIGLIO, Pulsed Field Facility, NHMFL, Los Alamos National Laboratory — A detailed understanding of the physics of the cuprate superconductors relies on an experimental determination of the thermodynamic phase diagram. Resonant ultrasound spectroscopy (RUS) is a unique thermodynamic probe, capable of measuring part per million changes in elastic moduli, and has access to symmetry information. Here we present a symmetry analysis of changes in the elastic moduli across the superconducting and pseudogap phase boundaries in several classes of cuprates: YBCO, LSCO, Hg-1201, and Tl-2201.

5:06PM C36.00014 Quantum Fluctuations of Superconductivity in Critically Underdoped La$_{2-x}$Sr$_x$CuO$_4$. N.P. ARMITAGE, Y. LUBASHEVSKY, L.S. BILBRO, R.V. AGUILAR, Department of Physics and Astronomy, The Johns Hopkins University, G. LOGVENOV, I. BOZOVIĆ, Brookhaven National Laboratory — In the underdoped pseudogap regime of the high-temperature superconductors, one expects that due to low superfluid densities and short correlation lengths, superconducting fluctuations will be very significant for transport and thermodynamic properties. We have used THz time-domain spectroscopy (TTDS) to probe the fluctuations of superconductivity in extremely underdoped La$_{2-x}$Sr$_x$CuO$_4$ films close to and beyond the superconducting quantum critical point. On the approach to the transition from above, we find a significant range of quantum superconducting fluctuations that we quantify through a comparison of the low and high frequency phase stiffnesses. An explicit measure of these fluctuations through the quantity we propose as a “quantum Debye-Waller factor” shows that these fluctuations diverge and drive the transition.
5:18PM C36.00015 Feedback effect on high-energy magnetic excitations in the model high-temperature superconductor \( \text{HgBa}_2\text{CuO}_4+\delta \). YUAN Li, International Center for Quantum Materials, Peking University, China, M. LE TACON, M. BAKR, D. TERRADE, D. MANSKE, Max Planck Institute for Solid State Research, Germany, R. HACKL, Walter Meissner Institute, Bavarian Academy of Sciences and Humanities, Germany, L. JI, M.K. CHAN, N. BARISIC, X. ZHAO, M. GREVEN, School of Physics and Astronomy, University of Minnesota, USA, B. KEIMER, Max Planck Institute for Solid State Research, Germany — Magnetic excitations might play an important role in the superconducting mechanism in the cuprates. Their contribution below \( \sim 60 \) meV is manifested by the generic neutron “resonance” feature, which signifies a feedback effect of pairing on the magnetic excitations. However, the spectral weight of the resonance is insufficient to explain the high superconducting temperature \( (T_c) \). Recent research has demonstrated that intense magnetic excitations exist above 100 meV up to high doping, but it remains unknown whether and how these excitations participate in the pairing mechanism. Here we present a systematic electronic Raman scattering study of the model cuprate superconductor \( \text{HgBa}_2\text{CuO}_4+\delta \). In an overdoped sample upon cooling below \( T_c \), we observe a pronounced enhancement of a high-energy peak related to two-magnon excitations in insulating cuprates, which is accompanied by the opening of the superconducting gap and can be understood as a high-energy feedback effect that implies a direct involvement of high-energy magnetic excitations in the Cooper pairing. The effect occurs already above \( T_c \) in two underdoped samples, demonstrating a related feedback mechanism associated with the pseudogap.

Tuesday, March 19, 2013 8:00AM - 11:00AM
Session F1 DCMP GSNP: Invited Session: Physics from the Laboratory to the Universe: Davison-Germer/Heineman/Onsager/Lilienfeld Prizes Ballroom I - Barbara Jones, International Business Machines

8:00AM F1.00001 Davison-Germer Prize in Atomic or Surface Physics Lecture: Line ’Em All Up: Macromolecular Assembly at Liquid Interfaces. GERALDINE RICHMOND, Department of Chemistry, University of Oregon — Advances in our molecular level understanding of the ubiquitous fluid interface comprised of a hydrophobic fluid medium, and an aqueous solution of soluble ions quanta have been slow until recently. Our progress from advances in both experimental and computational techniques as well as the increasingly important role that this interface is playing in such areas as green chemistry, nanoparticle synthesis, improved oil and mineral recovery and water purification. The presentation will focus on our most recent efforts in understanding (1) the molecular structure of the interface between two immiscible liquids, (2) the penetration of aqueous phase ions into the interfacial region and their effect on its properties, and (3) the structure and dynamics of the adsorption of surfactants, polymers and nanoparticles at this interface. To gain insights into these processes we use a combination of experimental methodology, including surface analysis, and computational and molecular dynamics simulations. The results demonstrate that weak interactions between interfacial oil and water molecules create an interface that exhibits a high degree of molecular structuring and ordering, and with properties quite different than what is observed at the air-water interface. As a consequence of these interfacial oil-water interactions, the interface provides a unique environment for the adsorption and assembly of ions, polymers and nanoparticles that are drawn to its inner-most regions. Examples of our studies that provide new insights into the unique nature of adsorption, adsorption dynamics and macromolecular assembly at this interface will be provided.

8:36AM F1.00002 Lars Onsager Prize Lecture: Statistical Dynamics of Disordered Systems. DANIEL S. FISHER, Stanford University — The properties of many systems are strongly affected by quenched disorder that arose from their past history but is frozen on the time scales of interest. Although equilibrium phases and universality classes can be well defined, the description of disordered materials can be very different from the corresponding pure systems, the most striking phenomena involve non-equilibrium dynamics. The state of understanding of some of these will be reviewed including approach to equilibrium in spin glasses and the onset of motion in driven systems such as vortices in superconductors or earthquakes on geological faults. The potential for developing understanding of short-term evolutionary dynamics of microbial populations by taking advantage of the randomness of their past histories and the biological complexities will be discussed briefly.

9:12AM F1.00003 Dannie Heineman Prize for Mathematical Physics Prize Lecture: Correlation Functions in Integrable Models: Ising Model and Monodromy Preserving Deformation. TETSUJI MIWA, Kyoto University — Studies on integrable models in statistical mechanics and quantum field theory originated in the works of Bethe on the one-dimensional quantum spin chain and the work of Onsager on the two-dimensional Ising model. This work marked the birth of integrable models and the theory of monodromy preserving linear ordinary differential equations. This work was the starting point of our journey with Michio Jimbo in integrable models, the journey which finally led us to the exact results on the correlation functions of quantum spin chains in 1992.

9:48AM F1.00004 Dannie Heineman Prize for Mathematical Physics Prize Lecture: Correlation Functions in Integrable Models II: The Role of Quantum Affine Symmetry. MICHIO JIMBO, Rikkyo University — Since the beginning of 1980s, hidden infinite dimensional symmetries have emerged as the origin of integrability: first in soliton theory and then in conformal field theory. Quen for symmetries in quantum integrable models has led to the discovery of quantum groups. On one hand this opened up rapid mathematical developments in representation theory, combinatorics and other fields. On the other hand it has advanced understanding of correlation functions of lattice models, leading to multiple integral formulas in integrable spin chains. We shall review these developments which continue up to the present time.

10:24AM F1.00005 Julius Edgar Lilienfeld Prize Lecture: Mapping the Universe: Physics Writ Large. MARGARET GELLER, Harvard-Smithsonian Center for Astrophysics — The age of mapping the universe began in earnest in the late twentieth century. I will describe the enormous strides we have made in mapping the galaxy distribution and in understanding its nature and history. I will show how techniques for measuring the (primarily dark) matter distribution in massive systems of galaxies are an astrophysical route to tests of fundamental physics.

Tuesday, March 19, 2013 8:00AM - 11:00AM
Session F2 DCMP: Invited Session: Low Energy Excitations in Iridates Ballroom II - Paolo Radaelli, University of Oxford

8:00AM F2.00001 Correlated phases and excitations in the iridates. LEON BALENTS, Kavli Institute of Theoretical Physics, UCSB — The iridium oxides form an intriguing set of materials controlled by a delicate balance of kinetic, spin-orbit, and Coulomb interaction energies. Many possible exotic phases and phenomena have been suggested for them in the literature. I will review the theoretical context for these compounds, emphasizing effects arising from the combination of strong spin-orbit coupling and electron-electron correlations. Finally, I will discuss our group’s on-going efforts to understand the excitations and magnetic phases in these materials.

1I acknowledge support from the DOE BES grant DE-FG02-08ER46524, and the NSF MRSEC program, grant DMR1121053
techniques. Specifically, following topics will be discussed: (i) Heisenberg-like nature of magnetic coupling in Sr$_2$IrO$_4$; (ii) origin of strong Ising anisotropy in Sr$_3$Ir$_2$O$_7$; and (iii) contrasting dynamics of "spin-orbit exciton" modes in the Heisenberg and Ising magnets.

9:12AM F2.00003 Interplay of spin-orbit coupling, correlations, and crystal anisotropy in 5d oxides. LIIVI HOZOL, Institute for Theoretical Solid State Physics, IFW Dresden, Germany — We investigate the correlated d-level electronic structure of 5d Ir and Os oxides by fully ab initio quantum-chemical many-body calculations on finite embedded clusters. The wave-function quantum-chemical methods provide a promising alternative to density-functional-based approaches to the electronic structure of solids. The computed d-d excitations in square-lattice, honeycomb, pyrochlore, and chain-like iridates compare well with recent RIXS (resonant inelastic x-ray scattering) data. We also perform a detailed analysis of the relativistic spin-orbit wave functions and compute observables such as the (L-S) ground-state expectation value of the spin-orbit operator. The latter is in principle accessible from x-ray absorption and provides information on the role of t$_2g$-e$_g$ couplings in the ground-state wave function and on the strength of non-cubic fields that lift the degeneracy of the t$_2g$ levels. As concerns the departure from cubic symmetry, interesting effects are found in A$_2$Ir$_2$O$_7$-pyrochlores, where the highly anisotropic, hexagonal configuration of the adjacent A-site ions breaks cubic symmetry even in the absence of O-ligand trigonal distortions and moreover competes with the latter. Our findings open new perspectives in pyrochlore oxides. In 227 iridates, the outcome of this competition is decisive for the actual realization of any type of non-trivial topological ground state. In 227 spin systems with S > 1/2, e.g., Cd$_2$Os$_2$O$_7$, this interplay decides the sign of the single-ion anisotropy and the degree of magnetic frustration.

9:48AM F2.00004 Low energy excitations in iridates studied with Resonant Inelastic X-ray Scattering. XUERONG LIU, 1) Brookhaven National Laboratory; 2) Institute of Physics, Chinese Academy of Sciences — In the iridium oxides, the strong spin-orbit coupling (SOC) of the 5d iridium electrons entangles the orbital and spin degrees of freedom, providing opportunities for exotic magnetic states with highly anisotropic exchange interactions. At the same time, the spatially extended 5d electrons are expected to have much stronger hybridization with the oxygen 2p orbitals, comparing with that in 3d transition element compounds. Both factors make crystal symmetry and local environment crucial in determining the electronic and magnetic properties of the iridates. We present here our resonant inelastic x-ray scattering (RIXS) studies of a number of octahedrally coordinated iridates with special structures, exploring these effects. In particular, for the 1-D spin 1/2 chain compound, Sr$_3$Ir$_2$O$_7$, the wavefunction of the hole in the t$_2g$ manifold was reconstructed based on the RIXS spectra. Our results show that it is significantly modified from the isotropic shape expected for J$_{xy}$ = 1/2 states in the strong SOC limit, due to the distortion of the oxygen octahedral cage. This distortion is comparable to, or smaller than, that present in most iridates and thus this work emphasizes the importance of local symmetry for the iridate families. Further, the magnetic excitations of this material were also measured. A large gap of ~30 meV, was found, comparable to the magnetic dispersion bandwidth. This is in contrast to the gapless dispersion expected for linear chain with isotropic Heisenberg exchange interaction. We also studied Na$_2$IrO$_3$ which has a hyperkagome lattice, and is a candidate quantum spin liquid. Here, a low energy continuum is observed below the d-d excitations. Optical conductivity measurements performed on the same sample and polarization dependence of the RIXS signal suggest that these excitations are magnetic in origin, agreeing with the spin-liquid state prediction.

10:24AM F2.00005 Spin Dynamics in Na$_2$IrO$_3$ Probed by Inelastic Neutron Scattering: Implications for Kitaev Physics. RADU COLDEA, University of Oxford — We explore the spin dynamics in the layered antiferromagnet Na$_2$IrO$_3$, a candidate for the Kitaev spin model on the honeycomb lattice [1]. Using powder inelastic neutron scattering with an optimised setup to minimise neutron absorption by Ir we observed evidence for dispersive spin wave excitations of the Ir moments below a zone-boundary energy of 5 meV [2]. Results are compared quantitatively with predictions of a Kitaev-Heisenberg model, as well as a Heisenberg model with further neighbour couplings, both with a magnetic ground state of zig-zag ferromagnetic chains ordered antiferromagnetically. By combining single-crystal x-ray diffraction and ab initio calculations we propose a revised crystal structure model with significant departures from the ideal case of regular IrO$_6$ octahedra and 90° Ir-O-Ir bonds required for large Kitaev exchanges.


1 This research was partly supported by EPSRC (UK).

Tuesday, March 19, 2013 8:00AM - 11:00AM – 207 - Jun Zhu, Pennsylvania State University

8:00AM F8.00001 Hydroxyl-decorated Graphene Systems: Organic metal-free Ferroelectrics, Multiferroics, and Proton battery Cathode Materials. MENGHAO WU, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, J.D. BURTON, EVGENY TSYMBA, Department of Physics, University of Nebraska, Lincoln, NE 68588; PURU JENA, Department of Physics, Virginia Commonwealth University, Richmond, VA 23284, PROF.JENA’S GROUP TEAM, PROF.BURTON’S GROUP TEAM, PROF.TSYMBA’S GROUP TEAM, PROF.JENA’S GROUP TEAM — Through density-functional-theory calculations we show that hydroxylized graphene systems are ideal candidates for light-weight organic ferroelectric materials with giant polarizations. For example, the polarization of semi-hydroxylized graphene and graphene as well as fully hydroxylized graphene are, respectively, 41.1, 43.7, 67.7 μC/cm$^2$, much higher than any organic ferroelectric materials known to date. In addition, hydroxylized graphene is multiferroic due to the coexistence of ferroelectricity and ferromagnetism. Zigzag graphene nanoribbons decorated by hydroxyl groups also exhibit ferroelectric properties with a large polarization of 27.0 μC/cm$^2$. Moreover, proton vacancies at the end of ribbons can induce large dipole moments that can be reversed by both hopping of protons and rotation of O-H bonds under an electric field. These materials have the potential as high-capacity cathode materials with specific capacity six times larger than lead-acid batteries and five times that of lithium-ion batteries.
8:12AM F8.00002 Quantum Stacking of Atomic Hydrogen to Graphene1, YANTING ZHANG, IBM Microelectronics, ADAM DOHERTY, University of Vermont, ANDREW GERACOTELIS, Siena College, DENNIS CLOUGHERTY, University of Vermont — We consider the low-energy behavior of the stacking probability of atomic hydrogen to suspended graphene. For energy transfer through the flexural modes of graphene, we find that the inelastic coupling falls in the subOhmic regime. Thus the effects of low-frequency fluctuations of the graphene sheet are crucially important for quantum sticking. We analytically solve for the low-energy asymptotic behavior of the sticking coefficient using a variational mean-field method [D.P. Clougherty and Y. Zhang, Phys. Rev. Lett. 109, 120401 (2012)]. We find that as a result of strong coupling to the low-frequency flexural modes of graphene, a new scaling law results. For suspended graphene at finite temperature, we find that at a critical incident energy, the sticking probability drops discontinuously; below this critical energy, the sticking probability is suppressed by the orthogonality catastrophe. We compare our nonperturbative variational results to those obtained by using Fermi's golden rule.

1We gratefully acknowledge support by the National Science Foundation under DMR-1062966.

8:24AM F8.00003 Electronic structure of oxygen functionalized graphene nanoribbons1, ADAM SIMBECK, DEYANG GU, Rensselaer Polytechnic Institute, NEERAJ KHARCHE, Brookhaven National Laboratory, SAROJ NAYAK, Rensselaer Polytechnic Institute — We investigate the electronic and magnetic properties of armchair graphene nanoribbons whose edges are passivated by oxygen. Using a first-principles density functional approach and the many-body GW method we find that the oxygen molecules distort the electronic and magnetic properties of the ribbon. For planar systems we report magnetic ground states whose electronic structure depends upon the magnetic coupling between edges. For non-planar ribbons we report a nonmagnetic ground state with a band gap that decreases as a function of increasing ribbon width. Our results will be discussed in light of previous experimental and computational studies.

8:36AM F8.00004 Optical properties of functionalized monolayer and bilayer graphene, JINLUO CHENG, CUAUHTEMOC SALAZAR, JOHN E. SIPE, Department of Physics and Institute for Optical Sciences, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — We use ab initio calculations to investigate the structures, band structures, and optical properties of functionalized monolayer and bilayer graphene, where a hydrogen atom is attached to only one carbon atom site periodically every few unit cells. The hydrogen atom distorts the carbon atoms vertically, but the inplane structure is approximately unchanged. The ground state acquires a bandgap due to adsorption depending on the supercell size, and shows magnetic order, which is in agreement with a recent experiment [1]. The calculated optical absorption spectra displays detailed structures at lower photon frequencies than that of the pristine graphene.


9:00AM F8.00006 Electronic structures and magnetism of hydrogenated and fluorinated graphene with vacancies1, BI-RU WU, Center for General Education, Chang Gung University, Kueishan, Taiwan, CHIH-KAI YANG, Graduate Institute of Applied Physics, National Chengchi University, Taipei 11605, Taiwan — Graphene is a gapless semiconductor. As graphene is covered with one layer of hydrogen or fluorine, it becomes a wide band gap insulator. However, vacancies are easily found during the hydrogenated or fluorinated processes. We investigate the electronic structure and magnetism of the hydrogenated and fluorinated graphene with a variety of configuration of vacancies. We found that a continuous zigzag chain distribution of vacancies will result linear energy dispersion both in the hydrogenated and fluorinated graphene. This finding should be very useful for the design of graphene based electronic devices.

1This work was supported by the National Science Council of the Republic of China under contract number NSC101-2112-M-182-002.

9:12AM F8.00007 First-principles study of the spin-orbit interaction in graphene induced by hydrogen adatoms1, MARTIN GMITRA, DENIS KOCHAN, JOARSLAV FABIAN, University of Regensburg — We have performed first principles calculations of the spin-orbit coupling effects in hydrogenated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent binding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles.

1This work is supported by the DFG SPP 1285, SFB 689, and GRK 1570.

9:24AM F8.00008 A Model for the Origin of Spin half Para-magnetism in Fluorinated Graphene, PIALI ADITYA, ALEJANDRO SUAREZ, Pennsylvania State University, TYLER MAUNU, School of Physics & Astronomy, University of Minnesota, DIEGO B. CARRASCO, Engineering Physics Department, Universidad Iberoamericana A.C., JORGE SOFO, Pennsylvania State University — We have performed first principles calculations of the spin-orbit coupling effects in fluorinated graphene structures, for varying hydrogen coverage densities, using the linearized augmented plane wave method as implemented in the FLEUR code. The covalent binding between the hydrogen and carbon atoms leads to a local structural puckering of graphene sheets, giving rise to an overlap between the Dirac and sigma electrons and a giant enhancement (from roughly 0.01 to 1 meV) of the local spin-orbit interaction. The calculated effects on the band structure and the emerging spin patterns of the electronic states can be well explained by effective Hamiltonian models derived from group theoretical principles. We propose that the magnetic response originates from regions with a small number of non-fluorinated carbon atoms surrounded by fluorinated ones. In support of this model we combine the exact response of the non-fluorinated regions with a stochastic model to account for the fluorination process. Our calculation reproduces the magnetic response of the samples and tracks the origin of this magnetic phenomenon to the grain boundary between fluorinated patches. If our model is correct, the number of spins in this sample is not an intrinsic quantity but is determined by the fluorination process.
9:36AM F8.00009 Analytic Local and Total Density of States for Hydrogen Adatoms on Graphene\(^1\), NICHOLAS PIKE, DAVID STROUD, The Ohio State University — Spin transport through graphene is strongly influenced by the presence of adatoms with unpaired spins, such as hydrogen adatoms. In this work, we calculate the local density of states (LDOS) for a simple model of hydrogen on graphene using a tight binding model. The model includes nearest neighbor hopping between carbon atoms, the value of the hydrogen energy level, hopping between the carbon and hydrogen atoms, and a Hubbard U-term to account for the on-site Coulomb interaction. When U = 0, we develop an exact analytic equation for the LDOS on the adatom site, and for the total density of states (DOS). When U ≠ 0, we carry out the same calculation but treat the Hubbard term using mean-field theory. We find that the hydrogen adatom has a net non-integer spin polarization, and that some of the electronic density is transferred from the hydrogen adatom to the graphene host. Possible implications of these results for spin transport through graphene will be discussed.

\(^1\)This work was supported by the Center of Emerging Materials at The Ohio State University, an NSF MRSEC (Grant No. DMR0820414).

9:48AM F8.00010 Electrical detection of phase changes in adsorbed neutral dipolar molecules on graphene\(^1\), YILIN WANG, Materials Research Science and Engineering Center (MRSEC), University of Maryland, College Park, WENZHONG BAO, SHUDONG XIAO, Department of Physics, University of Maryland, College Park, MICHAEL FUHRER, JANICE REUTT-ROBEY, Materials Research Science and Engineering Center (MRSEC), University of Maryland, College Park, MRSEC TEAM — Graphene is a very promising material for sensing application because its transport properties are highly sensitive to adsorbrates on its surface. Here, we study the carrier-density-dependent resistance of bilayer graphene to neutral dipolar adsorbates under ultra-high vacuum condition. Halocarbon molecules with known dipole moment are deposited on graphene at ∼ 20 K. After deposition of a few monolayers of molecules, the resistance of graphene near the Dirac point is measured as a function of carrier density (tuned by gate voltage) and temperature, from 20 K to room temperature. We observe negligible shifts of the gate voltage of maximum resistance, indicating negligible charge transfer from adsorbate to graphene. In the temperature-dependent-resistance curve, a sharp step-like increase and decrease in resistance occurs at ∼ 45 K and ∼ 65 K, respectively. We relate these abrupt changes in resistance to phase transitions in the adsorbate overlayer. The same molecules adsorbed on graphite are known to exhibit a complex temperature - coverage phase diagram. We will discuss the relationship between graphene resistance and the phases of molecules on graphite. This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471.

10:00AM F8.00011 Optical properties of hydrogenated graphene from first principles\(^1\), SEBASTIAN PUTZ, MARTIN GMITRA, JAROSLAV FABIAN, University of Regensburg — We investigate the effect of hydrogen coverage on the optical properties of single-side hydrogenated graphene from first principles. To account for different degrees of uniform hydrogen coverage we calculate the complex dielectric function for graphene supercells of various size, each containing a single additional H atom. We use the Linearized Augmented PlaneWave (LAPW) method, as implemented in WIEN2k, to show that the hydrogen coverage strongly affects the complex dielectric function and thus the optical properties of hydrogenated graphene. The absorption coefficient in the visible range, for example, has different characteristic features depending on the hydrogen coverage. This opens up new possibilities of determining the hydrogen coverage of hydrogenated graphene samples in the experiment by contact-free optical absorption measurements.

\(^1\)This work is supported by the DFG GRK 1570.

10:12AM F8.00012 A Theoretical Analysis of the Effect of the Hydrogenation of Graphene to Graphane on Its Mechanical Properties\(^1\), Q. PENG, CHAO LIANG, WEI JI, SUVRANU DE, Rensselaer Polytechnic Institute — We investigated the mechanical properties of graphene and graphane using first-principles calculations based on density-functional theory. A conventional unitcell containing a hexagonal ring made of carbon atoms was chosen to capture the finite wave vector “soft modes”, which affect the the fourth and fifth elastic constants considerably. Graphane has about 2/3 ultimate strengths in all three tested deformation modes — armchair, zigzag, and biaxial— compared to graphene. However, graphane has larger ultimate strains in zigzag deformation, and smaller in armchair deformation. We obtained the second, third, fourth, and fifth order elastic constants for a rigorous continuum description of the elastic response. Graphane has a relatively low in-plane stiffness of 240 N/m which is about 2/3 of that of graphene, and a very small Poisson ratio of 0.078, 44% of that of graphene. The pressure dependence of the second order elastic constants were predicted from the third order elastic constants. The Poisson’s ratio monotonically decreases with increasing pressure.

\(^1\)Acknowledge the financial support from DTRA Grant # BRBAA08-C-2-0130, the U.S. NRCFDP # NRC-38-08-950, and U.S. DOE NEUP Grant #DE-NE0000325.

10:24AM F8.00013 Fluorination of CVD graphene: the role of wrinkles, folds, multi-layer islands and grain boundaries, BEI WANG, JUNJIE WANG, J. ZHU, Department of Physics, Penn State University — Chemical functionalization, such as fluorination, can modify the gapless band structure of graphene and turn it into an insulator. Fluorinated graphene (FG) can potentially be integrated into graphene electronics and serve as ultrathin gate dielectrics or tunnel barriers. Here we present our effort in synthesizing and understanding the properties of FG. Graphene sheets synthesized by chemical vapor deposition (CVD) are fluorinated using CF\(_4\) plasma under varying conditions. The resulting FG is systematically examined using a wide range of spectroscopic and microscopic tools including XPS, Raman, FTIR, electrical transport and conductive AFM. We obtain high F:C ratio of 0.1-1. Our results show that 1. Morphological features of CVD graphene (wrinkles, folds, multi-layer islands) are less fluorinated and charge transport in FG occurs through the conductive network formed by these features. 2. Lattice defects and grain boundaries play a significant role in the chemical reactivity of CVD graphene. XPS studies indicate the formation and evolution of CF\(_x\). The defects, as well as oxygen-passivated defect sites in FG. In these studies highlight current challenges in realizing electronics-grade FG and point to the possible pathways forward.

10:36AM F8.00014 Theory of the hydrogen adatoms induced spin-orbit coupling in graphene\(^1\), DENIS KOCHAN, MARTIN GMITRA, JAROSLAV FABIAN, University Regensburg — We have analyzed the first-principles data of the electronic structure of hydrogenation in graphene by means of group theory derived effective Hamiltonians. We propose effective models for semi-hydrogenated graphene as well as for graphene with a single hydrogen adatom. The chemisorption of hydrogen modifies the structural symmetry of the plane graphene in two essential ways—it breaks the pseudospin (sublattice) symmetry and induces rippling. We show that in addition to the Rashba spin-orbit interaction there emerges another spin-orbit effect which is induced by the pseudospin inversion asymmetry due to the adatoms. Our realistic effective Hamiltonians should be useful for spin transport and spin relaxation investigations.

\(^1\)SFB 689 Spin phenomena in reduced dimensions
8:00AM F13.00001 Homological Order in Three and Four dimensions: Wilson Algebra, Entanglement Entropy and Twist Defects\textsuperscript{1}. ABHISHEK ROY, XIAO CHEN, JEFFREY TEO, University of Illinois at Urbana-Champaign — We investigate homological orders in two, three and four dimensions by studying $Z_2$ toric code models on simplicial, cellular or in general differential complexes. The ground state degeneracy is obtained from Wilson loop and surface operators, and the homological intersection form. We compute these for a series of closed 3 and 4 dimensional manifolds and study the projective representations of mapping class groups (modular transformations). Braiding statistics between point and string excitations in $(3+1)$-dimensions or between dual string excitations in $(4+1)$-dimensions are topologically determined by the higher dimensional linking number, and can be understood by an effective topological field theory. An algorithm for calculating entanglement entropy of any bipartition of closed manifolds is presented, and its topological signature is completely characterized homologically. Extrinsic twist defects (or disclinations) are studied in 2,3 and 4 dimensions and are shown to carry exotic fusion and braiding properties.

\textsuperscript{1}Simons Fellowship

8:08AM F13.00002 Weyl points and line nodes in gapless gyroid photonic crystals, LIANG FU, JOHN JOANNOPoulos, MARIN S\'OLJ\'ACIC, Department of Physics, Massachusetts Institute of Technology, MIT TEAM — Weyl points and line nodes are three-dimensional linear point- and line-degeneracies between two bands. In contrast to Dirac points, which are their two-dimensional analogues, Weyl points are stable in the momentum space and the associated surface states are predicted to be topologically non-trivial. However, Weyl points are yet to be discovered in nature. Here, we report photonic crystals, based on the double-gyroid structures, exhibiting frequency-isolated Weyl points with complete phase diagrams by breaking the parity and time-reversal symmetries. The surface states associated with the non-zero Chern numbers are demonstrated. Line nodes are also found in similar geometries; the associated surface states are shown to be at bands. Our results are based on realistic “numerical experiments” with true predictive power and should be readily experimentally realizable at both microwave and optical frequencies.

8:24AM F13.00003 The optical conductivity of quasicrystals: evidence of a Weyl semimetal with 3D Dirac spectrum, THOMAS TIMUSK, JULES CARBOTTE, McMaster University, CHRISTOPHER HOMES, Brookhaven National Laboratory, DIMITRI BASOV, University of California, San Diego, SERGEI SHARAPOV, Bogolyubov Institute for Theoretical Physics, Kiev — The optical conductivity of quasicrystals is characterized by an absence of the Drude peak and a conductivity that rises linearly over a wide range of frequencies. The absence of the Drude peak has been attributed to a pseudogap at the Fermi surface but a detailed explanation of the linear behavior has not been found. This unusual behavior is seen in allicosahedral quasicrystal families and their periodic approximants. A simple model that assumes that the entire Fermi surface is gapped, with the exception at a finite set of Dirac points, fits the data. There is no evidence of a semiconducting gap in any of the materials suggesting that the massless Dirac spectrum is protected by topology leading to a Weyl semimetal. The model gives rise to a linear conductivity with only one parameter, the Fermi velocity. In accord with this picture decagonal quasicrystals should have a frequency independent conductivity, without a Drude peak. This is in accord with the experimental data as well.

8:36AM F13.00004 Chiralmagnetic effect in Weyl semimentals and insulators, MOHAMMAD VAZ-IFEH, MARCEL FRANZ, University of British Columbia — It has been proposed recently, on the basis of field-theoretical considerations, that the effective electromagnetic action of Weyl semimetal (as well as the closely related Weyl insulators) contains an axion term with the $\theta$-angle dependent on time $t$ or spatial position $r$. If correct this would lead to a number of novel observable phenomena, such as the chiral magnetic effect, whereby an applied uniform magnetic field induces a dissipationless bulk current $j \propto B$. In this work we construct a simple lattice model for a Weyl semimetal (insulator) and use it to explicitly test for the chiral magnetic effect by means of numerical techniques combined with analytical calculations. We discuss possible ways to engineer a suitable material in layered nanostructures and comment on the physical observability of the effect.

8:48AM F13.00005 Axion field theory, chiral anomaly and anomalous non-dissipative transport properties of $(3+1)$-dimensional Weyl semi-metals and superconductors\textsuperscript{1}. PALLAB GOSWAMI, National High Magnetic Field Laboratory and Florida State University, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University — From a direct calculation of the anomalous Hall conductivity and an effective electromagnetic action obtained via Fujikawa’s chiral rotation technique, we conclude that an axion field theory with a non-quantized coefficient describes the electromagnetic response of the $(3+1)$-dimensional Weyl semi-metal. The coefficient is proportional to the momentum space separation of the Weyl nodes. Akin to the Chern-Simons field theory of quantum Hall effect, the axion field theory violates gauge invariance in the presence of the boundary, which is cured by the chiral anomaly of the surface states via the Callan-Harvey mechanism. A direct linear response calculation also establishes an anomalous thermal Hall effect and a Wiedemann-Franz law. But, thermal Hall conductivity does not directly follow from the well known formula for the $(3+1)$-dimensional gravitational chiral anomaly. By calculating the gravitational chiral anomaly at finite temperature we show the existence of a new term, which correctly accounts for the thermal Hall effect in $(3+1)$-dimensional Weyl materials, topological insulators and topological superconductors.

\textsuperscript{1}NSF
9:12AM F13.00007 Friedel oscillations due to Fermi arcs in Weyl semimetals. PAVAN HOSUR\textsuperscript{1}, Department of Physics, University of California at Berkeley — Weyl semimetals harbor unusual surface states known as Fermi arcs, which are essentially disjoint segments of a two-dimensional Fermi surface. We describe a prescription for obtaining Fermi arcs of arbitrary shape and connectivity by stacking alternate two-dimensional electron and hole Fermi surfaces and adding suitable interlayer coupling. Using this prescription, we compute the local density of states—a quantity directly relevant to scanning tunneling microscopy—on a Weyl semimetal surface in the presence of a point scatterer and present results for a particular model that is expected to apply to pyrochlore iridate Weyl semimetals. For thin samples, Fermi arcs on opposite surfaces conspire to allow nested backscattering, resulting in strong Friedel oscillations on the surface. These oscillations die out as the sample thickness is increased and Fermi arcs from the opposite surface retreat and weak oscillations, due to scattering between the top surface Fermi arcs alone, survive. The surface spectral function, accessible to photoemission experiments, is also computed. In the thermodynamic limit, this calculation can be done analytically and separate contributions from the Fermi arcs and the bulk states can be seen.

\textsuperscript{1}My present affiliation is Department of Physics, Stanford University

9:24AM F13.00008 Topological Phases of Point Group Symmetric Weyl Superconductors. VASUDHA SHIVAMOGGI, University of Illinois, Urbana-Champaign, CHEN FANG, Princeton University, TAYLOR HUGHES, MATTHEW GILBERT, University of Illinois. Urbana-Champaign — We study superconductivity in a Weyl semimetal with broken time-reversal symmetry and stabilized by a point-group symmetry. The resulting superconducting phase is characterized by topologically protected bulk nodes and surface states with Fermi arcs. We derive a phase diagram of possible superconducting phases which are distinguished by the number of bulk nodes and discuss novel properties of the corresponding surface states. We show how the topological behavior may be understood in terms of the properties of the parent Weyl semimetal at high-symmetry momenta.

9:36AM F13.00009 Excitonic Phases of Weyl Semi-Metals with Coulomb Interaction. HUAZHOU WEI, UC Riverside, SUNG-PO CHAO, National Tsing Hua University, VIVEK AJI, UC Riverside — Weyl semi-metals have an even number of nodes which are perfectly nested in the absence of a chemical chiral potential. For repulsive interactions these are susceptible to excitonic instabilities. The vanishing density of states requires that the coupling be larger than a critical value for the states to be realized. There are eight possible states in the particle-hole channel, only two of which gap out the weyl nodes for long range Coulomb interactions. The lowest energy state is the Charge Density Wave state, which is more stable than the ferromagnetic insulator that arises in the context of short range repulsion. The defects of the state, i.e. dislocations, have been shown in the literature, to carry gapless chiral modes.

9:48AM F13.00010 Excitonic Phases from Weyl Semi-Metals with short range interaction\textsuperscript{1}. SUNG-PO CHAO, National Tsing Hua University, HUAZHOU WEI, VIVEK AJI, UC Riverside — Weyl semimetal, possibly realized in Pyrochlore iridates or superlattice of 3D topological-normal insulators system, has strong spin orbit interactions leading to effective low energy described by massless linearly dispersing fermions. In the absence of interactions chirality is a conserved quantum number, protecting the semi-metallic physics against perturbations that are translationally invariant. We show that the interplay between short range repulsive interaction and topology yields a novel chiral excitonic insulator. The state is characterized by a complex vectorial order parameter leading to a gapping out of the Weyl nodes. An interesting feature is that it is ferromagnetic, with the phase of the order parameter determining the direction of the induced magnetic moment. The case of Coulomb interaction will be discussed by Huazhou Wei in his report.

\textsuperscript{1}The authors acknowledge the financial support by University of California at Riverside through the initial complement.

10:00AM F13.00011 Probing the Chiral Anomaly via Nonlocal Transport in Weyl Semimetals\textsuperscript{1}. SIDDHARTH PARAMESWARAN, UC Berkeley, TARUN GROVER, Kavli Institute for Theoretical Physics, UC Santa Barbara, ASHVIN VISHWANATH, UC Berkeley — Weyl semimetals are three-dimensional analogs of graphene in which a pair of bands touch at points in momentum space, known as Weyl nodes. Electrons originating from a single Weyl node possess a definite topological charge, the chirality. Consequently, they exhibit the Adler-Jackiw-Bell anomaly, which in this condensed matter realization implies that application of parallel electric (E) and magnetic fields (B) pumps electrons between nodes of opposite chirality at a rate proportional to E·B. We argue that this pumping is measurable via transport experiments, in the limit of weak internode scattering. Specifically, we show that injecting a current in a Weyl semimetal subject to an E·B term leads to nonlocal features in transport.

\textsuperscript{1}We acknowledge support of the Simons Foundation, NSF Grant PHY-1066293 and the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231

10:12AM F13.00012 Effective field theories for topological insulators by functional bosonization. PAK ON CHAN, TAYLOR L. HUGHES, SHINSEI RYU, EDUARDO FRADKIN, Department of Physics, University of Illinois at Urbana-Champaign — Effective field theories that describe the dynamics of electric current for topological insulators in general dimension D = d+1 are discussed using the functional bosonization. For non-interacting topological insulators with a conserved U(1) charge and characterized by an integer topological invariant, we derive the BF-type topological field theories supplemented with the Chern-Simons (when D is odd) or the Axion term (when D is even). For topological insulators characterized by a 2\textsuperscript{D} topological invariant, their topological field theories are obtained by dimensional reduction. Building on this effective field theory description for non-interacting topological phases, we also discuss, following the spirit of the parton construction of the fractional quantum Hall effect, the putative “fractional” topological insulators and their possible effective field theories.

10:24AM F13.00013 Physics of three dimensional bosonic topological insulators I. ASHVIN VISHWANATH, UC Berkeley, TODADRI SENTHIL, MIT — We discuss physical properties of “integer” topological phases of bosons in D=3+1 dimensions, protected by internal symmetries like time reversal and/or charge conservation. These phases invoke interactions in a fundamental way but do not possess topological order and are bosonic analogs of free fermion topological insulators and superconductors. Here we develop a field theoretic description of several of these states and show that they possess unusual surface states, which if gapped, must either break the underlying symmetry, or develop topological order. In certain cases the topological phases are characterized by a quantized magneto-electric response γ, which, somewhat surprisingly, is an odd multiple of 2π. A surface theory in which vortices transform under a projective representation of the symmetry group is shown to capture these properties. A bulk field theory of these states is also identified, which furthermore predicts phases characterized by the thermal analog of the magneto-electric effect, that lie beyond the current holography description.

10:36AM F13.00014 Physics of three dimensional bosonic topological insulators II. S. TODADRI, Massachusetts Institute of Technology, ASHVIN VISHWANATH, University of California Berkeley — We discuss physical properties of interacting boson/spin analogs of free fermion topological insulators and superconductors. We discuss general constraints on the surface theories of these phases, and their field theoretic descriptions. We illustrate some of the results in the context of quantum paramagnetic phases of spin systems. For the 3d states we describe the 2d surface either spontaneously breaks symmetry or is in a spin liquid phase. In the latter case the symmetry is realized in the surface spin liquid in a way that is forbidden in strictly two dimensional quantum magnets.
have a nonzero Chern number and exhibit a gapless chiral edge state within the Dirac gap.

Inorganic materials. Here, using first-principles calculations, we predict a family of 2D organic topological insulators (OTIs) for realizing the QAHE. Designed spin-orbit coupling give rise to a quantized Hall conductivity. So far, a number of theoretical proposals have been made to realize the QAHE, but all based on

is a fundamental transport phenomenon in the field of condensed-matter physics. Without external magnetic field, spontaneous magnetization combined with

ZHENGFEI WANG, ZHENG LIU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Quantum anomalous Hall effect (QAHE) effect transistor. At zero magnetic field, a conductance minimum close to

4

InAs/GaSb Field-Effect Transistors

InAs/GaSb Field-Effect Transistors

These helical edge states coexist with a residual bulk conductivity when the device is tuned into the minigap. We probe the spatial distribution of currents in

Energy Sciences — InAs/GaSb quantum wells have been predicted theoretically to exhibit the quantum spin hall phase in the inverted regime. In this phase,

, ERIC SPANTON, Stanford Institute for Materials and Energy Sciences, LINGJIE DU, Rice University, KATJA NOWACK, Stanford Institute for

Thousand Oaks, California 91630, USA — We have studied electrical transport in inverted InAs/GaAs quantum wells (QWs) made by molecular beam epitaxy,

RUI-RUI DU, Department of Physics and Astronomy, Rice University, Houston, Texas 77251-1892, USA, GERALD SULLIVAN, Teledyne Scientific and Imaging,

FAPESP, FAPEMIG, CNPq, CAPES

and the $Z_2$ crystalline Topological Insulator. A, ALEXANDRADINATA, Department of Physics, Princeton University, XI DAI, Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, B, ANDREI BERNEVIG, Department of Physics, Princeton University — In the context of translationally-invariant insulators, Wilson loops describe the adiabatic evolution of the ground state around a closed circuit in the Brillouin zone. We propose that the Wilson-loop eigenspectrum provides a complete characterization of (a) the inversion-symmetric topological insulator, and (b) the $Z_2$ crystalline topological insulator: time-reversal symmetric insulators with either $C_4$ or $C_6$ rotational symmetry, but with no spin-orbit coupling. For the 1D inversion-symmetric insulator, we formulate a $Z$ Wilson-loop index, which is identifiable with the number of protected boundary modes in the entanglement spectrum. For the 2D inversion-symmetric insulator, we identify a $Z$ relative-winding number, which is the inversion-analog of the first Chern class (for charge-conserving insulators). For the $Z_2$ crystalline topological insulator, we show how the $Z_2$ invariant can be extracted from the Wilson-loop eigenspectrum; this aids the identification of materials that realize this phase.

Tuesday, March 19, 2013 8:00AM - 11:00AM –

Session F18 DCMP: Two Dimensional Topological Insulators I

8:00AM F18.00001 Imaging currents in HgTe quantum wells in the quantum spin Hall regime, KATJA NOWACK, ERIC SPANTON, MATTHIAS BAENNINGER, MARKUS KÖNING, JOHN KIRTLYE, Stanford University, BEENA KALISKY, Stanford University, Bar-Ilan University, CHRISTOPHER AMES, PHILIPP LEUBNER, CHRISTOPH BRÜNE, HARTMUT BUHLMANN, LAURENS MOLENKAMP, Wuerzberg University, DAVID GOLDHABER-GORDON, KATHRYN MOLER, Stanford University — Dissipationless edge channels are a key feature of the quantum spin Hall (QSH) state, which was predicted and experimentally demonstrated to exist in HgTe quantum wells. The existence of the edge channels has been inferred from local and non-local transport measurements. Here we imagine the current in Hall bars made from HgTe quantum wells by probing the magnetic field generated by the current using a scanning superconducting quantum interference device. We observe that the current flows mainly along the edge of the device in the QSH regime, and furthermore that an identifiable edge channel exists even in the presence of disorder and considerable bulk conduction as the device is gated and its temperature is raised. Our results represent a versatile method for the characterization of new quantum spin Hall materials systems.

8:12AM F18.00002 Electronic properties of HgTe/CdTe heterostructure under perturbations preserving time reversal symmetry1, TOME SCHMIDT, Universidade Federal de Uberlândia, JONAS ANVERSA, PAULO PIQUINI, Universidade Federal de Santa Maria, ADALBERTO FAZZIO, Universidade de São Paulo — Using first principles calculations, the Dirac cone of HgTe/CdTe heterostructure is identified at the interface, inside the valence band. The spin texture of the 2D Dirac states is totally in-plane for all interface directions, different from the 3D topological insulators, where there is always some out-of-plane spin components. The masless Dirac states are strongly affected by applying positive or negative biaxial pressure. While negative pressure turns the system metallic, suppressing the Dirac states, positive pressure maintains the protected topological states, but dislocates the Dirac cone upward in energy. The protected Dirac states are kept up to a contraction of 3% in the lattice parameter. Larger compressive pressures leads to suppression of the protected metallic states.

1FAPESP, FAPEMIG, CNPq, CAPES

8:24AM F18.00003 Quantized Conductance in InAs/GaSb Quantum Wells1, LINGJIE DU, IVAN KNEZ, RUI-RUI DU, Department of Physics and Astronomy, Rice University, Houston, Texas 77251-1892, USA, GERALD SULLIVAN, Teledyne Scientific and Imaging, Thousand Oaks, California 91630, USA — We have studied electrical transport in inverted InAs/GaAs quantum wells (QWs) made by molecular beam epitaxy, in which the evidences for helical edge modes were observed in mesoscopic samples with either normal or superconductor contacts. Here we report on measurements of QWs that are doped with Si at the InAs/GaSb interface, where Si is a donor in InAs and an acceptor in GaSb. The influences of induced disorder in the quantum Spin Hall effect as well as outside this regime are systematically studied and results will be presented.

1The work is supported by NSF DMR-0706634 and DMR-1207562.

8:36AM F18.00004 Scanning SQUID measurements of current flow in InAs/GaSb Quantum Wells, ERIC SPANTON, Stanford Institute for Materials and Energy Sciences, LINGJIE DU, Rice University, KATJA NOWACK, Stanford Institute for Materials and Energy Sciences, GERRY SULLIVAN, Teledyne Scientific, RUI-RUI DU, Rice University, KATHRYN MOLER, Stanford Institute for Materials and Energy Sciences — InAs/GaSb quantum wells have been predicted theoretically to exhibit the quantum spin hall phase in the inverted regime. In this phase, spin-polarized helical edge modes are expected to exist. Previous published results on length and width dependence of InAs/GaSb 4-terminal devices suggests these helical edge states coexist with a residual bulk conductivity when the device is tuned into the minigap. We probe the spatial distribution of currents in devices using a scanning SQUID to measure the resulting magnetic fields. Specifically, we find that when the device is tuned into the gap with a front gate, current flows along the edge and coexists with bulk current. We also look at dependence on back gate voltage and temperature dependence.

8:48AM F18.00005 Quantum Transport near the Charge Neutrality Point in Inverted Type-II InAs/GaSb Field-Effect Transistors, W. PAN, J.F. KLEM, J.K. KIM, M. THALAKULAM, M.J. CICH, Sandia National Labs, S.K. LYO, University of California, Irvine — We present here our recent quantum transport results around the charge neutrality point (CNP) in a type-II InAs/GaSb field-effect transistor. At zero magnetic field, a conductance minimum close to $4e^2/h$ develops at the CNP and it follows semi-logarithmic temperature dependence. In quantized magnetic ($B$) fields and at low temperatures, well developed integer quantum Hall states are observed in the electron as well as hole regimes. Electron transport shows noisy behavior around the CNP at extremely high $B$ fields. When the diagonal conductivity $\sigma_{xx}$ is plotted against the Hall conductivity $\sigma_{xy}$, a conductivity circle law is discovered, suggesting a chaotic quantum transport behavior. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

9:00AM F18.00006 Quantum Anomalous Hall Effect in 2D Organic Topological Insulators1, ZHENGFEI WANG, ZHENG LIU, FENG LIU, Department of Materials Science and Engineering, University of Utah — Quantum anomalous Hall effect (QAHE) is a fundamental transport phenomenon in the field of condensed-matter physics. Without external magnetic field, spontaneous magnetization combined with spin-orbit coupling give rise to a quantized Hall conductivity. So far, a number of theoretical proposals have been made to realize the QAHE, but all based on inorganic materials. Here, using first-principles calculations, we predict a family of 2D organic topological insulators (OTIs) for realizing the QAHE. Designed by assembling molecular building blocks of triphenyl-transition-metal compounds into a hexagonal lattice, this new classes of organic materials are shown to have a nonzero Chern number and exhibit a gapless chiral edge state within the Dirac gap.

1This work was supported by US DOE-BES (Grant No. DE-FG02-04ER46027).
By Monte Carlo simulation, we discuss the stability of the anomalous Hall insulating region in the magnetic phase diagram. In the absence of Landau levels, spin-orbit coupling, and magnetic ordering, the new state is realized in itinerant electrons coupled with local spin textures. This has been generalized to topological insulators in the presence of the spin-orbit coupling. Besides, a noncoplanar magnetic order was shown to give rise to the formation of quantized Landau levels in external magnetic field. Later, a quantum anomalous Hall effect without Landau levels was proposed, and the idea of half-integer quantized spin Hall conductance and the electrical wire through which valley-polarized current can flow, and silicene can be used as a valley polarizer. We used to identify the topological domain walls as well as valley-polarized kink states. Our findings suggest that the one-dimensional domain wall may be used as an electrical wire through which valley-polarized current can flow, and silicene can be used as a valley polarizer. Based on first-principles calculations, our wavefunctions are related to color-dependent magnetic-flux inserted versions of Halperin and non-Abelian color-singlet states. We then provide large-size numerical results for both the $SU(2)$ and $SO(3)$ symmetry in 2D. There are infinite number of such phases, which can be described by $SU(2)/SO(3)$ nonlinear-sigma models with $N_c \times N_c$ full lattice translational symmetry. We implement the Haldane pseudopotential Hamiltonians in this new basis. Their ground states are the model FQH wavefunctions, and our Bloch basis allows for a mutatis mutandis transcription of these model wave functions to the fractional Chern insulator (FCI) of arbitrary Chern number $C$, obtaining wavefunctions different from all previous proposals. For $C > 1$, our wavefunctions are related to color-dependent magnetic-flux inserted versions of Halperin and non-Abelian color-singlet states. We then provide adiabatic numerical results for both the $C = 1$ and $C = 3$ cases. This new approach leads to improved overlaps compared to previous proposals. We also discuss the adiabatic continuation from the FCI to the FQH in our Bloch basis, both from the energy and the entanglement spectrum perspectives.

Quantum anomalous Hall effect with in-plane magnetization in HgMnTe.

9:12AM F18.00007 Quantum anomalous Hall effect with in-plane magnetization in HgMnTe. HSU-HUI HSU, XIN LIU, CHAO-XING LIU. Department of Physics, Pennsylvania State University — A quantum anomalous Hall (QAH) insulator carries quantized Hall conductance which is similar to Quantum Hall (QH) effect. However, it originates from the exchange coupling of magnetization instead of Landau levels. It was proposed that QAH effect can be realized in HgTe quantum wells doped with Mn (Phy. Rev. Lett. 101, 146802 (2008)) and evidenced by recent experiments. However, Mn is paramagnetic and an external magnetic field, which also leads to Landau levels, is required to obtain Mn polarization. Thus, it is essential to find an experimentally feasible way to distinguish between the two effects. In this study, we propose to distinguish QH effect and QAH effect by introducing the in-plane magnetization of Mn with an in-plane magnetic field. The in-plane magnetic field reduces the QAH effect by tilting the magnetization of Mn into the quantum well plane and reducing the out-of-plane magnetization. In contrast, the in-plane magnetic field has little influence on the conventional QH effect which only depends on the out-of-plane magnetic field. The phase diagram is identified based on the band structure calculation and Landau level calculation with the realistic material parameters of HgMnTe quantum wells, which can serve as the guidance for the future transport experiment.

9:24AM F18.00008 Engineering quantum anomalous Hall phases with orbital and spin. HONGBIN ZHANG, FRANK FREIMUTH, GUSTAV BIHLAYER, STEFAN BLUGEL, YURIY MOKROUSOV, Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA — Combining tight-binding models and first principles calculations, we demonstrate that under external exchange fields, non-zero Chern numbers and nontrivial QAH effect could be induced by on-site spin-orbit coupling (SOC) in buckled honeycomb lattices with sp orbitals. In the Haldane model [1], the occurrence of QAH effect is attributed to complex next nearest neighbor hopping. Detailed analysis of a generic tight-binding models reveals that there exist different mechanisms giving rise to complex hoppings, utilizing both orbital and spin degrees of freedom of electrons on a lattice. Furthermore, it is shown that in Bi/Sb(111) bilayers [2], different topological phases exist as function of the magnitude of SOC and external exchange fields. These phases are characterized using Chern and spin Chern numbers [3] together with transverse charge and spin conductivities. At last, we show that introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is modified due to incompletely filled d states around the Fermi energy.

By introducing ferromagnetic dopants provides a practical way to induce nontrivial topological phases, whereas the physics is modified due to incompletely filled d states around the Fermi energy.

9:36AM F18.00009 Effective field theory of nematic QAH for interacting fermions. YIZHI YOU, EDUARDO FRADKIN, University of Illinois at Urbana-Champaign — We consider 2D fermionic lattice models with quadratic band touching. By turning on a marginal relevant interaction of this system, the system condenses into a state that spontaneously breaks time reversal and/or rotation (point-group) symmetry. When both symmetries are broken the state is a nematic quantum anomalous Hall (QAH) phase. We derive an effective field theory which describes the quantum phase transition into this state from a spontaneous QAH state. The effective field theory has the form of Maxwell-Chern-Simons action for the hydrodynamic degrees of freedom of the spontaneous QAH state with a coupling to the nematic order-parameter field that induces a spatial anisotropy. The fluctuations of the nematic field modify the local spatial geometry and couples to the Maxwell term as the spatial components of a metric tensor. We will discuss the behavior at quantum criticality and the relation with recent theories that associate transitions of this type with quantum Lifshitz criticality [1]. We will also discuss extensions of our theory to nematic fractional QAH state. [1] M. Mulligan, C. Nayak, and S. Kachru, Phys. Rev. B 82, 085102 (2010); Phys. Rev. B 84, 195124 (2011) This work was supported in part by the NSF grant DMR-1064319 at the University of Illinois.

9:48AM F18.00010 Symmetry protected Spin Quantum Hall phases. ZHENGH-XIN LIU, Tsinghua university, Beijing, XIAO-GANG WEN, MIT, Perimeter institute — Symmetry protected topological (SPT) states are short-range entangled states with symmetry. Nontrivial SPT states have symmetry protected gapless edge excitations. Topological insulators are examples of nontrivial SPT phases. We study Bosonic SPT phases protected by $SU(2)$ or $SO(3)$ symmetry in 2D. There are infinite number of such phases, which can be described by $SU(2)/SO(3)$ nonlinear-sigma models with a quantized topological $\chi$-term. At open boundary, the $\chi$-term becomes the Wess-Zumino-Witten term and consequently the boundary excitations are decoupled gapless left movers and right movers. Only the left movers ($\theta > 0$) carry the $SU(2)/SO(3)$ quantum numbers. As a result, the $SU(2)$ SPT phases have a half-integer quantized spin Hall conductance and the $SO(3)$ SPT phases have an even-integer quantized spin Hall conductance. Both the $SU(2)/SO(3)$ SPT phases are symmetric under their $U(1)$ subgroup and can be viewed as $U(1)$ SPT phases with even-integer quantized Hall conductance.

10:00AM F18.00011 Bloch Model Wavefunctions and Pseudopotentials for All Fractional Chern Insulators. YANG-LE WU, Princeton University, N. REGNAULT, Princeton University, Ecole Normale Superieure and CNRS, B. ANDREI BERNEVIG, Princeton University — We introduce a Bloch-like basis in a C-component lowest Landau level fractional quantum Hall effect (FQH), which entangles the real and internal degrees of freedom and preserves an $N_c \times N_c$ full lattice translational symmetry. We implement the Haldane pseudopotential Hamiltonians in this new basis. Their ground states are the model FQH wavefunctions, and our Bloch basis allows for a mutatis mutandis transcription of these model wave functions to the fractional Chern insulator (FCI) of arbitrary Chern number $C$, obtaining wavefunctions different from all previous proposals. For $C > 1$, our wavefunctions are related to color-dependent magnetic-flux inserted versions of Halperin and non-Abelian color-singlet states. We then provide adiabatic numerical results for both the $C = 1$ and $C = 3$ cases. This new approach leads to improved overlaps compared to previous proposals. We also discuss the adiabatic continuation from the FCI to the FQH in our Bloch basis, both from the energy and the entanglement spectrum perspectives.

10:12AM F18.00012 First-principles study on quantum valley Hall effects in silicene. YOUNGKUK KIM, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea, HOSUB JIN, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA, KEUNSU CHOI, JISOON IHM, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Republic of Korea — Silicene is a two-dimensional honeycomb lattice of silicon atoms, similar to graphene. Based on first-principles calculations, considering the double-exchange model with spin-ice type Ising spins on a kagome lattice, we numerically show that a local spin correlation called kagome-ice opens a charge gap, resulting in quantization of the Hall conductivity in the absence of magnetic ordering. By Monte Carlo simulation, we discuss the stability of the anomalous Hall insulating region in the magnetic phase diagram.

10:24AM F18.00013 Quantum Topological Hall Effect in Kagome Ice. YUKITOSHI MOTOME, HIROAKI ISHIIZUKA, Dept. of Appl. Phys., Univ. of Tokyo — The quantum Hall state was originally discovered in two-dimensional electron systems associated with the formation of quantized Landau levels in external magnetic field. Later, a quantum anomalous Hall effect without Landau levels was proposed, and the idea has been generalized to topological insulators in the presence of the spin-orbit coupling. Beside, a noncoplanar magnetic order was shown to give rise to the quantum anomalous Hall effect through the Berry phase mechanism. Here, we present yet another example of the quantum anomalous Hall state which emerges in the absence of Landau levels, spin-orbit coupling, and magnetic ordering. The new state is realized in itinerant electrons coupled with local spin textures subject to geometrical frustration of lattice structure. Considering the double-exchange model with spin-ice type Ising spins on a kagome lattice, we numerically show that a local spin correlation called kagome-ice opens a charge gap, resulting in quantization of the Hall conductivity in the absence of magnetic ordering. By Monte Carlo simulation, we discuss the stability of the anomalous Hall insulating region in the magnetic phase diagram.
Critical behavior of the transport coefficients at the Chern-to-normal insulator transition

Increasing x will be discussed based on the results from penetration depth measurements.

This work was supported by the U.S. NSF grants DMS-1066045 and DMR-1056168.

Topological protection of localization against the hybridization

We are grateful for support from the Japan Society for the Promotion of Science (JSPS) through the ‘Funding Program for World-Leading Innovative R&D on Science and Technology (FIRST Program).’

Tuesday, March 19, 2013 8:00AM - 10:48AM –
Session F19 DCMP: Heavy Fermions and Quantum Criticality in 115’s

Stability of the Kondo Lattice and Field-tuned Antiferromagnetic Structures in the Ce$_{1-x}$Yb$_x$RhIn$_5$ System

Sample synthesis was funded by the US DOE (Grant No. DE-FG02-04-ER46105), and physical properties measurements were supported by the NSF (Grant No. DMR-08024478)

London penetration depth in Ce$_{1-x}$Yb$_x$RhIn$_5$ ($0 \leq x \leq 0.4$).

Work in Ames was supported by the Department of Energy Office of Science, Basic Energy Sciences under Contract No. DE-AC02-07CH11358. Work in San Diego was supported by the Department of Energy Office of Science (Grant DE-FG02-04-ER46105).
8:36AM F19.00004 Non-Fermi liquid behavior with and without quantum criticality in Ce$_{1-x}$Yb$_x$CoIn$_5$. Y.P. SINGH, T. HU, Kent State University, L. SHU, M. JANOSCHEK, University of California, San Diego, M. DZERO, Kent State University, M.B. MAPLE, University of California, San Diego, C.C. ALMANN, Kent State University — In a growing number of f-electron systems the non-Fermi liquid (NFL) behavior occurs in the absence of an obvious quantum phase transition (QPT), which takes place at a quantum critical point (QCP). An intriguing candidate is Ce$_{1-x}$Yb$_x$CoIn$_5$ that exhibits an unconventional T x phase diagram without an apparent QCP. Therefore, it is important to elucidate the nature of the NFL behavior and to search for possible QCPs in this system. Here we reveal a field induced QCP (H$_{QCP}$) through normal state magnetore sistivity measurements and find its evolution with x. The full suppression of H$_{QCP}$ for x > 0.2 has surprisingly little effect on the Kondo lattice coherence. At low Yb concentrations, resistivity consists of two contributions with linear and sub-linear temperature dependences, while at higher concentrations only the sub-linear term is present. These results imply that the NFL behavior could be a new state of matter in its own right rather than a consequence of the underlying QPT.

1 This work was supported by NSF (DMR-1006606 and DMR-084115), ICAM Branches Cost Sharing Fund from Institute for Complex Adaptive Matter, and Ohio Board of Regents (Grant OBR-RIP-220573) at KSU, and DOE (DE-FG02-04ER46105) at UCSD.

8:48AM F19.00005 Superfluid density in heavy fermion superconductor Ce$_{1-x}$Yb$_x$CoIn$_5$. LEI SHU, Fudan University, China, D.E. MACLAUGHLIN, University of California, Riverside, USA, O.O. BERNAL, California State University, Los Angeles, USA, X.P. SHEN, Fudan University, China, S. PHAM, California State University, Los Angeles, USA, I. LUM, M.B. MAPLE, University of California, San Diego, USA — Recent x-ray diffraction, electrical resistivity, magnetic susceptibility, and specific heat measurements on the superconducting heavy fermion system Ce$_{1-x}$Yb$_x$CoIn$_5$ reveal that the correlated electron state is stabilized throughout the range 0 < x < 0.8, apparently due to cooperative behavior of Ce and Yb ions involving their unstable valences. Phase separation occurs for x > 0.8. Interestingly, the superconducting transition temperature decreases linearly with x from 2.3 K at x = 0 to 0 K at x = 1. Transverse-field muon spin rotation experiments have been performed on Ce$_{1-x}$Yb$_x$CoIn$_5$ alloys. Based on these measurements, we report the absolute value of magnetic penetration depth as a function of x and discuss whether Tc is controlled by the superfluid density of superconducting carriers. The results are compared to a recently proposed theory for the superconductivity in Ce$_{1-x}$Yb$_x$CoIn$_5$.

2 This work was supported by Chinese NSF, grant 11204041, NSF of Shanghai, grant 12ZR1401200, the U.S. NSF, grants DMR-0801407 (Riverside), DMR-1105380 (Los Angeles), and the U.S. DOE, contract DE-FG02-04ER46105 (San Diego).

9:00AM F19.00006 Anomalous critical upper field in CeCoIn$_5$/YbCoIn$_5$ superlattices with a Rashba-type heavy fermion interface. MASAAKI SHIMOZAWA, Department of Physics, Kyoto University, S.K. GOH, Cavendish Laboratory, University of Cambridge, Y. MIZUKAMI, H. SHISHIDO, D. WATANABE, S. YASUMOTO, M. YAMASHITA, Department of Physics, Kyoto University, T. TERAISHIMA, Research Center for Light and Materials Science, Kyoto University, Y. YANASE, T. SHIBAUCH, Department of Physics, Kyoto University, A.I. BUZDIN, Universite Bordeaux I, LOMA, M. MATSUDA, Department of Physics, Kyoto University — We report the precise angular dependence of the upper critical field (H$_c2$) in the epitaxial superlattices CeCoIn$_5$(n)/YbCoIn$_5$(5), formed by alternating layers of n and 5 unit-cells thick CeCoIn$_5$ with a strong Pauli effect and normal metal YbCoIn$_5$, respectively [1]. For the n = 3 superlattice, H$_c2$($\theta$) changes smoothly as a function of the field angle $\theta$. However, near the superconducting transition temperature, H$_c2$($\theta$) shows a cusp near the angle parallel to the plane of the superlattice. This cusp behavior suggests the relative dominance of the orbital depairing effect in the n = 3 superlattice, which may be due to the suppression of the Pauli effect in a system with local inversion symmetry breaking [2].


9:12AM F19.00007 Strong pressure dependence of the magnetic penetration depth in single crystals of the heavy fermion system CeCoIn$_5$ studied by muon spin rotation. LUDOVIC HOWARD, ALEXANDER MAISURADZE, Institute of Physics, University of Zurich, Switzerland, PIERRE DALMAS DE REOTTIER, ALAIN YAOUANC, CEA Grenoble, France, CHRISTOPHER BAINES, Paul Scherrer Institut, Switzerland, GERARD LAPERTOT, KARINE MONTY, JEAN-PASCAL BRISON, CEA Grenoble, France, HUGO KELLER, University of Zurich, Switzerland — The pressure dependence (0 – 1 GPa) of the in-plane magnetic penetration depth ($\lambda$$_c$), the penetration depth anisotropy ($\gamma$ = $\lambda$$_c$/$\lambda$$_a$) and the temperature dependence of 1/$\lambda$$_c$$^2$ ($i$ = $a$, $c$) were studied in single crystals of the heavy fermion system CeCoIn$_5$ by means of muon spin rotation. A strong decrease of $\lambda$$_c$ with pressure was observed, while $\gamma$ and 1/$\lambda$$_c$$^2$(T) are pressure independent. A linear relationship between 1/$\lambda$$_c$$(T)$ and Tc was also found. The large decrease of $\lambda$$_c$ with pressure was the signature of an increase of the number of superconducting quasiparticles by a factor of about 2.

9:24AM F19.00008 STM Spectroscopic Mapping of Quasiparticle States in the Superconducting State of CeCoIn$_5$, SHASHANK MISRA, BRIAN ZHOU, EDUARDO H. DA SILVA NETO, PEGOR AYNAJIAN, Princeton University, RYAN BAUMBACH, J.D. THOMPSON, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The heavy fermion compounds provide an interesting playground to study strongly correlated physics, as a variety of unusual low-temperature states emerge in relatively close proximity to one another in their phase diagrams. However, to date, very little spectroscopic information about these low-temperature phases, including unconventional superconductivity, is known. Recently, at comparatively high temperatures, Aynajian and coworkers used scanning tunneling microscopy (STM) to visualize the formation of heavy quasiparticles in one of the prototype 115 compounds, CeCoIn$_5$. Here, we use a new home-built STM to extend the spatial mapping of the electronic states of CeCoIn$_5$ down to its superconducting state at mK temperatures. This work was supported by the DOE and NSF.


9:36AM F19.00009 STM Spectroscopic Mapping of Quasiparticle States in the Vortex State of CeCoIn$_5$. BRIAN ZHOU, SHASHANK MISRA, PEGOR AYNAJIAN, EDUARDO DA SILVA NETO, Princeton University, RYAN BAUMBACH, J.D. THOMPSON, ERIC BAUER, Los Alamos National Laboratory, ALI YAZDANI, Princeton University — The superconducting properties of the heavy-fermion CeCoIn$_5$ emerge from a remarkable backdrop of strong electron correlation and magnetic criticality. Fittingly, this superconducting phase is itself remarkable, displaying signatures of unconventional pairing with (d-wave) line nodes in the order parameter and a Pauli-limited upper critical field below 700 mK [1]. Through scanning tunneling microscopy at milli-Kelvin temperatures, we present, for the first time, atomically-resolved spectroscopy of CeCoIn$_5$ as the application of a magnetic field weakens and eventually destroys superconductivity.


Research funded by DOE and NSF.
Long range order and two-fluid behavior in heavy electron materials.

NICHOLAS CURRO, ABIGAIL SHOCKLEY, KENT SHIRER, ADAM DIOGUARDI, NICHOLAS ABROBERTS-WARREN, JOHN CROCKER, CHING LIN, DAVID NISSON, University of California at Davis — The heavy electron Kondo liquid is an emergent state of condensed matter that displays universal behavior independent of material details. Properties of the heavy electron liquid are best probed by NMR Knight shift measurements, which provide a direct measure of the behavior of the heavy electron liquid that emerges below the Kondo lattice coherence temperature as the lattice of local moments hybridizes with the background conduction electrons. Because the transfer of spectral weight between the localized and itinerant electronic degrees of freedom is gradual, the Kondo liquid typically coexists with the local moment component until the material orders at low temperatures. The two-fluid formula captures this behavior in a broad range of materials in the paramagnetic state. In order to investigate two-fluid behavior and the onset and physical origin of different long range ordered ground states in heavy electron materials, we have extended Knight shift measurements to URu$_2$Si$_2$, CeIn$_3$, and CeRhIn$_5$. Our results indicate that the ordered state can emerge from either the Kondo liquid or heavy electron component, and imply that the nature of the ground state is strongly coupled with the hybridization in the Kondo lattice.

Study of the Kondo lattice on La doped CeCoIn$_5$

G. KOUTROULAKIS, H. YASUOKA, Los Alamos National Laboratory, T. ZHOU, S. E. BROWN, UCLA, E. D. BAUER, J. D. THOMPSON, Los Alamos National Laboratory — The effect of non-magnetic impurities on the properties of the Kondo lattice was investigated through nuclear magnetic/quadrupolar resonance (NMR/NQR) experiments on Ce$_{1-x}$La$_x$CoIn$_5$. Specifically, comprehensive $^{115}$In and $^{139}$La NQR and NMR measurements were carried out on single crystals of various La concentration levels ($x=0, 2, 3, 5$%) for temperatures 1.5K-80K and applied magnetic field values 0T-7T. Our results indicate that the ramifications of the Kondo-ion substitution extend well beyond the vicinity of the particular site, readily affecting the heavy-fermion forming hybridization. It is suggested that the spin polarization around La impurities is modulated on a much larger length scale than that of charge oscillations.

High Field Knight shift studies in CeIrIn$_5$

ABIGAIL SHOCKLEY, NICHOLAS APROBERTS-WARREN, DAVID NISSON, University of California, Davis, PHIL KÜHNS, ARNEIL REYES, National High Magnetic Field Lab, PETER KLAIVINS, NICHOLAS CURRO, University of California, Davis — All heavy fermion compounds that have been measured with NMR exhibit a Knight shift anomaly, in which the Knight shift does not scale with the bulk susceptibility below a characteristic temperature, $T^*$. Typically this temperature corresponds with the Kondo lattice coherence temperature as measured by other probes. In order to investigate the microscopic origin of this anomaly, we have conducted high field measurements of the In-115 Knight shift in CeIrIn$_5$ up to 30 T. We find that although the onset temperature $T^*$ is field independent, the overall low temperature shift below $T^*$ is suppressed. In the context of the two-fluid model, these results suggest that the dominant change is in the local moment channel.

Probing the hybridization gap in heavy fermions by temperature dependent ARPES

CRIS ADRIANO, University of Illinois at Chicago, FANNY RODOLAKIS, Argonne National Laboratory, PRISCILA ROSA, University of Campinas, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, MUCIO CONTINENTINO, Centro Brasileiro de Pesquisas Físicas, ZACHARY FISK, University of California at Irvine, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas — We report temperature dependent angle-resolved photoemission spectroscopy (ARPES) for pure and Cd-doped Ce$_x$Rh$_{1-x}$In$_5$ heavy fermion compounds. Our results reveal that for Ce$_x$Rh$_{1-x}$In$_5$ at $T = 100$ K once the $f$-conduction electrons magnetic scattering becomes larger than the phonon scattering, even states of different parities can hybridize, forming many-body quasiparticles with heavy masses. We further show that at a temperature of 20 K, where the hybridization of conduction electrons and $f$ states is stronger, a spectral gap is observable in the ARPES spectra. Interestingly, when replacing In by Cd to tune the local density of conduction electrons states at the Ce$^{3+}$ site, we find a strong reduction of the $f$-conduction electrons hybridization strength, and the suppression of the hybridization gap at low temperatures. We also observe that the $f$ states near the chemical potential hybridize mostly with out-of-plane $p$ states (presumably from In). These findings have important consequences for the understanding of the different antiferromagnetic and exotic superconducting ground states that occur in these families of materials.

Fermi Surface evolution as a function of temperature in heavy fermion Ce$_2$RhIn$_5$ probed by ARPES

FANNY RODOLAKIS, Argonne National Laboratory, CRIS ADRIANO, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago — The crossover of $f$ localized magnetic moments at high temperatures into itinerant states of heavy mass at low temperatures in Cerium-based heavy fermion materials is a fundamental problem in condensed matter physics, involving a temperature-dependent hybridization between the $f$ levels immersed in a sea of conduction electrons (ce). Due to the Luttinger theorem, this hybridization leads to a Fermi surface (FS) enlargement at low temperature: as the $f$ electrons become itinerant, their contribution to $\rho_F$ increases. We have studied the evolution of the heavy fermion FS in Ce$_2$RhIn$_5$ as a function of temperature using angle resolved photoemission. We observed topological changes that emerge at a temperature scale much higher than the onset of the coherence character of the $f$ electrons. This behavior can be related to the evolution of the electrical resistivity as a function of temperature: as typically found for Kondo lattice materials, it first decreases when temperature is lowered, but increases below $\sim 150$K as the magnetic scattering of the ce by the localized $f$ electrons becomes larger than the phonon scattering. It reaches a maximum and then drops when the magnetic scattering becomes coherent for $T^* \sim 5$K. This multiple scale behavior of the $f$ electrons is in good agreement with a recent theoretical study performed in the parent compound CeRhIn$_5$.[1].

The hybridization gap in heavy fermions by temperature dependent ARPES

CRIS ADRIANO, University of Illinois at Chicago, FANNY RODOLAKIS, Argonne National Laboratory, PRISCILA ROSA, University of Campinas, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas — We report temperature dependent angle-resolved photoemission spectroscopy (ARPES) for pure and Cd-doped Ce$_x$Rh$_{1-x}$In$_5$ heavy fermion compounds. Our results reveal that for Ce$_x$Rh$_{1-x}$In$_5$ at $T = 100$ K once the $f$-conduction electrons magnetic scattering becomes larger than the phonon scattering, even states of different parities can hybridize, forming many-body quasiparticles with heavy masses. We further show that at a temperature of 20 K, where the hybridization of conduction electrons and $f$ states is stronger, a spectral gap is observable in the ARPES spectra. Interestingly, when replacing In by Cd to tune the local density of conduction electrons states at the Ce$^{3+}$ site, we find a strong reduction of the $f$-conduction electrons hybridization strength, and the suppression of the hybridization gap at low temperatures. We also observe that the $f$ states near the chemical potential hybridize mostly with out-of-plane $p$ states (presumably from In). These findings have important consequences for the understanding of the different antiferromagnetic and exotic superconducting ground states that occur in these families of materials.

Fermi Surface evolution as a function of temperature in heavy fermion Ce$_2$RhIn$_5$ probed by ARPES

FANNY RODOLAKIS, Argonne National Laboratory, CRIS ADRIANO, FRANCISCO RESTREPO, DIMITAR TENEV, University of Illinois at Chicago, PASCOAL PAGLIUSO, University of Campinas, JUAN CARLOS CAMPUZANO, University of Illinois at Chicago — The crossover of $f$ localized magnetic moments at high temperatures into itinerant states of heavy mass at low temperatures in Cerium-based heavy fermion materials is a fundamental problem in condensed matter physics, involving a temperature-dependent hybridization between the $f$ levels immersed in a sea of conduction electrons (ce). Due to the Luttinger theorem, this hybridization leads to a Fermi surface (FS) enlargement at low temperature: as the $f$ electrons become itinerant, their contribution to $\rho_F$ increases. We have studied the evolution of the heavy fermion FS in Ce$_2$RhIn$_5$ as a function of temperature using angle resolved photoemission. We observed topological changes that emerge at a temperature scale much higher than the onset of the coherence character of the $f$ electrons. This behavior can be related to the evolution of the electrical resistivity as a function of temperature: as typically found for Kondo lattice materials, it first decreases when temperature is lowered, but increases below $\sim 150$K as the magnetic scattering of the ce by the localized $f$ electrons becomes larger than the phonon scattering. It reaches a maximum and then drops when the magnetic scattering becomes coherent for $T^* \sim 5$K. This multiple scale behavior of the $f$ electrons is in good agreement with a recent theoretical study performed in the parent compound CeRhIn$_5$.[1].

Spin flip in spin-orbit split quantum wires in magnetic field

OLEG A. TRETIAKOV, Tohoku University and Texas A&M University, K. S. TIKHONOV, V. L. POKROVSKY, Texas A&M University and Landau Institute for Theoretical Physics We study spin-flip processes induced by ac electromagnetic field in quantum wires with strong spin-orbit coupling in the presence of an external magnetic field. The dc magnetic field is essential to enable the electric dipolar excitation of the spin-flip processes. We consider the electron spin-flip resonance in the framework of Luttinger liquid theory. The electron-electron interaction is strong in quantum wires and changes the shape of the spin-flip resonance curve at the spin wave frequency and produces an additional capacit at the frequency of collective charge excitation. We discuss how this spin flip is affected by the dissipation processes and the dispersion curvature.

This work has been supported by the DOE under the grant DE-FG02-06ER46278, by NSF under Grants No. DMR-0757992, ONR-N000141110780, and by NHARP.

**Tuesday, March 19, 2013 8:00AM - 11:00AM — Session F22 DCMP: Strongly Correlated Electron Theory I**

**8:00AM F22.00001 Spin flip in spin-orbit split quantum wires in magnetic field**

TOHOKU UNIVERSITY AND TEXAS A&M UNIVERSITY, K. S. TIKHONOV, V. L. POKROVSKY, TEXAS A&M UNIVERSITY AND LANDAU INSTITUTE FOR THEORETICAL PHYSICS — We study spin-flip processes induced by ac electromagnetic field in quantum wires with strong spin-orbit coupling in the presence of an external magnetic field. The dc magnetic field is essential to enable the electric dipolar excitation of the spin-flip processes. We consider the electron spin-flip resonance in the framework of Luttinger liquid theory. The electron-electron interaction is strong in quantum wires and changes the shape of the spin-flip resonance curve at the spin wave frequency and produces an additional capacit at the frequency of collective charge excitation. We discuss how this spin flip is affected by the dissipation processes and the dispersion curvature.

This work has been supported by the DOE under the grant DE-FG02-06ER46278, by NSF under Grants No. DMR-0757992, ONR-N000141110780, and by NHARP.
8:12AM F22.00002 Theoretical study of a one-dimensional chain of alternating spin-1 and electron sites with spin-mediated hopping. WING-HO KO, HDONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106, USA; JEFFREY RAU, Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada, LEON BAULENTS, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106, USA — Motivated by the nickel valence controversy in the perovskite nickelate RNiO₃, we consider a one-dimensional chain consisting of alternating spin-1 (“nickel”) and electron (“oxygen”) sites, in addition to the usual electron hopping and spin-spin interaction between the spin-1 and the electron also contains a spin-1 mediated electron hopping term. Using density-matrix renormalization group (DMRG), we obtain the phase diagram of such model, as well as various correlation functions in each phase. Importantly, for certain range of parameters the model exhibits a quasi-long-range spiral (QS) order. To understand the DMRG results, we construct a mean-field theory based on Schwinger fermion decomposition of the spin-1 spins, from which we argue that the QS phase corresponds to a phase in proximity to the spin Bose metal state proposed by Sheng, Motrunich, and Fisher [Phys. Rev. B, 79, 205112 (2009)].

8:24AM F22.00003 Magnetic Phase Transition Induced by the Hubbard and Spin-orbit Interactions in a Nanoribbon Geometry. HYEONG JUN LEE, MOO YOUNG CHOI, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea, GUN SANG JEON, Department of Physics, Ewha Womans University, Seoul 120-750, Korea — The local repulsive Coulomb interaction between the electrons tends to cause a Mott transition into a magnetically ordered phase. In a honeycomb lattice, particularly, the magnetic order is known to emerge on the edges of graphene, which is attributed to the electron interactions. Meanwhile, the introduction of the spin-orbit interaction gives rise to metallic boundary states, which is a prominent characteristic of the topologically nontrivial materials. We study the effect of the spin-orbit interaction on the edge states as well as the bulk properties of the electron system on the honeycomb lattice. By employing a Hartree-Fock approximation, we compute the local magnetization in the half-filled nanoribbon system at zero temperature. We pay particular attention to the decaying behavior of the local magnetization from the edge toward the center. It is found that the characteristic length associated with the decay is divergent on the phase boundaries. Such slow decay is found to be algebraic in the thermodynamic limit. We discuss the relation between the bulk phase transitions and the decay of magnetization at the edges.

8:36AM F22.00004 Nonequilibrium thermal transport and its relation to linear response. CHRISTOPH KARRASCH, RONI ILAN, JOEL MOORE, UC Berkeley — We study the real-time dynamics of spin chains driven out of thermal equilibrium by an initial temperature gradient \( T_1 \neq T_2 \). We demonstrate that the nonequilibrium energy current saturates fast to a finite value if the linear-response thermal conductivity is infinite, i.e. if the Drude weight \( D \) is nonzero. Our data suggests that a nonintegrable dimerized chain might support such dissipationless transport \( D > 0 \). We show that the steady-state value of the current for arbitrary \( T_1 \neq T_2 \) is completely determined by the linear conductance. Inhomogeneous systems exhibiting different bulk parameters as well as Luttinger liquid boundary physics induced by single impurities are discussed shortly.

8:48AM F22.00005 Quantum Monte-Carlo simulation of spin-one antiferromagnets with single-ion anisotropy¹. YASUYUKI KATO, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, KEOLA WIERSCHEM, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371, YUSUKE NISHIDA, Theoretical division, T-2, Los Alamos National Laboratory, CRISTIAN BATISTA, Theoretical division, T-4 and CNLS, Los Alamos National Laboratory, PINAKI SENGUPTA, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371 — We study a spin-one Heisenberg model with uniaxial single-ion anisotropy, \( D \), and Zeeman coupling to a magnetic field, \( B \), parallel to the symmetry axis. We compute the \( (D/J, B/J) \) quantum phase diagram for square and simple cubic lattices by combining analytical and Quantum Monte Carlo approaches, and find a transition between XY-antiferromagnetic and ferromagnetic phases that spontaneously break the \( U(1) \) symmetry of the model. In the language of bosonic gases, this is a transition between a Bose-Einstein condensate (BEC) of single bosons and a BEC of pairs. For the efficient simulation of ferromagnetic phase, we developed and implemented a new multi-discontinuity algorithm based on the directed-loop algorithm. The ordinary quantum-Monte-Carlo methods fall into freezing problems when we apply them to this system at large \( D/J \) and finite \( B/J > 1 \). The new method does not suffer from the freezing problems.

¹This research used resources of the NERSCC (DOE Contract No. DE-AC02-05CH1123I). Work at LANL was performed under the auspices of a J. Robert Oppenheimer Fellowship and the U.S. DOE contract No. DE-AC52-06NA25396 through the LDRD program.

9:00AM F22.00006 Majorana dimerised order in magnetic systems. EDMUND BENNETT, University of St Andrews — We consider the analysis of quantum critical points (QCPs) using a Majorana fermion representation of spin. Majorana fermions are a useful spin representation as they obey Wick’s theorem and automatically provide the correct quantum phase diagram for square and simple cubic lattices. We consider an Ising model in various dimensions in an applied transverse field, a model which exhibits a QCP and has an exact solution in 1D. In the Majorana fermion representation, the interaction vertex may be decoupled into a Majorana dimerisation (MD) decoupling or an Ising magnetic decoupling. A mean-field analysis of the MD decoupling (which involves two Majorana fermions of the same flavour on adjacent lattice sites) suggests an ordered phase in the region above the QCP extant in the model, which extends through to high magnetic fields. Full RPA corrections to this mean-field theory are also presented, which give insight into the stability of this ordered phase to quantum perturbations.

9:12AM F22.00007 Spin Orbit Magnetism and Unconventional Superconductivity. YI ZHANG, KEVIN BEDELL, Boston College — We find an exotic spin excitation in a magnetically ordered system with spin orbit magnetism in 2D, where the order parameter has a net spin current and no net magnetization. Starting from a Fermi liquid theory, similar to that for a weak ferromagnet, we show that this excitation emerges from an exotic magnetic Fermi liquid (EMFL) state that is protected by a generalized Pomeranchuk condition. We derive the propagating mode using the Landau kinetic equation, and find that the dispersion of the mode has a \( q^{1/2} \) behavior in leading order in 2D. We find an instability toward superconductivity induced by this exotic mode, and a further analysis based on the forward scattering sum rule strongly suggests that this superconductivity has p-wave pairing symmetry. We perform similar studies in the 3D case, with a slightly different magnetic system and find that the mode leads to a Lifshitz-like instability most likely toward an inhomogeneous magnetic state in one of the phases.

9:24AM F22.00008 Magnetic properties of \( d \)-atomic systems with unquenched orbital moments. VICTOR ANTONOV, (1). Ames Laboratory USDOE, Ames, IA 50011 (2). Institute for Metal Physics, 36 Vernadsky blvd., Kiev, Ukraine, 03680, LIQIN KE, ANTON JESCHE, VLADIMIR ANTROPOV, Ames Laboratory USDOE, Ames, IA 50011 — Many systems of \( d \)-atoms with unquenched orbital moments demonstrate unusually large values of atomic magnetic moments, high magnetic anisotropy and small magnetic ordering temperatures. Using electronic structure analysis, we study a mechanism of the formation of strong on-site electronic correlations that lead to a strong orbital polarization, and in turn, generate a highly orbitally polarized hybridization with non-magnetic host atoms. In this case, even a small spin orbital coupling of \( 3d \)-atoms can create a significant effect. We introduce a consistent model of the formation of large orbital moments and magnetic anisotropy both in the metallic and insulating cases, and apply it to several realistic systems. Detailed calculations of magnetic properties, including magneto-optical studies of the Kerr angle rotation, are performed for several nitrometallates of Mn, Fe and Co where a rather large (3-5 degrees) Kerr angle rotation is predicted for the first time. We further discuss the nature of critical temperature in magnetic phase transition in such systems and the opportunity to increase it.
We present magnetotransport studies of Na$_{x}$KIM, E.D. MUN, R.D. MCDONALD, V. ZAPF, NHMFL/MPA-CMMS, LANL, J.D. THOMPSON, MPA-CMMS, LANL, L. BALICAS, NHMFL, I. MARTING, the composition with metallic behavior. It also has frustrated local spin texture owing to its hexagonal structure. Previous works report a very large Hall signal for coplanar spin texture. This compound exhibits a unique insulating state below temperature ($T_{\text{transition}}$) suggesting a structural quantum critical point. Here in an attempt to characterize this phase further, we present a picture of the evolution of the temperature—suggesting a structural quantum critical point. Here in an attempt to characterize this phase further, we present a picture of the evolution of the structural and magnetic behavior in Ca$_3$Ir$_4$(Sn$_{1-x}$Sb$_x$)$_{13}$ via a combined transport, magnetization and neutron scattering study. We find that this Hall signal reaches a maximum around $T \sim 30$ K and $B \sim 27$ T and on further cooling the absolute change of $\rho_{xy}$ decreases significantly. Interestingly, we found no significant changes in field-dependent magnetization which suggests that this behavior does not come from the ordinary anomalous Hall effect. We discuss the origin of this unique Hall signal by existence of a non-coplanar spin structure that may exist in this compound (I. Martin, C. D. Batista, Phys. Rev. Lett. 101, 156402 (2008)).

Our preliminary results indicate that DMBTDMA is more disposed from the supramolecular aggregated structures influenced by the different extractant tails. To test our hypothesis, atomistic molecular dynamics simulations were performed on DMDBTDMA in bulk oil system and DMDOHEMA in bulk oil system. Our preliminary results indicate that DMBTDMA is more disposed towards formation of chain-like aggregates, especially at lower water concentration, in comparison with the branched structures observed in DMDOHEMA.

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**Tuesday, March 19, 2013 8:00AM - 11:00AM**

Session F30 DCMP: Membranes, Micelles, Vesicles, Gels and Complex Fluids

### 8:00AM F30.00001 For a Safe Diamide Extraction Process, Elucidated by Atomistic Simulations

**BAOFU QIAO**, Department of Materials Science and Engineering, Northwestern University. ROSS J. ELLIS, Chemical Sciences and Engineering Division, Argonne National Laboratory, MONICA OLVERA DE LA CRUZ

The diamine extraction process has been successfully employed in separating trivalent actinides from used nuclear fuels. The extractant, which is an amphiphilic molecule with a metal-binding polar headgroup and hydrophobic tail, binds the actinides, thus extracting them from the aqueous phase into the oil phase. However, the oil phase will split into two phases, once a critical concentration of actinide is reached. This phase splitting is suggested to have caused the Red Neck effect, which can decompose explosively. Therefore, it is extremely important for an extractant to have a high extraction efficiency, on one hand, and resist phase splitting, on the other. In comparison with DMDBTDMA, DMDOHEMA has both higher extraction efficiency and phase stability, which we suspect stem from the supramolecular aggregated structures influenced by the different extractant tails. To test our hypothesis, atomistic molecular dynamics simulations were performed on DMDBTDMA in bulk oil system and DMDOHEMA in bulk oil system. Our preliminary results indicate that DMBTDMA is more disposed toward formation of chain-like aggregates, especially at lower water concentration, in comparison with the branched structures observed in DMDOHEMA.

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The formation of equilibrium vesicles and the L3 phase is facilitated by ion exchange between the cationic surfactant and the ionic liquid, as well as the strength spontaneously via different thermodynamic routes, with the same size distribution, which strongly supports that they exist in a true thermodynamic equilibrium. Density highly viscous solution containing giant vesicles and a sponge phase coexists with a dilute high density phase containing large vesicles. Vesicles form scattering, rheology and bright field microscopy, we identify the coexistence of two vesicle containing phases in compositions ranging from 2 to 68 wt %. A low double tail surfactant (didodecyldimethylammonium bromide) in a protic ionic liquid (ethylammonium nitrate) [1-2]. Using small and ultra-small angle neutron scattering, we are generally challenging due to the complex structure of the energy landscape. We show results for the lipid bilayer formation process obtained by newly developed parallel Wang–Landau Monte Carlo and statistical temperature molecular dynamics simulations. By applying those methods to a generic coarse-grained model for amphiphilic molecules in solution, we were able to obtain the thermodynamical data over the whole relevant temperature and energy range and to unravel the membrane formation process including all structural sub-transitions between different fluid and gel-phase bilayers. [3] Research supported by NSF.

8:48AM F30.00005 Amphiphilic lipids in solution: a simulational study of lipid bilayer formation. THOMAS VOGEL, DAVID P. LANDAU, The University of Georgia, LILI GAI, KATIE A. MAERZKE, CHRISTOPHER R. IACOVELLA, CLAIRE M. MCCABE, Vanderbilt University, PETER T. CUMMINGS, Vanderbilt University and Oak Ridge National Laboratory — Amphiphilic molecules consisting of hydrophilic head and hydrophobic tail groups self-assemble into a wide variety of structures, such as bilayers (membranes), micelles, or vesicles (liposomes) when mixed with a suitable solvent. The understanding of this lipid self-assembly is essential for industrial, biological, or medical applications, but computer simulations are generally challenging due to the complex structure of the energy landscape. We show results for the lipid bilayer formation process obtained by newly developed parallel Wang–Landau Monte Carlo and statistical temperature molecular dynamics simulations. By applying those methods to a generic coarse-grained model for amphiphilic molecules in solution, we were able to obtain the thermodynamical data over the whole relevant temperature and energy range and to unravel the membrane formation process including all structural sub-transitions between different fluid and gel-phase bilayers. [3] Research supported by NSF.

9:00AM F30.00006 Study of vesicle size distribution dependence on pH value based on nanopore resistive pulse method. YUQING LIN, YAUHENI RUDZEVICH, ADAM WEARNE, DANIEL LUMPKIN, JOSELYN MORALES, KATLÉENN NEMEC, SUREN TATULIAN, OLEG LUPAN, LEE CHOW, Department of Physics, University of Central Florida — Vesicles are low-micron to sub-micron spheres formed by a lipid bilayer shell and serve as potential vehicles for drug delivery. The size of vesicle is proposed to be one of the instrumental variables affecting delivery efficiency since the size is correlated to factors like circulation and residence time in blood, the rate for cell endocytosis, and efficiency in cell targeting. In this work, we demonstrate accessible and reliable detection and size distribution measurement employing a glass nanopore device based on the resistive pulse method. This novel method enables us to investigate the size distribution dependence of pH difference across the membrane of vesicles with very small sample volume and rapid speed. This provides useful information for optimizing the efficiency of drug delivery in a pH sensitive environment.

9:12AM F30.00007 Spontaneous Thermoreversible Formation of Cationic Vesicles in a Protic Ionic Liquid. DONGCUI LI, CARLOS LOPEZ-BARRON, LEO DERITA, MADIVALA BASAVARAJ, NORMAN WAGNER, University of Delaware — The search for stable vesicular structures is a long-standing topic of research because of the usefulness of these structures and the scarcity of surfactant systems that spontaneously form vesicles in true thermodynamic equilibrium. We report the first experimental evidence of spontaneous formation of vesicles for a cationic double tail surfactant (didecyldimethylammonium bromide) in a protic ionic liquid (ethylammonium nitrate) [1-2]. Using small and ultra-small angle neutron scattering, rheology and bright field microscopy, we identify the coexistence of two vesicle containing phases in compositions ranging from 2 to 68 wt %. A low density highly viscous solution containing giant vesicles and a sponge phase coexists with a dilute high density phase containing large vesicles. Vesicles form spontaneously via different thermodynamic routes, with the same size distribution, which strongly supports that they exist in a true thermodynamic equilibrium. The formation of equilibrium vesicles and the L3 phase is facilitated by ion exchange between the cationic surfactant and the ionic liquid, as well as the strength of the solvophobic effect in the protic ionic liquid.

9:24AM F30.00008 Phase separation in a DMPC/Dchol mixed Langmuir Film: A combined Brewster Angle, Fluorescence and Light Scattering Microscopy study\(^1\), PRITAM MANDAL, FANINDRA BHATTA, Department of Physics, Kent State University, ARNE GERICKE, Department of Chemistry & Biochemistry, Worcester Polytechnic Institute, EDGAR KOUJMAN, Department of Biophysics, The Netherlands, ANKE SCHUTZ, Department of Biophysics, Kent State University, DAVID ALLENDEER, ELIZABETH MANN, Department of Physics, Kent State University — Fluorescence microscopy (FM) is one of the most direct imaging techniques for in situ observation of morphology and phase-separation at the macroscopic scale \([1]\) in lipid mono- or bi-layers. However, the presence of fluorescent dye-molecules can affect the system. In Brewster Angle Microscopy (BAM), one can image monomolecular Langmuir films without probes. Here, using a composite set-up of BAM, FM and Light Scattering Microscopy (LSM), we present a comparative study of the three techniques on a binary lipid mixture in the presence of two different probes. In most cases, all three techniques show precisely the same domains. However, depending on conditions, some domain types were more evident in one technique than the others. This established, we can directly test the influence of probe on the domain structure.

\(\text{1NSF CBET-0730475}\)

9:36AM F30.00009 Mesoscopic Membrane Morphology Regulated by Molecular Crystallization, CHEUK-YUI LEUNG, LIAM PALMER, BAO FU QIAO, SUMIT KEWALRAMANI, RASTKO SKNEPNEK, CHRISTINA NEWCOMB, MEGAN GREENFIELD, GRAZIANO VERNIZZI, SAMMUEL STEPP, MICHAEL BEDZYK, MONICA OLVERA DE LA CRUZ, Northwestern University — A grand challenge in self-assembly of multi-component systems is to control the geometric symmetries and the resulting geometries of co-assembled molecular structures. We generate herein crystal-like materials in a variety of geometries, which resemble unusual cellular shell shapes, by mixing \(\pm 3\) and \(-1\) ionic amphiphiles. To structurally characterize the co-assemblies from the mesoscopic to nanometer scale, we combine electron microscopy with small and wide angle x-ray scattering. We use pH to control the degree of ionization of the amphiphiles and hence their intermolecular electrostatic interactions. At low and high pH, closed faceted vesicles with 2D hexagonal molecular arrangements were observed, while at intermediate pH ribbons with rectangular-C packing of the amphiphiles were observed. Thus pH acts as a switch to control the morphology of the ionic bilayers via transitions in the crystalline lattice. This work promotes the design of nanocontainers for various applications and improves our understanding of the origin of polyhedral shells in nature.

9:48AM F30.00010 Thermodynamics of protein driven self assembly in membranes, RAMAKRISHNAN NATENASAN, RICHARD TOURDOT, RYAN BRADLEY, RAVI RADHAKRISHNAN, University of Pennsylvania — Recent experimental evidences strongly point to the role of proteins and other membrane binding macromolecules in reshaping biological membranes, at length scales of the molecule and the structure enclosed by the membrane. In this work, we investigate the interplay between the membrane curvature induced at the molecular scale, mainly due to peripheral membrane proteins, and the resulting membrane morphologies, of varying complexity, observed at the mesoscale. The biological membrane, in our approach, is represented by a dynamically triangulated surface while the proteins are modeled as curvature fields on the membrane, which can either be isotropic or anisotropic. Thermal undulations in the membrane and cooperativity in the curvature field, due to the stabilization of a nematic phase, drives the membrane into conformations that resemble those in experiments in vivo and vitro. The stability of these structures are examined by two approaches to compute the free energy of the system: (i) Widom insertion technique to compute excess chemical potentials and (ii) thermodynamic integration using the Kirkwood coupling parameter to compute absolute free energies. Building on these methods, we propose a hybrid scheme that couples both the approaches for computing free energies.

10:00AM F30.00011 Morphology and Performance of PLLA Based Porous Membranes by Phase Separation Control\(^1\), QIAN XING, XIA DONG, Beijing National Laboratory for Molecular Sciences, CAS Key Laboratory of Engineering Plastics, Institute of Chemistry, Chinese Academy of Sciences, RONGBO LI, PetroChina Petrochemical Research Institute, CHARLES C. HAN, DUJIN WANG, Nanjing University of Technology, Nanjing, China, MARIA SANTOS, Imperial College London, UK, JUREK KULWICKI, Northwestern University, USA. — The biological membrane, in our approach, is represented by a dynamically triangulated surface while the proteins are modeled as curvature fields on the membrane, which can either be isotropic or anisotropic. Thermal undulations in the membrane and cooperativity in the curvature field, due to the stabilization of a nematic phase, drives the membrane into conformations that resemble those in experiments in vivo and vitro. The stability of these structures are examined by two approaches to compute the free energy of the system: (i) Widom insertion technique to compute excess chemical potentials and (ii) thermodynamic integration using the Kirkwood coupling parameter to compute absolute free energies. Building on these methods, we propose a hybrid scheme that couples both the approaches for computing free energies.

10:12AM F30.00012 Correlating bulk properties and nanoscale rearrangement during UV-initiated gelation of hybrid nanoparticle/ block copolymer systems, K. ANNE JUGGERNAUTH, Macromolecular Sci. & Eng. Research Center, Dept of Materials Sci. & Eng., University of Michigan, Ann Arbor, SOENKE SEIFERT, X-Ray Sciences Division, Advanced Photon Source, Argonne National Labs, Argonne, IL, BRIAN LOVE, Macromolecular Sci. & Eng. Research Center, Dept of Materials Sci. & Eng., University of Michigan, Ann Arbor — The photoinduced behavior of amphiphilic block copolymers is highly dependent on the interplay between the interfacial properties of the copolymer and the state of the surrounding medium, which can be externally controlled by varying the conditions of the environment. Here, we investigate the interplay between the microphase separation and structural rearrangement in a model system, namely a blend of polystyrene and poly(ethylene oxide)-block-poly(propylene oxide)-block-poly(ethylene oxide) (PEO-b-PPO-b-PEO) block copolymer surfactants, under UV exposure. We use time resolved synchrotron SAXS and WAXS with simultaneous UV exposure to investigate the structural dynamics of the system. Our results show that the kinetics for local structural changes between particles and bulk gelation from UV exposure are strongly correlated.

10:24AM F30.00013 Cooperative Processes in Restructuring Gel Networks, JADER COLOMBO, Microstructure and Rheology, Institute for Building Materials, ETH Zurich, ASAPH WIDMER-COOPER, School of Chemistry, University of Sydney, EMANUELA DEL GADO, Microstructure and Rheology, Institute for Building Materials, ETH Zurich — Colloidal gel networks are disordered elastic solids that can form even in extremely dilute particle suspensions. Similarly to other network-forming soft materials, including many with important biological function or technological potential, they can locally restructure via breaking and reforming interparticle bonds. Although controlling the link between local restructuring and mechanical response bears enormous potential for designing smart nanocomposites, there is at present little understanding of how local bond changes affect the dynamics of the gel network and the stress transmission through it. Here, using numerical simulations of a model system and a space-resolved analysis of dynamical heterogeneities, we show that bond breaking has non-local consequences and induces cooperative relaxation further away along the network. This provides explicit microscopic insight into why non-local constitutive relations are required to rationalize the non-trivial mechanical response of colloidal gels.
10:36AM F30.00014 Elimination of branching in self assembled beta-hairpin based peptide hydrogels. SAMEER SATHAYE, DARRIN POCHAN, Department of Materials Science and Engineering, University of Delaware, DARRIN POCHAN RESEARCH GROUP TEAM — Hydrophobic collapse of amphiphilic β-hairpin peptides (e.g. MAX1 VKVKVKVKVKVDPTKVKVKVKV-NH₂) into fibrils and their hierarchical assembly into branched, hydrogel networks has been extensively studied. A physically crosslinked hydrogel network is formed due to fibrillar entanglement and branched defects in hydrophobic collapse during fibril formation. Alternating valine residues with side chains of the same size are responsible for the hydrophobic collapse of the molecule into a b-hairpin and fibril nanostructure with branching. In a new sequence LNK1 (LNK1 (NaI)K(NaI)KAKAKVKDPTKAKAK(NaI)(K(NaI))-NH₂) the non-beta turn valines were replaced with Naphthylalanine and alanine amino acid residues, with hydrophobic side chains of larger and smaller volume, respectively, than valine. Thus, formation of a 'lock and key' type structure was attempted in the hydrophobic core of the peptide fibrils that would eliminate fibril branching. The folding and network formation of LNK1 has been studied by Circular Dichroism spectroscopy (CD), Transmission Electron Microscopy (TEM) and Oscillatory Rheology. Preliminary rheological characterization suggests the elimination of branching in the fibrils and also a possibility that LNK1 networks, unlike MAX1, are just nanofibrillar suspensions rather than permanently physically crosslinked hydrogels.

10:48AM F30.00015 Microstructure and rheology of a thermoreversible gel under large amplitude oscillatory shear (LAOS) deformation using time-resolved oscillatory rheo-small-angle neutron scattering (tOr-SANS). JUNG MIN KIM, A. KATE GURNON, NORMAN WAGNER, University of Delaware, AARON EBERLE, NCNR NIST — Large amplitude oscillatory shear (LAOS) rheology is an effective way of studying the nonlinear dynamics of complex fluids. Here, we present a new method for a direct, quantitative study of the microstructure under LAOS deformation in the framework of the alignment factor, Af. We use a model thermoreversible adhesive hard-sphere system composed of octadecyl-coated silica particles suspended in n-tetradecane. With temperature the particle potential is controlled and the system is shifted from behaving as a near hard-sphere to an adhesive hard-sphere system leading to aggregation and ultimately a dynamical arrest transition to macroscopic gelation. Time-resolved oscillatory rheo-small-angle neutron scattering (tOr-SANS) measurements in the 1-3 plane are performed by stroboscopically probing the structural evolution as a function of time during LAOS. Under strong shear, the 2D scattering pattern of the system in the gel state exhibits a strong anisotropy commonly known as a “butterfly” pattern, which corresponds to the stretching of the microstructure along the flow direction. The first structure-Lissajous plots of this model system are presented in terms of an order parameter and Af as a function of instantaneous strain and strain rate. This new analysis demonstrates a novel method for simultaneously measuring the rheology and microstructure during a time-dependent deformation (LAOS).

Tuesday, March 19, 2013 8:00AM - 11:00AM —
Session F34 DPOLY DCMP DBIO: Charged Colloids with Short-Range Attractions I

8:00AM F34.00001 POLYMER PHYSICS PRIZE BREAK —

8:36AM F34.00002 A colloidal perspective of protein solutions manipulated by multivalent ions: Phase behavior and associated dynamics. FRANK SCHREIBER, Tuebingen University — After a brief overview of interactions in aqueous protein solutions, we will discuss how ions can be used to manipulate these interactions and the associated phase behavior as well as the diffusion dynamics. We show that multivalent ions do not only influence the ionic strength and the resulting interactions including effective attraction, but lead to qualitatively new effects. Particular attention will be given to the reentrant condensation of proteins (F. Zhang et al, PRL 101 (2008) 148101; F. Zhang et al, Soft Matter 8 (2012) 1313) and its relationship with liquid-liquid phase separation and protein crystallization. In particular, we attempt to rationalize crystallization controlled by trivalent ions and discuss the role of specific ions and their impact on the effective interaction potential. These results are compared to the diffusion dynamics in these systems studied using neutron spectroscopy and light scattering (F. Roosen-Runge et al, PNAS 108 (2011) 11815; Heinen et al, Soft Matter 8 (2012) 1404) and the question of transient clusters is discussed. Finally, we critically discuss to which extent proteins can be described by colloidal concepts. The work was performed in collaboration with F. Zhang, T. Seydel, M. Hennig, F. Roosen-Runge, M. Skoda, R. Jacobs and others.

9:12AM F34.00003 ABSTRACT WITHDRAWN —

9:24AM F34.00004 Protein clusters in biomembranes. NICOLAS DESTAINVILLE, University Paul Sabatier - Toulouse 3 — We propose that proteins embedded in lipidic bio-membranes can spontaneously self-organize into stable membrane nano-domains (or clusters), due to the competition between short-range attractive and longer-range repulsive forces between proteins, specific to these systems, and propagated by the lipidic membrane. We compare different long-range potentials (including notably three-body terms) and we demonstrate that the existence of cluster phases in this context should be quite generic. Furthermore, a real membrane contains hundreds of different protein species that are far from being randomly distributed in these nano-domains, which is crucial in terms of biological functions. We take this protein diversity into account by modulating protein-protein interactions both at short and longer range. Both theoretical and numerical investigations explain why protein clusters recruit only a few protein species, thus leading to cluster biological specialization. In this respect, we highlight that cluster phases can turn out to be an advantage at the biological level, for example by enhancing the cell response to external stimuli.

9:36AM F34.00005 Assembly of Spherical Colloids by Short-range Out-of-plane Attraction and Long-range In-plane Repulsion. FUDUO MA, DAVID T. WU, NING WU, Colorado School of Mines — The electric-field assembly of spherical colloids with isotropic surface properties has been studied in both two- and three- dimensions. Structures, such as FCC, HCP, and BCT crystals were observed. Recently, we have found surprisingly new types of structures within a previously unexplored experimental regime: low frequency regime (100 Hz to 10 kHz) and low salt concentrations (below 10⁻³ M). At low particle concentrations, a family of well-defined clusters, ranging from 3 to 10 was observed. Statistical analysis of the population distribution revealed non-trivial peaks for trimers, tetrarmers, hexamers, and nonamers. We attribute these new types of non-planar structures to a short-range out-of-plane (the plane refers to the substrate) attraction and a long-range in-plane repulsion. For example, the double layer and in-plane dipolar repulsion could make bottom particles in the clusters separate from each other. While the out-of-plane dipolar attraction and particle-substrate attraction could be responsible for the formation of the clusters, i.e., the top central sphere is associated with the bottom spheres. Phase diagrams from experiments and simulation will be compared. These clusters could be used as building blocks for making photonic crystal, filtration, and plasmonic structures.
9:48AM F34.00006 Colloidal stability in concentrated electrolyte solutions using large counterions, GUILLERMO GUERRERO GARCIA, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA, PEDRO GONZALEZ MOZUELOS, Departamento de Física, Cinvestav del I. P. N., Av. Instituto Politecnico Nacional 2508, Distrito Federal, C. P. 07360, Mexico, MONICA OLVERA DE LA CRUZ, Department of Materials Science, Northwestern University, Evanston, IL 60208, USA — The stability of charged colloids in solution has been widely studied because it has ubiquitous applications in science and engineering. According to the classical DLVO theory, the electrostatic repulsion among charged colloids is significantly screened at high electrolyte concentrations. As a result, highly charged particles are expected to aggregate due to short-range van der Waals attractive interactions. Nevertheless, the classical DLVO theory relies in the linear Poisson-Boltzmann equation, which is usually restricted to low electrolyte concentrations and weakly charged colloids. In this work, we propose a novel mechanism beyond the classical DLVO picture that uses large counterions to prevent highly charged nanoparticles from aggregating in salt solutions with concentrations up to 1 M, in agreement with experimental observations.

10:00AM F34.00007 Size and interaction-strength effects on the phase behavior of colloidal particle assemblies, RAY SEHGAL, DAVID FORD, DIMITRIOS MAROUDAS, University of Massachusetts Amherst — We report the findings of a systematic computational study of the inherently complex phase behavior of thermodynamically small assemblies (clusters) of colloidal particles interacting via a potential that includes electrostatic repulsion and depletion-based short-ranged attraction. Using Monte Carlo umbrella sampling with coarse graining in two order parameters and a biasing scheme based on a genetic algorithm, we generate free-energy landscapes (FELs) that can indicate coexistence between fluid-like and crystalline phases. We have used the data mining technique of diffusion mapping to determine the dimensionality of the order-parameter space and assess the suitability of chosen order parameters that represent metrics of cluster density and crystallinity. Evaluation of phase behavior metrics from analysis of the FELs leads to predictions of conditions for formation of stable phases of such small colloidal clusters. A stable crystalline phase emerges as the number of particles in the assembly increases beyond a critical value. We find that the critical cluster size for the onset of crystallization decreases with increasing strength of the interparticle attraction. This FEL analysis also enables a mean-field description of the phase transitions undergone by these assemblies.

10:12AM F34.00008 Distinguishing cluster phases as a unique scenario of intermediate range order in colloidal suspensions and protein solutions, PAUL DOUGLAS GODFRIN, University of Delaware, RAMON CASTANEDA-PRIEGO, Universidad de Guanajuato, YUN LIU, National Institute of Standards and Technology, NORMAN J. WAGNER, University of Delaware — A state of stable clusters is characterized by the reversible aggregation of colloidal particles to a finite, energetically favored size. Clusters can arise from a competition between short range attraction, driving aggregation, and long range repulsion, stabilizing clusters. Recent interest in systems with these interactions has brought attention to the formation of a low-q peak in the structure factor and the proposition that this peak directly indicates cluster formation. To understand the structures that produce a low-q peak, Metropolis Monte Carlo simulations are performed to calculate the partial structure factors by decomposing the system into cluster-cluster, monomer-monomer, and cross-correlations. We find that a low-q peak appears in fluids with strong cluster-cluster correlations but also in systems dominated by monomer-monomer correlations and percolated states. Thus, this low-q peak is more appropriately termed the intermediate range order (IRO) peak. Consequently, an IRO peak does not necessarily signal the existence of a cluster state in solution. Rather, it reflects the presence of a preferred length scale related to the two competing potential features. Determining cluster formation is most accurately accomplished by combining experiment with simulation.

10:24AM F34.00009 Changing the state and structure of charged colloids with short-range attraction in shear flows, ALESSIO ZACCONE, Cavendish Laboratory, University of Cambridge, MASSIMO MORBIDELLI, Department of Chemistry, ETH Zurich — Under static conditions, the superposition of short-range (e.g. van der Waals) attraction and electrostatic repulsion gives rise to interesting phases such as equilibrium clusters in globular protein suspensions. What is much less understood is their behavior under external flow, which is important for the physiological aggregation of proteins and for industrial systems as well. I will present theoretical and experimental results showing that clustering of these systems in shear flow is characterized by the crossover from a reaction-limited clustering kinetics at low shear into a convection-dominated aggregation regime at high Peclet numbers. The kinetics may rise by up to many orders of magnitude in the crossover regime. This behavior is due to the singularly-perturbed character of the governing diffusion equation where the shear drift term induces a singularity and a boundary-layer at large interparticle distances. This understanding, together with a theoretical description of cluster breakup, is used to rationalize the peculiar nonequilibrium state diagram (including gelation) of these colloidal suspensions in shear flow with applications ranging from microfluidic self-assembly to proteins.

10:36AM F34.00010 Percolation and local density fluctuations for a Colloidal System with competing interactions, NESTOR VALADEZ-PEREZ, NIST Center for Neutron Research and Science and Engineering Division, University of Guanajuato, YUN LIU, NIST Center for Neutron Research and Department of Chemical and Biomolecular Engineering, University of Delaware, RAMON CASTANEDA-PRIEGO, Science and Engineering Division, University of Guanajuato — The gelation is believed to result from the particle aggregation in a complex structure. The aggregate span in the entire volume gives it a capability for supporting stresses. Gelled systems possess a high degree of inhomogeneity, while locally the particles and their near neighbors present a defined array as can be seen in their coordination number and bonding angles. Using Monte Carlo simulations, we investigate the structure of a system of hard spheres interacting through a combined potential: a short-ranged Square Well (SW) and a long-ranged repulsive Yukawa potential (RY). We made an exhaustive study for several conditions of temperature (T*) and concentration (\(\phi\)) corresponding to different repulsion strengths (\(\lambda\)). Our results show that the percolation threshold is shifted to lower concentrations when the repulsion is increased, but this shift gradually disappears at low temperature. Besides we also computed the local density through the system; we particularly identified a length scale at which counter-ion motion is unknown. Using optical tweezers to trap a colloidal particle in a low-frequency electric field, we found the drag coefficient of the particle in the field to be non-Stokes. We discuss how the non-Stokes’ drag coefficient as a function of salt concentration and particle size may be useful for interpreting different models of Zeta potential.

Tuesday, March 19, 2013 8:00AM - 10:48AM — Session F36 DCMP: Superconductivity: Josephson Effect
8:00AM F36.00001 High Temperature Superconducting Terahertz Emitters with Various Mesa Structures
KAVEH DELFANAZARI, M. TSUJIMOTO, T. KASHIWAGI, Univ. of Tsukuba, University of Tsukuba, CREST-JST, WPI-MANA, H. ASAI, AIST, T. KITAMURA, University of Tsukuba, CREST-JST, WPI-MANA, T. YAMAMOTO, JAE, M. SAWAMURA, K. ISHIDA, C. WATANABE, S. SEKIMOTO, H. MINAMI, M. TACHIKI, T. HATTORI, University of Tsukuba, CREST-JST, WPI-MANA, R. A. KLEMM, Univ. of Central Florida, USA, K. KADOWAKI, University of Tsukuba, CREST-JST, WPI-MANA — In 2007, the first observation of the coherent terahertz (THz) electromagnetic (EM) waves from a mesa structures of intrinsic Josephson junctions (IJJs) in high temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212) is reported [1]. The ac-Josephson effect as well as the cavity resonance conditions is considered as the principle mechanism of the THz radiation [1, 2]. In order to understand the cavity effect in THz radiation from IJJ mesas more clearly, we studied mesas with various geometries; various kinds of triangles [3], and pentagonal mesas with various sizes and thicknesses. The focused ion beam (FIB) milling technique is used in all mesa fabrications. In this talk, we discuss our recent progress in THz emission observation in pentagonal mesas.


This work has been supported in part by CREST-JST (Japan Science and Technology Agency), WPI-MANA project (NIMS).

8:12AM F36.00002 Tunable THz radiation from intrinsic Josephson junctions in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ in a localized phase rotating mode
MANABU TSUJIMOTO, KAVEH DELFANAZARI, TAKEO KITAMURA, MASASHI SAWAMURA, KAZUYA ISHIDA, SHUNSUKE SEKIMOTO, CHIHARU WATANABE, University of Tsukuba, TAKASHI YAMAMOTO, Japan Science and Technology Agency, TAKANARI KASHIWAGI, HIDETOSHI MINAMI, KAZUO KADOWAKI, University of Tsukuba — After the first report of intense continuous THz electromagnetic wave radiation from high-T$_c$ superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [L. Ozyuzer et al., Science 318, 1291 (2007)] with remarkably higher intensity, a great deal of interest has been drawn not only to the physical mechanism of the radiation but also to the possible variety of applications in the vast fields of THz science and technology. Recently, the authors pointed out that the contributions to the output power from the Josephson current source was found to be comparable in magnitude [K. Kadowaki et al., J. Phys. Soc. Jpn. 79, 023703 (2010); M. Tsujimoto et al., Phys. Rev. Lett. 108, 107006 (2012)]. As R. Kleiner et al. observed in 1992 [R. Kleiner et al., Phys. Rev. Lett. 68, 2394 (1992)], the intrinsic junctions in the phase rotating mode produce an equal number of $1$-$V$ characteristic branches. Here we show clear evidence that the mesas can emit radiation at many frequencies in various localized phase rotating modes, and that the resulting radiation is tunable over a broad range of frequencies, allowing us to construct a powerful THz source device that could fill the THz gap.

1. JST-CREST, WPI-MANA

8:24AM F36.00003 Direct imaging of hot spot in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ mesa terahertz sources
TIMOTHY BENSEMAN, KEN GRAY, ALEXEI KOSHELEV, WAI-KWONG KWOK, ULRICH WELP, VITALII VLASKO-VLASOV, Materials Science Division, Argonne National Laboratory, KAZUO KADOWAKI, HIDETOSHI MINAMI, University of Tsukuba, Japan — Stacks of intrinsic Josephson junctions (IJJs) made from high-temperature superconductors such as Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212) are a promising source of coherent continuous-wave terahertz radiation. When electrical power is applied to these devices, it is thought that hot spots may form due to resistive self-heating, and that these spots may be highly beneficial for the generation of high levels of THz power from Bi-2212 stacks. In order to better understand these hot spots, we have performed a thermal imaging study of SSCCO stacks which generate approximately 50 microwatts of radiation power at 0.59 THz. Utilizing the temperature-dependent 612nm fluorescence line of Eu$^{3+}$, we are able to directly measure the temperature distribution at the top surface of these stacks with a resolution of +/- 1K. The images reveal a highly non-uniform temperature distribution in which the temperature in the middle of the stack can exceed the superconducting transition temperature by tens of Kelvin under biasing conditions typical for THz-emission.

This research was funded by the Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

8:36AM F36.00004 Magnetic field effects on THz radiation from Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ mesa structures
TAKEO KITAMURA, TAKANARI KASHIWAGI, MANABU TSUJIMOTO, KAVEH DELFANAZARI, MASASHI SAWAMURA, KAZUYA ISHIDA, SHUNSUKE SEKIMOTO, CHIHARU WATANABE, University of Tsukuba, TAKASHI YAMAMOTO, Japan Atomic Energy Agency, HIDETOSHI MINAMI, MASASHI TACHIKI, KAZUO KADOWAKI, University of Tsukuba — In a previous study, coherent and continuous electromagnetic radiation phenomena in mesa structures of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ single crystal have been investigated precisely in magnetic fields up to only 150 Oe [1]. This experimental result showed that the emission intensity decreases sharply for the field parallel to the c-axis, while it decreases gradually as increasing magnetic field for the in-plane field. In order to improve the measurement, we developed a new system with a better angular resolution and much wider magnetic field range up to 6 T, and a mesa having much stronger THz emission power. The mesa structure is also changed to the stand-alone type of mesa, which produces higher power THz radiation with ideal distribution of radiation [2]. In this presentation, the recent detailed results will be shown in magnetic fields both parallel and perpendicular to the ab-plane of Bi2212, where the Josephson and pancake vortices are playing an important role for THz radiation.


This work was supported in part by CREST-JST, WPI-MANA project (NIMS) and Strategic Initiative category (A) at the University of Tsukuba.

8:48AM F36.00005 Simultaneous observation of temperature distribution and THz emitting spectra of Bi2212 THz devices
CHIHARU WATANABE, HIDETOSHI MINAMI, University of Tsukuba, TAKASHI YAMAMOTO, Quantum Beam Science Directorate, TAKANARI KASHIWAGI, KAZUO KADOWAKI, University of Tsukuba — When the intrinsic Josephson junctions in high-Tc superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ are fabricated to a mesa structure and biased by a dc-voltage, it is known to emit coherent, stable and continuous THz electromagnetic waves [1] whose frequency lies between 0.3-1 THz with the line width of 0.5 GHz and the radiation maximum power of 30 µW. Recently, we have succeeded in measuring the temperature distribution of the mesa directly while the mesa is emitting THz radiation and found an extreme temperature inhomogeneity (hot-spot) in the mesa [2]. By this way, we could determine the temperature of a mesa, as a result we could observe inhomogeneous temperature distribution, and we found that relation between THz emitting characteristics and temperature distribution. The simultaneous observation of the emission frequency by FTIR strongly indicates that the THz emission phenomenon is not influenced by the formation of the hot-spot at all. In this meeting, we would like to discuss the relations between THz emission phenomena hot-spot formation.


9:00AM F36.00006 ABSTRACT WITHDRAWN —
9:12AM F36.00007 Control of Spin-Triplet Josephson Junctions with Perpendicular Anisotropy\textsuperscript{1} \hfill \textsuperscript{1}Funding provided in part by DOE grant DEFG02-06ER46341 and in part by IARPA contract N66001-12-C-2017

Eric Gingrich, Michigan State University, Simon Diesch, University of Konstanz, William Pratt, Norman Birge, Michigan State University — We present recent work on S/F'/F/F"/S Josephson Junctions with the magnetic multilayer Ni/[Co/Ni]\textsubscript{m}. as the central F layer \textsuperscript{1}. This multilayer possesses strong intrinsic perpendicular (out-of-plane) anisotropy at Co and Ni thicknesses of a few monolayers. If a hard ferromagnet is used for F\textsuperscript{'} and a softer ferromagnet is used for F\textsuperscript{"}, both with magnetizations in plane, the direction of the F\textsuperscript{"} layer’s magnetization is predicted to control the state of the junction \textsuperscript{2}. We are currently working toward a SQUID-based experiment that should be able to distinguish the 0 and \(\pi\) states. By integrating these junctions in a SQUID device, a measurement of the (and \(\pi\) state of the junction can be performed. We will report on our progress.

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9:24AM F36.00008 Search for \(\pi/2\) state in large-area spin-triplet ferromagnetic Josephson junctions\textsuperscript{1}, Yixing Wang, Norman O. Birge, William P. Pratt, Jr., Department of Physics and Astronomy, Michigan State University — The current-phase relationship of ferromagnetic spin-triplet Josephson junctions was predicted to be tuned by the magnetization orientations of different magnetic layers \textsuperscript{1}. Given the random domain structure in large-area ferromagnetic junctions, the possibility of a random distribution of 0 or \(\pi\) subjunctions across the area could lead to a global \(\pi/2\) junction \textsuperscript{2}. Critical current measurements as a function of area provide indirect evidence for \(\pi/2\) coupling \textsuperscript{3}, but they do not provide phase-sensitive information. Unfortunately, there are technical difficulties faced by a direct current-phase measurement, especially for large area junctions. We are currently working on a SQUID-based experiment that should be able to distinguish the \(\pi/2\) state from either the 0 or \(\pi\) states. In this talk we will report on our progress toward this goal.

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9:36AM F36.00009 Odd-Frequency Triplet Josephson Current Through an Exchange Spring\textsuperscript{1}, Andreas Bill, California State University Long Beach, Thomas E. Baker, California State University Long Beach and University of California, Irvine, Adam Richielle-Halford, Adam K. Moke, California State University Long Beach — The existence of an odd-frequency long range triplet component in the order parameter of a proximity system with singlet superconductors is a recent prediction that has garnered great interest. The experimental fingerprint of this phenomenon is difficult to establish. We investigate a hybrid structure in which the emergence of the long range triplet component may be measured and identified. We consider a superconductor - exchange spring - superconductor Josephson junction as a function of increasing twist of the magnetic domain wall in the exchange spring. We show that as the domain wall is generated the long range triplet component emerges and modifies the current flowing through the Josephson junction. The critical temperature is also affected by the increased twist of the domain wall. The calculations lead us to propose an experiment where the long range triplet component can unequivocally be identified.

\begin{itemize}
  \item [\textsuperscript{1}] Work supported by the US Department of Energy under Grant No. DE-FG02-06ER46341.
\end{itemize}

9:48AM F36.00010 Spin-triplet supercurrent in planar geometry ferromagnetic Josephson junctions\textsuperscript{1}, William M. Martinez, W.P. Pratt, Jr., Norman O. Birge, Michigan State University — The spin-triplet supercurrent in ferromagnetic Josephson junctions is obtained by surrounding the central ferromagnet with noncollinear ferromagnetic layers, F\textsuperscript{'} \textsuperscript{1}. In metallic ferromagnets, the long-range nature of the spin-triplet supercurrent has only been tested to lengths of a few tens of \textit{nm} \textsuperscript{2}. In this work, we are fabricating and measuring S/F'/F/F''/S junctions where the central F layer has a lateral geometry with lengths up to a few hundred \textit{nm}. We will report on our recent progress.

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10:00AM F36.00011 Skewness and Kurtosis of the Switching Current Distribution in Superconductor-Graphene-Superconductor Junctions and Superconductor-Nanowire-Superconductor Devices, Andrew Murphy, Thomas Aref, Ulas Coskun, University of Illinois Urbana-Champaign, Phillip Weinberg, Alex Levchenko, Michigan State University, Victor Vakaryuk, The Johns Hopkins University, Alexey Bezryadin, University of Illinois Urbana-Champaign — We study statistical properties of the switching current in superconductor-graphene-superconductor proximity junctions and superconductor-nanowire-superconductor devices. The fluctuations of the switching current are related to Little’s phase slips, generated by thermal and quantum fluctuations of the superconducting order parameter. The study focuses on higher moments of the statistical probability distributions of the switching current. Namely we study the skewness, which defines the asymmetry of the distribution, and kurtosis, which is a measure of the “peakedness.” The skewness is defined as \(sk = m_3/m_2^2\) where \(m_2\) is the second moment of the distribution, called the variance, and \(m_3\) is the third moment. Kurtosis is defined as \(kur = m_4/m_2^2\), where \(m_4\) is the fourth moment of the distribution. It is known that for Gaussian distributions \(sk = 0\) and \(kur = 3\). On our devices we find, in most cases, \(sk \sim -1\) and \(kur \sim 5\). These results are in agreement with numerical simulations as well as an analytic model. Finally we present preliminary experimental results for a two-nanowire device. We have found that the standard deviation, skewness and kurtosis of the switching current distributions in these devices vary periodically with magnetic field.

10:12AM F36.00012 Realization of short ballistic vertical graphene Josephson junction, Gil-Ho Lee, Hui-Jong Lee, POSTECH — We realized short ballistic vertical graphene Josephson junctions (vGJJs), where a monolayer graphene sheet is sandwiched between two superconducting electrodes along the c-axis of graphene. To enhance the transparency between electrodes and graphene layer we thermally deposited aluminum superconducting electrodes on both surfaces of the graphene sheet by using a “flip-transfer” scheme instead of transferring graphene onto the bottom electrode. With the highly transparent contacts and atomically short channel length, vGJJ shows a very large value of \(I_{c}\) product (\(2.2\Delta_{A_{1}}\)). This value is in sharp contrast to much suppressed value of \(I_{c}\) product of planar graphene Josephson junctions. Surprisingly, \(I_{c}\) decreases superlinearly with increasing temperature (\(T\)) from 50 mK up to the junction critical temperature, which is a typical character of a short ballistic Josephson junction. To our best knowledge, this feature has long been predicted but never been reported in proximity-coupled Josephson junctions. \(I_{c}-T\) curve fits well to the short ballistic Josephson junction model (KO-2) \textsuperscript{3} with the transparency of 0.94.

\begin{itemize}
  \item [\textsuperscript{3}] K. K. Likharev, Rev. Mod. Phys. 51, 101 (1979)
\end{itemize}
10:24AM F36.00013 Direct measurements of the current-phase relation in graphene Josephson junctions. CHRISTOPHER ENGLISH, DAVID HAMILTON, DALE VAN HARLINGEN, NADYA MASON, University of Illinois at Urbana-Champaign — The current-phase relation (CPR) of a Josephson junction can provide key information about the microscopic processes and symmetries that control the supercurrent. In this talk, we present CPR measurements on Josephson junctions incorporating single-layer graphene as a weak link between Al superconducting electrodes with spacing <100nm that are in the quasi-ballistic regime. We use a phase-sensitive SQUID technique to determine the supercurrent amplitude and phase as a function of temperature and electrostatic doping (gate voltage). As the critical current is varied, we observe a crossover from forward skewing in the CPR that arises from the low density of discrete electronic states in the junction to backward skewing induced by noise-rounding in the CPR measurement. We compare our results to theoretical models.

10:36AM F36.00014 Josephson currents in semiconductor nanowire / s-wave superconductor nanostructures. LI MAO, Department of Physics, the University of Texas at Dallas, Richardson, TX, 75080 USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, SC, 29634 USA, CHUANWEI ZHANG, Department of Physics, the University of Texas at Dallas, Richardson, TX, 75080 USA — It has been theoretically predicted that a nanostructure composed of a semiconductor nanowire with strong spin-orbit coupling and an s-wave superconductor can support two Majorana fermions at the ends of the nanowire in the presence of a Zeeman field. Recently, following the theoretical proposals, some preliminary experimental signatures (e.g., zero-bias conductance peak) which may be related to the existence of Majorana fermions have been observed in the charge transport experiments. Here we investigate the Josephson currents with the zero-bias voltage in the topologically trivial region of a superconductor-insulator-superconductor junction in the presence of strong spin-orbit coupling and Zeeman field. This structure may be relevant to the Delft experiment by considering the possible proximity effect of the superconductor lead to the normal part of the nanowire. Our results indicate that the experimentally observed zero-bias conductance peak may not originate from Majorana fermions.

Tuesday, March 19, 2013 8:00AM - 11:00AM — Session F40 DCMP: Surfaces, Interfaces, and Thin Films: Molecules on Surfaces 349 - Daniel Dougherty, North Carolina State University

8:00AM F40.00001 Molecular Ordering in PCBM Monolayer Films on Ag and Au (111): From μ-aerosol deposited glasses to hep packing. QIAN SHAO, University of Maryland-College Park, LEVAN TSKIPURI, None, JANICE REUTT-ROBEY, University of Maryrdl College Park — Functionalized C60 and C70 fullerenes are increasingly employed as active components in organic electronic devices. The structure of the PCBM electrode interface is expected to strongly impact charge transfer processes in photovoltaic devices. Here we report molecularly-detailed studies of PCBM ordering at coinage metal surfaces. We have developed a vacuum-compatible liquid delivery source to generate thin films of C60 and C70-PCBM from organic solvents. Structure is tracked from the sub-monolayer to multilayer regime on (111)-oriented Ag and Au surfaces with molecular detail by UHV-STM. Glassy morphologies of as-grown films reflect solvant retention. Upon thermal annealing solvent molecules are released and films evolve into ordered packing arrangements that depend upon the PCBM density in the original films. The hcp monolayer phase of C60 and C70-PCBM are newly produced and characterized, indicating the accessibility of new growth phases by μ-aerosol deposition. Acknowledgement: This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471.

8:12AM F40.00002 Doping of Grain Boundaries in diF TESADT Transistors1, COURTNEY BOUGHER, SHAWN M. HUSTON, Appalachian State University, JEREMY W. WARD, ABDUL OBAID, Wake Forest University, MARSHA A. LOTHE, JOHN E. ANTHONY, University of Kentucky, OANA D. JURCHESCU, Wake Forest University, BRAD R. CONRAD, Appalachian State University — We utilize Atomic Force Microscopy (AFM) and Kelvin Probe Force Microscopy (KPFM) to characterize the dynamics of electronic transport across 2,8-difluoro-5,11-triethylsilylethynylanthradiithiophene (diF-TES-ADT) grain boundaries. We show that the morphology of grain boundaries and the adsorption of atmospheric dopants at these local boundaries have a direct impact on the electrical behavior of diF TESADT in thin film transistor (TFT) devices. Device voltage drops at grain boundaries are characterized as a function of both atmospheric dopants and transition time between dopants. The morphology, including crystallization and packing motifs, of diF TESADT grown on thermally grown SiO2 will be discussed and related to other semiconducting small organic molecules. This work will be put in the context of other, recent advances in small molecule organics.

1 Funded by: Ralph E Powe Junior Faculty Enhancement Award, Appalachian State University Office of Student Research, and NC Space Grant Consortium.

8:24AM F40.00003 Scanning Tunneling Microscopy investigation of multilayer diF-TES-ADT on Au(111), SHAWN HUSTON, Appalachian State University, JIUYANG WANG, North Carolina State University, MARSHA LOTHE, JOHN ANTHONY, University of Kentucky, BRAD CONRAD, Appalachian State University, DANIEL DOUGHERTY, North Carolina State University — Organic thin film transistors (OTFT) partially composed of solution processed 2,8-difluoro-5,11-bis(triethylsilyl)anthradiihophene (diF-TES-ADT) have shown high performance with hole mobilities up to 1 cm²/Vs. Pretreatment of the gold electrodes results in growth of large diF-TES-ADT crystals extending well out into the channel of the OTFT. Without pretreatment, the crystal sizes are small and possess a non-preferred molecular orientation. We have chosen to investigate the reasons for the reduced crystal size of these films on untreated gold electrodes by studying a model system generated by vapor deposition of multilayers of diF-TES-ADT on Au(111). The initial wetting layer forms a highly ordered film such that the anthradithiophene backbone is oriented parallel to the substrate and the unit cell is 1.49 nm x 1.25 nm with an included angle of 56.8°. Growth beyond the second layer appears essentially bulk-like and crystalline with domain sizes that are potentially limited by the disordered bilayer growth.

8:36AM F40.00004 STM and optical investigations of molecules on graphene1, OZGUN SIZER, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA, JOSEPH SMERDON, Surface Science Research Centre, University of Liverpool, Liverpool L69 3BX, UK, NATHAN QUISINGER, JEFFREY GUEST, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL 60439, USA — We describe efforts to understand the structural, electronic and optical properties of an archetypal organic molecular building block for graphene-based nano-electronic devices. The structure of the PCBM electrode interface is expected to strongly impact charge transfer processes in photovoltaic devices. Here we report molecularly-detailed studies of PCBM ordering at coinage metal surfaces. We have developed a vacuum-compatible liquid delivery source to generate thin films of C60 and C70-PCBM from organic solvents. Structure is tracked from the sub-monolayer to multilayer regime on (111)-oriented Ag and Au surfaces with molecular detail by UHV-STM. Glassy morphologies of as-grown films reflect solvant retention. Upon thermal annealing solvent molecules are released and films evolve into ordered packing arrangements that depend upon the PCBM density in the original films. The hcp monolayer phase of C60 and C70-PCBM are newly produced and characterized, indicating the accessibility of new growth phases by μ-aerosol deposition. Acknowledgement: This work was supported by the NSF-MRSEC at the University of Maryland, DMR 0520471.

1 This work was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02- 06CH11357 and SISGR Contract No. DE-FG02-09ER16109
on Cleaved GaP Surfaces

9:00AM F40.00006 Bonding of anthracene derivatives to a Cu (111) surface: a combined STM and DFT study JONATHAN WRICK, YEMING ZHU, DANIEL SALIB, CONNOR HOLZKE, University of California at Riverside, ZHIHAI CHENG The National Center for Nanoscience and Technology, China, LUDWIG BARTELS, University of California at Riverside — We compare and contrast three anthracene derivatives whose 9,10 hydrogens are replaced by the elements O, S, and Se respectively that act as “feet” binding the molecules to a Cu (111) substrate. DFT calculations are compared with and shed light on STM data for the three molecules. We analyze the three species in terms of their geometric and electronic structure upon adsorption, taking into account the competing effects that the “feet” have with the anthracene moiety in their interactions with the underlying Cu surface.


1At the time of contributed research, Zhihai was at University of California at Riverside

9:12AM F40.00007 Substrate Mediated Short-range and Long-range Adsorption Pattern of CO on Ag(110) WAI-LEUNG YIM YIM, Institute of High Performance Computing, Singapore, THORSTEN KLUENER, Institute for Pure and Applied Chemistry, Theoretical Chemistry, University of Oldenburg, Germany — Substrate-mediated intermolecular interactions were proposed in the literature to explain the adsorption of CO on Ag(110) but the underlying mechanism is yet to be known. Here, short-range and long-range relaxation patterns for CO adsorption on Ag(110) surfaces have been investigated. The relaxation mode can be explained by the interaction of heavy electrons on metal substrates in electron momentum space. We identified two relaxation modes for CO on Ag(110). The long-range relaxation involved a (6×6) commensurate phase, while the short-range relaxation involved an alleviation of Fermi surface nesting along the (110) direction of the Ag(110) substrate. The symmetry broken ground state structure at high CO coverage can be rationalized, and this structure is consistent with the interpretation of available experimental data.

WLY acknowledges the IIHC Independent Investigatorship. Computations have been performed on the computers allocated at the A*STAR Computational Resource Centre (A*STAR).

9:24AM F40.00008 ABSTRACT WITHDRAWN

9:36AM F40.00009 5,6,7-trithiapentacene-13-one on vicinal gold (788): a STM study AMANDA LARSON, JEREMIAH VAN BAREN, JEREMY KINTIGH, JUN WANG, GLEN MILLER, KARSTEN POHL, University of New Hampshire — Scanning tunneling microscopy was used to examine the atomic interface between gold and 5,6,7-trithiapentacene-13-one (TTPO), an electron donor of potential interest for photovoltaic applications. TTPO is a polar species of pentacene with centered oxygen and sulfur bridge substituents. TTPO is a thermally and photo-oxidatively robust molecule with a HOMO-LUMO gap of 1.90 eV that can be thermally evaporated onto an electrode. The vicinal gold (788) surface is a well-studied surface on which pentacene molecules and other pentacene derivatives self assemble in long range order. We examined TTPO on gold to gain a better understanding of the structure of photovoltaic interfaces at the nanoscale.


1At the time of contributed research, Zhihai was at University of California at Riverside

10:00AM F40.00011 First Principles Study of the Electronic Structure of Organic Adsorbates on Cleaved GaP Surfaces MIN YU, PETER DOAK, JEFFREY NEATON, Lawrence Berkeley National Laboratory — We report a first principles calculations of structural, electronic, and spectroscopic properties of organic molecules, such as ethylene and benzene, adsorb on cleaved GaP (110) surface to assess their potential to allow controlled coupling and to modify charge transport between light absorbing semiconductors and catalysts for applications in artificial photosynthesis. We compute adsorbate geometries, binding energetics, surface band structures, constant current scanning tunneling microscopy images, and electronic energy level alignment of organic molecules on GaP surfaces using density functional theory and many-body perturbation theory within the GW approximation. We quantify the impact of coverage, interface dipoles, hybridization, and nonlocal polarization effects on level alignment, and validate our understanding through direct comparison recent measurements. Work supported by JCAP and computational resources provided by NERSC.

1Supported by JCAP and computational resources provided by NERSC.

10:12AM F40.00012 Low Temperature STM Study of Single-Molecule Attachment to GaP(110) AARON BRADLEY, Department of Physics, UC Berkeley, M.M. UGEDA, M. YU, JCAP, LBNL, K.L. MEAKER, Department of Physics, UC Berkeley, J. NEATON, Molecular Foundry, LBNL; JCAP, LBNL; UC Berkeley, G. MOORE, I. SHARP, JCAP, LBNL, M.F. CROMMIE, Department of Physics, UC Berkeley; Materials Science Division, LBNL; JCAP, LBNL — Engineering efficient artificial photosystems for catalytic and photovoltaic (PV) purposes is a major challenge for the development of viable solar fuel generators. One possible route toward this goal is to employ molecular catalysts covalently attached to semiconductor light absorbers through molecular linkages. The effect of such linkage on local electronic structure, however, remains an important question. Scanning tunneling microscopy (STM) is a useful tool for answering this question since it enables characterization of molecular interfaces at the atomic level. Here we describe our progress at measuring the structural and electronic properties of single organic molecules adsorbed to a p-doped GaP(110) surface. Low temperature STM was used to explore the surface chemistry and reactivity of GaP(110) by exposing UHV-cleaved GaP surfaces to sub-monolayer coverages of ethylene (C2H4) and iodobenzene (IC6H6), the latter being a candidate linker for connecting catalysts and PV molecules to semiconducting light absorbers. Our high-resolution STM images in combination with DFT calculations provide guidance for future attachment strategies involving improved molecule/semiconductor interfaces.
tunneling microscope-induced light emission, KUNIYUKI MIWA, MAMORU SAKAUE, HIDEAKI KASAI, Department of Applied Physics, Osaka University, Japan — Scanning tunneling microscope (STM)-induced light emission spectroscopy of molecules has unique advantage to investigate the luminescence properties of molecules with the atomic-scale spatial resolution. Recently, many attempts have been made to control the molecular luminescence by using the intense electromagnetic field generated by surface plasmons localized near the tip-substrate gap region. In this study, the nonequilibrium Green’s function method is utilized to investigate effects of coupling between an exciton composed by electron and hole in the molecule and the surface plasmons on the luminescence properties of the molecule and the surface plasmons. It is found that the luminescence intensities of the molecule are suppressed due to the re-absorption of the surface plasmons by the molecule. Molecular absorption and enhancement by molecular electronic and vibrational modes lead to peak structures in the luminescence spectra of the surface plasmons. Corresponding structures can be seen in a recent experiment. Moreover we found that the re-absorption by the surface plasmons plays important roles in determining the luminescence spectral profiles. We will discuss the detailed mechanisms of variation in these luminescence spectral profiles.

In-situ spectro-microscopy on organic films: Mn-Phtalocyanine on Ag(100)1, ABDULLAH AL-MAHBOOB, JERZY T. SADOWSKI, Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, ELIO VESCOVO, Photon Sciences, Brookhaven National Laboratory, Upton, NY 11973 — Metal phthalocyanines are attracting significant attention, owing to their potential for applications in chemical sensors, solar cells and organic magnets. As the electronic properties of molecular films are determined by their crystallinity and molecular packing, the optimization of film quality is important for improving the performance of organic devices. Here, we present the results of in situ low-energy electron microscopy / photoemission electron microscopy (LEEM/PEEM) studies of incorporation-limited growth [1] of manganese-phthalocyanine (MnPc) on Ag(100) surfaces. MnPc thin films were grown on both, bulk Ag(100) surface and thin Ag(100)/Fe(100) films, where substrate spin-polarized electronic states can be modified through tuning the thickness of the Ag film [2]. We also discuss the electronic structure and magnetic ordering in MnPc thin films, investigated by angle- and spin-resolved photoemission spectroscopy.

Research carried out at the Center for Functional Nanomaterials and National Synchrotron Light Source, Brookhaven National Laboratory, which are supported by the U.S. Dept. of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

Adorption structure analysis of co-adsorption dye-sensitized solar cells by the NEXAFS and XPS, MITSUNORI HONDA, MASATOSHI YANAGIDA, LIYUAN HAN, National Institute for Materials Science, NIMS TEAM — Adsorption structures of N719 dye alone and a N719+D131 co-adsorption system on a TiO₂ electrode were studied with the objective of increasing the efficiencies of dye-sensitized solar cells (DSCs). However, adsorption structure of isothiocyanate (R-N=C=S) in the alone and co-adsorption system was not completely understood because the surface morphology around nanocrystalline TiO₂ is complex. Therefore, we have investigated the adsorption structure on nanocrystalline TiO₂ surface using the Sulfur K absorption edge (S K-edge) and core level (S 1s) in details by using the near edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS), respectively. To consider the co-adsorption effect on DSCs, we analyze the depth profiling by the angle dependent NEXAFS spectroscopy and the chemical state on top of surface by the XPS analysis. As the results, we can determine the electronic structure around S atom in R-N=C=S in N719 on nanocrystalline TiO₂ surface. We clarify the adsorption structure of alone and co-adsorption system from the S K-edge NEXAFS and S 1s XPS analysis. I will talk about these results in my presentation.

Tuesday, March 19, 2013 8:00AM - 11:00AM — Session F47 DBIO DCMP: Invited Session: Solid-State Nanopores: Translocation and Applications
Hilton Baltimore Holiday Ballroom 6 - Gustavo Stolovitzky, IBM Research

The time distribution of charged biopolymers translocation through voltage-biased solid-state nanopores1, JIALI LI, Department of Physics, University of Arkansas. Fayetteville, AR 72701 — When a charged DNA or protein molecule is passing through a voltage biased solid-state nanopore in an ionic solution, it generates a current blockage signal characterized by its amplitude and time duration (or translocation time). Many parameters such as solution viscosity, applied voltage, the size, conformation, charge, and the charge sequence of the molecule could all contribute to the translocation time and its distribution. By fitting the translocation times to the solution of a Smoluchowski-type equation for 1D-biased diffusion and using the Einstein relation, the viscous drag force on uniformly charged DNA molecules and the uncertainty in determining the DNA chain length due to the contribution of Brownian motion can be evaluated. Furthermore, the time distribution of globular shaped particles and not uniformly charged unfolded protein molecules will also be discussed.

8:00AM F47.00001 The time distribution of charged biopolymers translocation through voltage-biased solid-state nanopores1, JIALI LI, Department of Physics, University of Arkansas. Fayetteville, AR 72701 — When a charged DNA or protein molecule is passing through a voltage biased solid-state nanopore in an ionic solution, it generates a current blockage signal characterized by its amplitude and time duration (or translocation time). Many parameters such as solution viscosity, applied voltage, the size, conformation, charge, and the charge sequence of the molecule could all contribute to the translocation time and its distribution. By fitting the translocation times to the solution of a Smoluchowski-type equation for 1D-biased diffusion and using the Einstein relation, the viscous drag force on uniformly charged DNA molecules and the uncertainty in determining the DNA chain length due to the contribution of Brownian motion can be evaluated. Furthermore, the time distribution of globular shaped particles and not uniformly charged unfolded protein molecules will also be discussed.

8:00AM F47.00001


1This work was supported by NIH R21HG003290 and NIH R21HG004776.

Surface Charge Modulation, AMIT MELLER, Boston University and The Technion, Haifa, Israel — The Nanopore method is an emerging technique, which extends gel-electrophoresis to the single-molecule level and allows the analysis of DNA, RNAs and DNA-protein complexes. The strength of the technique stems from two fundamental facts: First, nanopores due to their nanoscale size can be used to uncoil biopolymers, such as DNA or RNA and slid them in a single file manner that allows scanning their properties. Consequently, the method can be used to probe short as well as extremely long biopolymers, such as genomic DNA with high efficiency. Second, electrostatic focusing of charged biopolymers into the nanopore overcomes thermally driven diffusion, thus facilitating an extremely efficient end-threading (or capture) of DNA. Thus, nanopores can be used to detect minute DNA copy numbers, circumventing costly molecular amplification such as Polymerase Chain Reaction. A critical factor, which determines the ability of nanopore to distinguish fine properties within biopolymers, such as the location of bound small-molecules, proteins, or even the nucleic acid’s sequence, is the speed at which molecules are translocated through the pore. When the translocation speed is too high the electrical noise masks the desired signal, thus limiting the utility of the method. Here I will discuss new experimental results showing that modifying the surface charge inside the pore can effectively reduce the translocation speed through solid-state nanopores fabricated in thin silicon nitride membranes. I will present a simple physical model to account for these results.

8:36AM F47.00002 Controlling DNA Translocation Speed through Solid-State Nanopores by Surface Charge Modulation, AMIT MELLER, Boston University and The Technion, Haifa, Israel — The Nanopore method is an emerging technique, which extends gel-electrophoresis to the single-molecule level and allows the analysis of DNA, RNAs and DNA-protein complexes. The strength of the technique stems from two fundamental facts: First, nanopores due to their nanoscale size can be used to uncoil biopolymers, such as DNA or RNA and slid them in a single file manner that allows scanning their properties. Consequently, the method can be used to probe short as well as extremely long biopolymers, such as genomic DNA with high efficiency. Second, electrostatic focusing of charged biopolymers into the nanopore overcomes thermally driven diffusion, thus facilitating an extremely efficient end-threading (or capture) of DNA. Thus, nanopores can be used to detect minute DNA copy numbers, circumventing costly molecular amplification such as Polymerase Chain Reaction. A critical factor, which determines the ability of nanopore to distinguish fine properties within biopolymers, such as the location of bound small-molecules, proteins, or even the nucleic acid’s sequence, is the speed at which molecules are translocated through the pore. When the translocation speed is too high the electrical noise masks the desired signal, thus limiting the utility of the method. Here I will discuss new experimental results showing that modifying the surface charge inside the pore can effectively reduce the translocation speed through solid-state nanopores fabricated in thin silicon nitride membranes. I will present a simple physical model to account for these results.
9:12AM F47.0003 Advanced Solid State Nanopores Architectures — From Early Cancer Detection to Nano-electrochemistry. RASHID BASHIR, University of Illinois at Urbana-Champaign — Solid-state nanopores (ssNPs) are potentially low-cost and highly scalable technologies for rapid and reliable sequencing of the human diploid genome for under $1000. The ssNPs detect ionic current changes while molecules translocate through the pore. Several key challenges must be overcome in order for ssNPs to become ubiquitous in the fields of medical diagnostics and personalized healthcare. One major challenge is to reduce the speed at which DNA translocates through the nanopore from microseconds to milliseconds per nucleotide, enabling reliable identification of single nucleotides. The other major challenge is to improve the sensitivity of the approach requiring new sensing modalities and novel device architectures. In this paper, we review our recent efforts to (i) develop ssNPs for early cancer detection, (ii) to embed graphene electrodes in dielectric nanolaminates to form 3 and 4 terminal nanopore devices, and (iii) to demonstrate a nanopore based structure consisting of stacked graphene and Al$_2$O$_3$ dielectric layers to study electrochemical activity at graphene edges. The electrochemical signal corresponding to the atomically thin graphene layer could also provide a pathway to DNA sequencing.

1Supported by National Institute of Health.

9:48AM F47.0004 Nonlinear transport of fd virus particles through a solid-state nanopore. XINSHENG LING, Brown University — In this talk I will discuss our recent experiments on fd virus particles. The fd particles provide an interesting model system for testing the first-passage time theory of electro-field-driven translocation. We find that the distribution of translocation time can be understood using Schrodinger's first-passage time distribution function. The extracted diffusion constant for fd is significantly larger than the expected value from the Stokes-Einstein relation. We also find that the extracted translocation velocity is a nonlinear function of the electric field. We attribute the large effective diffusion constant to a Taylor dispersion effect in the electroosmotic flow profile in the nanopore and the nonlinear electrophoretic mobility to a Stötz-Wien effect.

10:24AM F47.0005 Nanopore Graphene-based Electronic Devices, MARIJA DRNDIC, Department of Physics and Astronomy, University of Pennsylvania — Graphene is an exceptional material for high-speed electronics, as well as a revolutionary membrane material due to its strength and atomic thickness. Nanopores in suspended graphene membranes are currently regarded as candidates for ultrafast DNA sequencing. When a single DNA molecule passes through a nanopore, it blocks the field-driven ions passing through the pore and is detected by measuring the ion current reduction. Due to the thin nature of graphene membranes and reduced pore resistance, we observe larger current signals than in the case of traditional solid-state nanopores. Use of graphene as a membrane material opens the door to a new class of nanopore devices in which electronic sensing and control are performed directly at the pore.

3We acknowledge support from NIH Grants R21HG004767 and R21HG006313.

Tuesday, March 19, 2013 11:15AM - 2:15PM —

11:15AM G1.00001 The “Higgs” amplitude mode at the two-dimensional superfluid-Mott insulator transition, IMMANUEL BLOCH, Max-Planck Institute of Quantum Optics — Spontaneous symmetry breaking plays a key role in our understanding of nature. In relativistic quantum field theory, a broken continuous symmetry leads to the emergence of two types of fundamental excitation: massless Nambu-Goldstone modes and a massive ‘Higgs’ amplitude mode. An excitation of Higgs type is of crucial importance in the standard model of elementary particle physics, and also appears as a fundamental collective mode in quantum many-body systems. Whether such a mode exists in low-dimensional systems as a resonance-like feature, or whether it becomes overdamped through coupling to Nambu-Goldstone modes, has been a subject of debate. Here we experimentally find and study a Higgs mode in a two-dimensional neutral superfluid close to a quantum phase transition to a Mott insulating phase. We unambiguously identify the mode by observing the expected reduction in frequency of the onset of spectral response when approaching the transition point. In this regime, our system is described by an effective relativistic field theory with a two-component quantum field, which constitutes a minimal model for spontaneous breaking of a continuous symmetry. Additionally, all microscopic parameters of our system are known from first principles and the resolution of our measurement allows us to detect excited states of the many-body system at the level of individual quasiparticles. This allows for an in-depth study of Higgs excitations that also addresses the consequences of the reduced dimensionality and confinement of the system. Our work constitutes a step towards exploring emergent relativistic models with ultracold atomic gases.

11:51AM G1.00002 Higgs Excitations in Dimer Antiferromagnets, CHRISTIAN RÜEGG, Paul Scherrer Institute — In three-dimensional dimer antiferromagnets a generic quantum critical point (QCP) separates a quantum-disordered ground state with a spin gap from a phase with long-range antiferromagnetic order and finite ordering temperature. While this QCP and related phases have been studied intensely in theoretical and numerical work using among other methods bond-operators and quantum Monte-Carlo, real materials in which they can be explored experimentally are rare. Structurally dimerised antiferromagnets are located on the disordered or ordered side of the QCP and application of pressure offers a way to control the ration of exchange interactions in the material across a critical value, so the compressibility and pressure dependence of the exchange are favourable. In TiCuCl$_3$ this QCP was realised for the first time and was studied in great detail by neutron scattering. These experiments provide unprecedented insights into the effects of thermal and quantum fluctuations, and of the elementary excitations near QCPs. A unique phenomena is the emergence of longitudinal modes near the QCP, which are the Higgs exceptions in dimer antiferromagnets proposed by S. Sachdev and coworkers. These Higgs exceptions follow precisely scaling predications and are involved in both the quantum and thermal melting of order in such systems.

12:27PM G1.00003 Higgs Bosons in Superconductors, CHANDRA VARMA, University of California, Riverside — Spurred by some strange experimental observations in some superconductors, the theory of a new collective mode in superconductors and how it can be experimentally found very easily under certain circumstances was proposed in 1981. It was called the “Amplitude Mode” to distinguish it from the “Phase Modes” which provide Josephson effects and which in homogeneous superconductors are coupled to charge density fluctuations and are at the energies of the plasmons. More generally [this mode is the amplitude mode of a particle-hole symmetric $U(1)$ field, i.e the model treated by Higgs and others in the1960’s whose generalization have played an important role in the standard model of particle physics. Recently the amplitude or Higgs mode for d-wave superconductors have also been discussed where its various cousins may also be found. I will tell the story of the above and why such modes were missed in the theory of superconductivity for so long and the applications of the ideas to modes for cold bosons and fermions in optical lattices. I will also comment, as a very interested outsider and an enthusiast, on the Higgs in particle physics being discovered at LHC from the point of view of the theory of superconductivity.

scanning tunneling microscopy. We have shown proximity-induced superconductivity up to a temperature of at least 80K – an order of magnitude higher than any previous observations. We have also demonstrated hybrid high-Tc-superconductor-semiconductor tunnel junctions combining Bi$_2$Sr$_2$CaCu$_3$O$_{8+δ}$ with graphite, with bulk semiconductors and with semiconductor quantum wells. Our approach provides a simple method of constructing high-T$_c$ tunnel junctions which can conceptually facilitate tunneling spectroscopy studies of novel materials.

11:51AM G2.00002 Topological superconductivity in IV-VI semiconductors, LIANG FU, Department of Physics, MIT — No abstract available.

12:27PM G2.00003 The Coexistence of Superconductivity and Topological Order in the Bi$_2$Se$_3$ Thin Films, JIN-FENG JIA, Department of Physics, Shanghai Jiao Tong University — No abstract available.

1:03PM G2.00004 Gate-tuned superconducting transport at the surface of a topological insulator, ALBERTO MORPURGO, Department of Condensed Matter Physics, Ecole de Physique — No abstract available.

1:39PM G2.00005 Majorana Bound States and Disclinations in Topological Crystalline Superconductors$^1$, JEFFREY TEO, University of Illinois at Urbana-Champaign — We prove a topological criterion for the existence of zero-energy Majorana bound-state on a disclination, a rotation symmetry breaking point defect, in topological crystalline superconductors (TCS). We first establish a complete topological classification of TCS using the Chern invariant and a few integral rotation invariants. By analytically and numerically studying disclinations, we algebraically deduce a $Z_2$-index that identifies the parity of the number of Majorana zero-modes at a disclination. Surprisingly, we also find weakly-protected Majorana fermions bound at the corners of superconductors with trivial Chern and weak invariants.

$^1$Simons Fellowship


11:15AM G8.00001 Towards a Rigorous Proof of Magnetism on the Edges of Graphene Nanoribbons$^1$, HAMED KARIMI, IAN AFFLECK, University of British Columbia — A zigzag edge of a graphene nanoribbon supports localized zero modes, ignoring interactions. Based mainly on field arguments and numerical approaches, it has been suggested that interactions can produce a large magnetic moment on the edges. By considering the Hubbard model in the weak coupling limit, $U \ll t$, for bearded as well as zigzag edges, we argue for such a magnetic state, based on Lieb’s theorem. Projecting the Hubbard interactions onto the flat edge band, we then prove that resulting 1 dimensional model has a fully polarized ferromagnetic ground state. We also study excitons and the effects of second neighbor hopping as well as a potential energy term acting on the magnetic state, based on Lieb’s theorem. Projecting the Hubbard interactions onto the flat edge band, we then prove that resulting 1 dimensional model has a fully polarized ferromagnetic ground state. We also study excitons and the effects of second neighbor hopping as well as a potential energy term acting on the magnetic state, based on Lieb’s theorem. Projecting the Hubbard interactions onto the flat edge band, we then prove that resulting 1 dimensional model has a fully polarized ferromagnetic ground state. We also study excitons and the effects of second neighbor hopping as well as a potential energy term acting on the magnetic state, based on Lieb’s theorem. Projecting the Hubbard interactions onto the flat edge band, we then prove that resulting 1 dimensional model has a fully polarized ferromagnetic ground state.

$^1$NSERC, CIFAR

11:27AM G8.00002 Quantum Monte Carlo study of edge-state magnetism on chiral graphene nanoribbons, MICHAEL GOLOR, Institute for Theoretical Solid State Physics, RWTH Aachen University, THOMAS C. LANG, Department of Physics, Boston University, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We investigate the edge-state magnetism of chiral graphene nanoribbons using projective quantum Monte Carlo (QMC) simulations and a self-consistent mean-field approximation of the Hubbard model. Previous QMC simulations support edge-state ferromagnetism in sufficiently wide zigzag terminated ribbons. We extended these calculations to include the class of chiral graphene nanoribbons and investigate the influence of chirality and ribbon width on spin-spin correlations. The static magnetic correlations are found to rapidly increase with the width of the ribbons for all chiralities, such that already for ribbons of moderate widths we observe a strong trend towards mean-field-type ferromagnetic correlations along the edges. We extract dynamical edge state signatures which can be used to detect edge-state magnetism by scanning tunneling microscopy.
11:39AM G8.00003 Strain induced magnetism in graphene, LUCIAN COVAČI, FRANCOIS PEETERS, University of Antwerp — Electron-electron interactions are believed not to be very important in graphene since the strength of the on-site Hubbard repulsion is moderate and the electron density of states is small near the Dirac points. Even so, graphene is believed to be in the proximity of a phase transition between a conducting state and an insulating one (antiferromagnetic or spin liquid). Finding a way to bring graphene across the transition is thus an important issue. We consider the effect of inhomogeneous strain from deformations induced by imperfections or steps in the substrate or from specific strain configurations that give almost constant pseudo-magnetic fields. We perform self-consistent mean field calculations for a tight-binding Hamiltonian where we consider only a repulsive on-site Hubbard term. We show that due to strain induced modifications of the kinetic energy, the staggered magnetization will become finite near regions where the strain is large. We also uncover that near deformations, spin-polarized states will appear, in a similar way the spin-polarized states appear at zig-zag edges of graphene nanoribbons.

11:51AM G8.00004 Friction, Adhesion, and Elasticity of Graphene Edges1, D. PATRICK HUNLEY, TYLER FLYNN, TOM DODSON, ABHISHEK SUNDARARAJAN, MATHIAS BOLAND, DOUGLAS STRACHAN, University of Kentucky, Department of Physics and Astronomy — Frictional, adhesive, and elastic characteristics of graphene edges are determined through lateral force microscopy. Measurements reveal a significant local frictional increase at exposed graphene edges, whereas a single overlapping layer of graphene removes this local frictional increase. Comparison of lateral force and atomic force microscopy measurements shows that local forces on the probe are successfully modeled with a vertical adhesion in the vicinity of the atomic-scale graphene steps. Lateral force microscopy performed with carefully maintained probes shows evidence of elastic straining of graphene edges which are consistent with out-of-plane bending of the edges.

1The work was supported in part by the NSF Grant DMR-0805136, the KY NSF EPSCoR award EPS-0814194, the UK Center for Advanced Materials (CAM), and a Research Support Grant from the UK Office of the Vice President for Research.

12:03PM G8.00005 Single point defect states in an armchair-graphene nanoribbon1, CHI-HSAUN CHIU, C.S. CHU, National Chiao Tung University, Taiwan — We investigate in detail the electronic states induced by a single or a few defects in an armchair-graphene nanoribbon (AGNR). A semi-analytical approach is developed for the Lippmann-Schwinger formulation within the tight-binding model. The dependences of the local density of states (LDOS) in the vicinity of the defects on both the defect locations and the nanoribbon widths are explored. In particular, the LDOS characteristics in the gapped or gapless AGNR will be discussed. Our results are compared with exact diagonalization approach. The effects of these point defect states on the transport property of the AGNR will also be presented.

1NSC 101-2112-M-009-014

12:15PM G8.00006 Ab initio electronic structure and transport studies of N4A-doped armchair and zigzag graphene nanoribbons, JONATHAN OWENS, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts Amherst, VINCENT MEUNIER, Rensselaer Polytechnic Institute — Recent work by Lu, et al. (Nature Scientific Reports, DOI: 10.1038) on large sheets of nitrogen-doped graphene, determined that a highly predominant amount of nitrogen dopants (80 %) form in pairs on the same sub-lattice. Graphene nanoribbons, which are essentially narrow strips of graphene, have a natural band gap and tunable electronic properties, making them a promising candidate for scalable nanoelectronics. In this work we explore various electronic structural (density of states, local density of states, and STM images) and transport properties of armchair (aAGNR) and zigzag (zAGNR) graphene nanoribbons under different orientations of the N4A dopants with respect to the ribbon growth direction. For all configurations of zAGNRs and aAGNRs, we see a substantial decrease in conductance due to the dopants, as well as spatially localized states opening around the dopant sites. Most notably, however, we observe the emergence of a new stable spin configuration, wherein the spin-up spin-down polarizations of the edges in zAGNRs (denoted the antiferromagnetic state) flip near the doping sites, while being in the normal zAGNR AFM ground state away from the dopants.

12:27PM G8.00007 Atypical structural, electronic, and thermoelectric properties of assembled graphene nanoribbons1, LIANGBO LIANG, VINCENT MEUNIER, Rensselaer Polytechnic Institute, EDUARDO CRUZ-SILVA, University of Massachusetts, EDUARDO GIRÃO, Universidade Federal do Piauí — Highly ordered assembly of individual graphene nanoribbons (GNRs) into graphene nanowiggles (GNWs) has been recently demonstrated using a surface-assisted bottom-up chemical approach. GNWs are characterized by a periodic repetition of wiggle-like junctions where armchair- or zigzag-edged GNRs sectors alternate. We employed both density functional theory (DFT) and Tight-Binding+U to demonstrate their versatile electronic properties [Girão et al, Phys. Rev. Lett. 107 (2011)]. The coexistence of parallel and oblique sectors leads GNWs to offer a broader set of geometrical parameters to fine tune the electronic band gap from 0.0 eV to 1.7 eV than GNRs [Girão et al, Phys. Rev. B 85 (2012)]. Also, the presence of wiggle-like edges dramatically degrades thermal conductance but retains excellent electronic conduction, resulting in significant enhancement of the thermoelectric performance [Liang et al, Phys. Rev. B 86 (2012)]. Finally, many-electron GW calculations show quasiparticle band gaps of GNWs generally more than twice of their DFT band gaps, reaching 3.7 eV. Furthermore, the gold substrate where GNWs are synthesized is found to lead to band gap reduction owing to substrate polarization effect, consistent with experiments [Liang et al, Phys. Rev. B 86 (2012)].

1Liangbo Liang is supported by New York State under NYSTAR contract C080117. All the calculations were performed on resources from the Computational Center for Nanotechnology Innovation at Rensselaer Polytechnic Institute.

12:39PM G8.00008 Quasiparticle Band Gap modulation in Graphene Nanoribbons Supported on Weakly interacting Surfaces, XUEPING JIANG, Rensselaer Polytechnic Institute, NEERAV KHARCHE, Brookhaven National Laboratory, PAUL KOHL, Georgia Institute of Technology, TIMOTHY BOYKIN, The University of Alabama in Huntsville, GERHARD KLIMECK, Purdue University, MATHIEU LUISIER, Integrated Systems Laboratory, PULICKEL AJAYAN, Rice University, SAROJ NAYAK, Rensselaer Polytechnic Institute — Low dimensional nanostructures such as graphene nanoribbons (GNRs) and hexagonal boron nitride (hBN) have been successfully synthesized in experiments and attract a lot of attention recently. The strong electron-electron interactions due to quantum confinement could alter band gaps of nanostructures, which has been studied thoroughly for GNRs. Band gaps could also be changed by the effect of dielectric screening arising from the surrounding materials such as the substrate. However, this effect has not been thoroughly investigated for GNRs. In contrast, almost all the experiments GNRs are deposited on different dielectric substrates leaving a gap between theoretical estimates and experimental measurements. The effect of dielectric screening cannot be captured in an effective single particle theory such as the density functional theory (DFT) and the many-body approaches such as GW are required. We show the band gaps of the free standing GNRs are reduced as much as 1 eV in spite of weak van der Waals interactions between the GNR and the underlying substrate. This non-local effect can be explained by a semi-classical image charge model and such understanding is critical to the band gap engineering of graphene based devices.

12:51PM G8.00009 ABSTRACT WITHDRAWN —
non-trivial topological insulators and superconductors support gapless modes localized at the boundary. When a boundary is introduced, which is reflected into itself, these symmetry operators and the reflection symmetry operator. By using the construction of bulk Dirac Hamiltonians, we provide the complete classification, which logical invariants. Furthermore, those topological invariants are also determined by commutation or anticommutation relations between the discrete non-spatial $\mathbb{Z}$ and $\mathbb{Z}'$ valley.

1:15PM G8.00011 Evidence for edge state photoluminescence in graphene quantum dots, KIRAN LINGAM, RAMAKRISHNA PODILA, Department of Physics, Clemson University, SC 29634, HAIJUN QIAN, Electron Microscope facility, Clemson research park, Department of Physics, Anderson, SC USA 29625., STEVE SERKIZ, Savannah River National Laboratory, Aiken, SC USA 29808, APPARAO M. RAO, Department of Physics and Astronomy, Clemson University, Clemson, SC 29634 — For a practical realization of graphene-based logic devices, opening of a band gap in graphene is crucial and has proved challenging. To this end, several synthesis techniques including unzipping of carbon nanotubes, chemical vapor deposition and other bottom-up fabrication techniques have been pursued for the bulk production of graphene nanoribbons (GNRs) and graphene quantum dots (GQDs). However, only a limited progress has been made towards a fundamental understanding of the electronic and optical properties of GQDs. In particular, the origin of strong photoluminescence (PL) in GQDs, which has been attributed to the presence of emissive surface traps and/or the edge states in GQD, remains inconclusive to date. Here, we experimentally show that the PL is independent of the functional groups attached to the GQDs. Following a series of annealing experiments, we further show that the PL in GQDs originates from the edge states, and an edge-passivation subsequent to synthesis quenches PL. These results are consistent with comparative studies on other carbon nanostructures such as GNRs and carbon nano-onions.

1:27PM G8.00012 Spontaneous Gap Formation in an Uniaxially Strained Graphene, ANAND SHARMA, VALERI N. KOTOV, University of Vermont, ANTONIO H. CASTRO NETO, National University of Singapore — We study the condition of spontaneous gap generation due to Coulomb interaction between anisotropic Dirac fermions in an uniaxially strained graphene. The gap equation is realized as a self-consistent solution for the self-energy i.e., Dyson-Schwinger equation, with static Random Phase Approximation. The mass gap not only depends on the momentum due to long-range nature of the interaction but also on the anisotropy due to uniaxial strain. Using standard numerical analysis we solve the integral equation on a finite grid. We evaluate the mass gap as a function of dimensionless coupling constant for different values of anisotropy parameter and obtain the critical coupling at which the gap becomes non-zero. Our study indicates that with an increase in uniaxial strain in graphene, the critical coupling decreases which is in agreement with our perturbative renormalization group analysis.

1:39PM G8.00013 Band Gap Opening in Periodically Modified Graphene, MARC DVORAK, ZHIGANG WU, Department of Physics, Colorado School of Mines — The gapless electronic structure of graphene must be modified to allow a meaningful on-and-off ratio for use in field-effect transistors. Many attempts to create semiconducting graphene have been made; among them, application of periodic structural modifications, such as patterned defects or nanoscale perforation creating a graphene nanomesh, is particularly promising. Extensive theoretical efforts have been spent to investigate such graphene structures, but the precise role of periodic perturbation on band gap opening remains unclear. Here, we show analytically that band gap opening in graphene under a periodic perturbation can be accurately predicted by mapping the perturbative reciprocal lattice vectors onto Dirac points. The modified graphene alternates between a semi-metal and a semiconductor with 8/9 gapless and 1/9 semiconducting. Furthermore, semiconducting modified graphene can be mapped to exactly two corresponding semimetallic carbon nanotubes or graphene nanoribbons. These predictions reveal the fundamental physics of band gap opening in periodically defected graphene and are in excellent agreement with previous and present first-principles results for graphene nanomeshes.

1:51PM G8.00014 Gauge fields for rippled graphene membranes under central load, SALVADOR BARRAZA-LOPEZ, JAMES V. SLOAN, University of Arkansas, ALEJANDRO A. PACHECO, Universidad del Norte, CEDRIC M. HORVATH, University of Arkansas, ZHENFENG WANG, University of Utah — Gauge fields on graphene are invariably expressed in the language of continuum elasticity. Following an approach where the atomic positions play the preponderant role, a model of strain on graphene was developed where all relevant quantities —including gauge fields— are directly expressed in terms of atomic displacements only. Suspended, rippled graphene membranes under central load by a sharp object were studied using this approach. The effects from both the pseudo-magnetic field and the deformation potential were included in calculations of the electron density at different spatial locations (the deformation potential acts as an on-site potential energy). The deformation potential —neglected without proper justification in many published works— appears to modify the electronic spectrum dramatically in a qualitative way. Discussion of experiments relevant to the model will also be given.

2:03PM G8.00015 Theory of electromechanical coupling in dynamical graphene, MIRCEA TRIF, PRAKASH UPADHYAYA, YAROSLAV TSERKOVNYAK, University of California, Los Angeles — We study the coupling between mechanical motion and Dirac electrons in a dynamical sheet of graphene. We show that this coupling can be understood in terms of an effective gauge field acting on the electrons, which has two contributions: quasistatic and purely dynamic of the Berry-phase origin. As is well known, the static gauge potential is odd in the $K$ and $K'$ valley index, while we find the dynamic coupling to be even. In particular, the mechanical fluctuations can thus mediate an indirect coupling between charge and valley degrees of freedom.

Tuesday, March 19, 2013 11:15AM - 2:15PM –
Session G13 DCMP: Topological Insulators: Theory II 315 - Roman Lutchyn, Microsoft Station Q

11:15AM G13.00001 The strong index classification of reflection symmetric topological insulators and superconductors, CHING-KAI CHIU, University of Illinois at Urbana-Champaign, HONG YAO, Institute for Advanced Study, Tsinghua University, SHINSEI RYU, University of Illinois at Urbana-Champaign — We discuss the topological invariants of topological insulators and superconductors protected by spatial reflection symmetry in any spatial dimensions. In the presence of both (non-spatial) discrete symmetries in the Altland-Zirnbauer classification and reflection symmetry, we introduce two new topological invariants: a mirror integral number and a binary integral number, which is determined by the larger one of the $Z$ number and mirror integral number. We claim that the topological states are characterized by one of $0'$, $Z_2$, $Z$, and the two new topological invariants. Furthermore, those topological invariants are also determined by commutation or anticommutation relations between the discrete non-spatial symmetry operators and the reflection symmetry operator. By using the construction of bulk Dirac Hamiltonians, we provide the complete classification, which still has the same dimensional periodicities with the original Altland-Zirnbauer classification. When a boundary is introduced, which is reflected into itself, these non-trivial topological insulators and superconductors support gapless modes localized at the boundary.
11:27AM G13.00002 Symmetry protected topological phases from decorated domain walls. XIÉ CHEN, YUAN-MING LU, ASHVIN VISHWANATH, University of California, Berkeley — Symmetry protected topological phases are gapped quantum phases with gapless edge excitations protected by certain symmetries of the system. While SPT phases in lower dimensions (especially 1D) are relatively well understood, less is known about higher dimensional (2D and 3D) SPT phases including what their edge excitations are like and how to detect them. In this work, we present a construction of d dimensional SPT phases with Zd × G symmetry by decorating the Zd domain walls in the d dimensional bulk with d−1 dimensional SPT phases with G symmetry. Such a construction not only provides a simple understanding of higher dimensional SPT phases starting from lower dimensional ones, but also reveals a special topological feature of such SPT phases. That is, on the boundary of the system, the domain wall end points/loops carry gapless edge states of the d−1 dimensional SPT phase with G symmetry. We discuss in detail a 2D SPT phase with Z2 × Z2 symmetry and a 3D SPT phase with Z2 × Z2 symmetry, which illustrate a more general hierarchical structure of SPT phases related to the cup product of group cohomology.

11:39AM G13.00003 Lattice model for the surface states of a topological insulator. MARCEL FRANZ, DOMINIC MARCHAND, University of British Columbia — A surface of a strong topological insulator (STI) is characterized by an odd number of linearly dispersing gapless electronic surface states. It is well known that such a surface cannot be described by an effective two-dimensional lattice model (without breaking the time-reversal-symmetry), which often hampers theoretical efforts to quantitatively understand some of the properties of such surfaces, including the effect of strong disorder, interactions and various symmetry-breaking instabilities. Here we describe a lattice model that can be used to describe a pair of STI surfaces and has an odd number of Dirac fermion states with wavefunctions localized on each surface. The Hamiltonian consists of two planar tight-binding models with spin-orbit coupling, representing the two surfaces, weakly coupled to each other by terms that remove the redundant Dirac points from the low-energy spectrum. The utility of this model is illustrated by studying the magnetic and exciton instabilities of the STI surface state driven by short-range repulsive interactions.

11:51AM G13.00004 3D Dirac Electrons on a Cubic Lattice with Noncoplanar Multiple-Q Order. SATORU HAYAMI, TAKAHIRO MISAWA, YOUHEI YAMAJI, YUKITOSHI MOTOME, Dept. of Appl. Phys., Univ. of Tokyo — Noncoplanar multiple-Q orders often lead to new low-energy excitations and/or topologically nontrivial states. In particular, triple-Q orders have attracted much interest due to the emergence of topological (Chern) insulators and associated anomalous quantum Hall effects. In the present study, we explore the possibility of such multiple-Q orderings on a simple cubic lattice and their influence on the electronic structure. We find that a four-sublattice triple-Q magnetic order significantly affects the low-energy single-particle spectrum which is described by the three-dimensional massless Dirac electrons. In order to clarify the stability of such noncoplanar magnetic order in microscopic models, we investigate the ground-state phase diagram of an extended periodic Anderson model on a cubic lattice by mean-field approximation. As a result, we find that the triple-Q phase appears in a wide range of parameters at 3/2 filling. The 3D Dirac nature gives rise to a characteristic gapless surface state. We discuss the bulk and surface electronic states in details. We also discuss a possible realization of a topological insulating phase by opening an energy gap in the triple-Q phase.

12:03PM G13.00005 Fermi loop in interface states and surface flat bands in diamond lattice models. RYUJI TAKAHASHI, SHUICHI MURAKAMI, Tokyo Institute of Technology — Previously we have shown the gapless interface states between two topological insulators with different chiralities by means of the mirror Chern number [1]. In this presentation we use the Fu-Kane-Mele tight-binding model on diamond lattice with the spin-orbit interaction, and calculate their gapless interface states. We find that when the particle-hole symmetry is imposed in the whole system the Fermi surface of the gapless states becomes a loop in the interface Brillouin zone. We show how to characterize the existence of such Fermi loop in terms of topology. Next we report flat band states in the surface of the diamond lattice model with anisotropic hopping integrals without the spin-orbit interaction. When anisotropy is not so strong, the surface flat band exits in some part of the Brillouin zone. Moreover when the anisotropy becomes sufficiently strong, the surface flat band covers the whole surface Brillouin zone. [1] R. Takahashi, S. Murakami, Phys. Rev. Lett. 107,166805 (2011).

12:15PM G13.00006 Effect of electron-phonon interaction on the velocity renormalization of the surface state of 3D topological insulator. QIUI LI, SANKAR DAS SARMA, University of Maryland-College Park — Explicitly taking into account of electron-phonon interaction, we consider the velocity renormalization of the surface state of 3D topological insulator. The velocity renormalization is shown to be strongly dependent on the carrier density of the system. We compare our theoretical calculation to recent experimental data. We further consider the correction to the compressibility arising from electron-phonon coupling, and discuss its implication in experiments.

3This work is supported by ONR-MURI, LPS- CMTC, and NRI-SWAN.

12:27PM G13.00007 ABSTRACT WITHDRAWN –

12:39PM G13.00008 2D compressibility of surface states on 3D topological insulators. DAVID ABERGEL, SANKAR DAS SARMA, University of Maryland — We develop a theory for the compressibility of the surface states of 3D topological insulators and propose that surface probes of the compressibility via scanning single electron transistor microscopy will be a straightforward way to access the topological states without interference from the bulk states. We describe the single-particle nature of the surface states taking into account an accurate Hamiltonian for the bands and then include the contribution from electron-electron interactions and discuss the implications of the ultra-violet cutoff, including the universality of the exchange contribution when expressed in dimensionless units. We also compare the theory with experimentally obtained dµ/dn as extracted from angle-resolved photoemission spectroscopy measurements. Finally, we point out that interaction-driven renormalization of the Fermi velocity may be discernible via this technique.

3We thank the US-ONR for support.

12:51PM G13.00009 Dislocations in topological phases of matter and their topological terms. AKIHIRO TANAKA, TORU KIKUCHI, AKIHIRO TANAKA, National Institute for Materials Science — When dislocations are present in topological insulators/superconductors and their variants, they are known to endow subgap boundstates. We revisit their physics from the viewpoint of topological field theories, discussing several issues among which are 1) the interplay of the Nieh-Yan torsional invariant with other topological terms, 2) possible appearance of Nieh-Yan-like terms in nonlinear sigma models of competing orders, 3) the subtle controversy on the absence/existence of Callan-Harvey-like anomaly-inflow in the dual formulation.

1:03PM G13.00010 Massless Axions: the Callan-Harvey effect revisited. TORU KIKUCHI, AKIHIRO TANAKA, National Institute for Materials Science — Axion-like degrees of freedom appear in the low energy physics of various condensed matter systems, which range from quantum spin systems and superconductors to topological insulators and their variants. When topological defects such as domain walls and vortices are formed by the axion fields, their responses to external fields are dominated by the current inflow from the surrounding bulk (Callan-Harvey effect). However, a dual reformulation due to Izquierdo-Townsend is known to present a controversy regarding the existence of this inflow in the case when axions are massless, and can have important consequences. We revisit this problem and discuss its possible relevance to condensed matters.
1:15PM G13.00011 Semi-metal-insulator transition at the surface of a topological insulator with in-plane magnetization\(^1\). FLAVIO NOGUEIRA, ILYA EREMIN, Theoretische Physik III, Ruhr-Universitaet Bochum — We discuss the role of quantum fluctuations when the surface of a topological insulator (TI) is used as a substrate for a layered ferromagnetic (FM) material. As is well known, an out-of-plane magnetization gaps the surface states and modifies the Landau-Lifshitz-Gilbert equation in an essential way, due to the topological magnetoelectric effect. On the other hand, for the case of in-plane magnetization the surface states are gapless. We show that quantum fluctuations may modify this picture if the exchange interaction between the TI and the FM is sufficiently large. Indeed, we will show that a gap is dynamically generated in this case, turning in this way the semi-metallic state into an insulating one. Another situation of interest where a similar mechanism applies involves the Coulomb interaction between the fermions at the interface between the TI and the FM. The interplay between the magnetization dynamics and the Coulomb interaction is discussed in detail.

\(^1\)Work supported by SFB TR 12 of the German Research Council (DFG)

1:27PM G13.00012 Theory of a quantum critical phenomenon in a topological insulator: (3+1)-dimensional quantum electrodynamics in solids. HIROKI ISOBE, NAOTO NAGAOSA, Department of Applied Physics, University of Tokyo — We study theoretically the quantum critical phenomenon of the phase transition between the trivial insulator and the topological insulator in (3+1) dimensions, which is described by a Dirac fermion coupled to the electromagnetic field. The intriguing result is the recovery of the Lorentz invariance in the infrared limit, and the electrons in solids obey the conventional QED. In detail, the renormalization group (RG) equations for the running coupling constant \(\alpha\), the speed of light \(c\), and electron \(\nu\) are derived by using perturbative RG method to one-loop level. The almost exact analytic solutions to these RG equations are obtained to reveal that (i) \(c\) and \(\nu\) approach to the common value with combination \(c^2\nu\) being almost unrenormalized, (ii) the RG flow of \(\alpha\) is the same as that of usual QED with \(c^2\nu\) being replaced by \(\nu^2\) and, (iii) there are two crossover momentum/energy scales separating three regions of different scaling behaviors. The dielectric and magnetic susceptibilities, angle-resolved photoemission spectroscopy (ARPES), and the behavior of the gap are discussed from this viewpoint. Reference: H. Isobe and N. Nagaosa, Phys. Rev. B 86, 165127 (2012).

1:39PM G13.00013 Nonequilibrium Transport Through a Gate-Controlled Barrier on the Quantum Spin Hall Edge\(^1\). RONI ILAN, University of California, Berkeley, JEROME CAYSSOL, Max-Planck-Institut für Physik Komplexer Systeme, Dresden, Germany and LOMA (UMR-5798), CNRS and University Bordeaux, Talence, France, JENS BARDARSON, JOEL MOORE, University of California, Berkeley and the Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA — The quantum spin Hall insulator is characterized by the presence of gapless helical edge states where the spin of the charge carriers is locked to their direction of motion. In order to probe the properties of the edge modes, we propose a design of a tunable quantum impurity realized by a local gate under an external magnetic field. Using the integrability of the impurity model, the conductance is computed for arbitrary interactions, temperatures and voltages, including the effect of Fermi liquid leads. The result can be used to infer the strength of interactions from transport experiments.

\(^1\)The authors acknowledge support from AFSOR MURI (RI), the ONR EU/FP7 under contract TEMSOCC and from ANR through project 2010-BLANC-041902 (ISOTOP) (JC), the Nanostructured Thermoelectrics program of LBNL (JHB), and DARPA (JEM).

1:51PM G13.00014 Magnetic translation algebra with or without magnetic field. CHRISTOPHER MUDRY, Paul Scherrer Institute, CLAUDIO CHAMON, Boston University — The magnetic translation algebra plays an important role in the quantum Hall effect. Murthy and Shankar have shown how to realize this algebra using fermionic bilinears defined on a two-dimensional square lattice. We show that, in any dimension \(d\), it is always possible to close the magnetic translation algebra using fermionic bilinears, be it in the continuum or on the lattice. We also show that these generators are complete in even, but not odd, dimensions, in the sense that any fermionic Hamiltonian in even dimensions that conserves particle number can be represented in terms of the generators of this algebra, whether or not translation-invariance is broken. As an example, we reproduce the \(s\)-sum rule of interacting electrons at vanishing magnetic field using this representation. We also show that interactions can significantly change the bare bandwidth of lattice Hamiltonians when represented in terms of the generators of the magnetic translation algebra.

2:03PM G13.00015 Spin-orbital Texture in Topological Insulators. CHAOXING LIU, Department of Physics, Pennsylvania State University, HAIJUN ZHANG, SHOU-CHENG ZHANG, Department of Physics, McCullough Building, Stanford University — Relativistic spin-orbit coupling plays an essential role in the field of topological insulators and quantum spintronics. It gives rise to the topological non-trivial band structure and enables electric manipulation of the spin degree of freedom. Because of the spin-orbit coupling, rich spin-orbital coupled textures can exist both in momentum and in real space. For three dimensional topological insulators in the Bi2Se3 family, topological surface states with pz orbitals have a left-handed spin texture for the upper Dirac cone and a right-handed spin texture for the lower Dirac cone. In this work, we predict a new form of the spin-orbital texture associated with the pz and the py orbitals. For the upper Dirac cone, a left-handed (right-handed) spin texture is coupled to the “radial” ("tangential") orbital textures, whereas for the lower Dirac cone, the coupling of spin and orbital textures is the exact opposite. A spin-resolved and photon polarized angle-resolved photoemission spectroscopy experiment is proposed to observe this novel spin-orbital texture.

Tuesday, March 19, 2013 11:15AM - 1:51PM – Session G18 DCMP: Two Dimensional Topological Insulators II: Graphene and Related Materials 320 - Shaffique Adam, Yale University

11:15AM G18.00001 Is graphene on the edge of being a topological insulator? JOSÉ GONZALEZ, Instituto de Estructura de la Materia (CSIC), Madrid, Spain — We show that, at sufficiently large strength of the long-range Coulomb interaction, a mass term breaking parity (so-called Haldane mass) is dynamically generated in the many-body theory of Dirac fermions describing the graphene layer. While the tendency towards a conventional excitonic instability is stronger than for the dynamical breakdown of parity at spatial dimension \(D\) greater than 2, we find that the situation is reversed at \(D = 2\). The need to regularize the many-body theory in a gauge-invariant manner (taking the limit \(D = 2\) from below) is what leads to the dominance of the parity-breaking pattern in graphene. We compute the critical coupling for the generation of a parity-breaking mass from the finite radius of convergence of the ladder series supplemented with electron self-energy corrections, finding a value quite close to the effective interaction strength for graphene in vacuum after including Fermi velocity renormalization and static RPA screening of the Coulomb interaction.

11:27AM G18.00002 ABSTRACT WITHDRAWN
Here, we argue that by growing such designer lattices on metals or semiconductors with strong spin-orbit interactions, one can realize an analog of graphene. Honeycomb lattices with graphene-like "Dirac" band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. However, the insulating gap is immeasurably small owing to the weakness of spin-orbit interactions in graphene. A recent experiment demonstrated that designer lattices on metals or semiconductors with strong spin-orbit interactions can result in various topological phases. However, at certain adatom coversages, the intervalley scattering renders the system a trivial insulator. Using both finite-size scaling method and transport calculation, we showed that when the adatom distribution becomes random, the intervalley scattering is weakened, but other quantities (e.g. spin-orbit couplings, and exchange field) are not affected. This finding points out that the topological states are graphene-favored ground states in the presence of randomly distributed adatoms.


Bound States of Conical Singularities in Graphene-Based Topological Insulators. ANDREAS RUEGG, UC Berkeley, CHUNGWEI LIN, University of Texas at Austin — We investigate the electronic structure induced by wedge-disclinations (conical singularities) in a honeycomb lattice model realizing Chern numbers $\gamma = \pm 1$. We establish a correspondence between the bound state of (i) an isolated $\Phi_0/2$-flux, (ii) an isolated pentagon $(n = 1)$ or heptagon $(n = -1)$ defect with an external flux of magnitude $n\Phi_0/4$ through the center, and (iii) an isolated square or octagon defect without external flux, $\Phi_0 = h/e$ is the flux quantum. Due to the above correspondence, the existence of isolated electronic states bound to the disclinations is robust against various perturbations. These results are also generalized to graphene-based time-reversal invariant topological insulators.

Topological kink states at the tilt boundary in gapped multi-layer graphene. EUN-AH KIM, ABOLHASSAN VAEZI, Cornell University, YUFENG LIANG, Washington University, DARRYL NGAI, Cornell University, LI YANG, Washington University — Search for new realization of symmetry protected topological states with protected edge states is an active area of research. We show that a tilt boundary in gapped multi-layer graphene supports topologically protected gapless kink states. We investigate such kink states from two perspectives: the microscopic perspective of tight-binding model and an ab-initio calculation on bilayer, and the perspective of symmetry protected topological (SPT) states for general multi-layer. We show that the bilayer tilt boundary supports gapless kink states that are undetected by strain concentrated at the boundary. Further, we establish the kink state of (i) an isolated conical singularity of edge state protected by $Z_2$-type SPT, protected by $T$ and two $U(1)$ symmetries in the absence of inter-valley mixing. Recent observations of such boundaries in multi-layer samples suggest that transport through these topological kink states might explain the long standing puzzle of sub-gap conductance. We discuss possible topological phase transitions upon breaking subset of symmetries from SPT perspective.

Topological Proximity Effects in Graphene Nanoribbon Heterostructures. GUFEFENG ZHANG, Univ. of Sci. & Tech. of China, Fudan University, XIAOGUANG LI, Fudan University, Univ. of Sci. & Tech. of China, GUANGFEN WU, Univ. of Sci. & Tech. of China, Shenzhen Institutes of Advanced Technology, JIE WANG, DIMITRIE CULCER, Univ. of Sci. & Tech. of China, EFTHIMIOS KAXIRAS, Harvard University, ZHENYU ZHANG, Univ. of Sci. & Tech. of China, Harvard University — Topological insulators (TI) are bulk insulators that possess robust chiral conducting states along their interfaces with normal insulators. A tremendous research effort has recently been devoted to TI-based heterostructures, in which conventional proximity effects give rise to many exotic physical phenomena. Here we establish the potential existence of "topological proximity effect" at the interface of a topological graphene nanoribbon (GNR) and a normal GNR. Specifically, we show that the location of the topological edge states exhibits versatile tunability as a function of the interface orientation, as well as the strengths of the interface coupling and spin-orbit coupling in the normal GNR. For zigzag and bearded GNRs, the topological edge state can be tuned to be either at the interface or outer edge of the normal ribbon. For armchair GNR, the potential location of the topological edge state can be further enriched to be at the edge of or within the normal ribbon, at the interface, or diving into the topological GNR. We also discuss possible experimental realization of the predicted topological proximity effects, which may pave the way for integrating the salient functionality of TI and graphene in future device applications.

Designer quantum spin Hall phase transition in molecular graphene. POUYAN GHAEMI, University of Illinois at Urbana-Champaign, SARANG GOPALAKRISHNAN, University of Illinois at Urbana-Champaign, Harvard University, TAYLOR HUGHES, University of Illinois at Urbana-Champaign — Graphene was the first material predicted to be a time-reversal-invariant topological insulator; however, the insulating gap is immeasurably small owing to the weakness of spin-orbit interactions in graphene. A recent experiment demonstrated that designer honeycomb lattices with graphene-like “Dirac” band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. Here, we argue that by growing such designer lattices on metals or semiconductors with strong spin-orbit interactions, one can realize an analog of graphene. Honeycomb lattices with graphene-like "Dirac" band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. However, the insulating gap is immeasurably small owing to the weakness of spin-orbit interactions in graphene. A recent experiment demonstrated that designer honeycomb lattices with graphene-like “Dirac” band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. Here, we argue that by growing such designer lattices on metals or semiconductors with strong spin-orbit interactions, one can realize an analog of graphene. Honeycomb lattices with graphene-like "Dirac" band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. However, the insulating gap is immeasurably small owing to the weakness of spin-orbit interactions in graphene. A recent experiment demonstrated that designer honeycomb lattices with graphene-like “Dirac” band structures can be engineered by depositing a regular array of carbon monoxide atoms on a metallic substrate. Here, we argue that by growing such designer lattices on metals or semiconductors with strong spin-orbit interactions, one ca...
Semiconductor devices.

Effective low-energy $k$-Hamiltonian, we show that the intrinsic polarization of materials can be utilized to simultaneously reduce the energy gap and enhance the SOI, driving the system to a TI state. The proposed system consists of ultrathin InN layers embedded into GaN, a layer structure that is experimentally achievable. We found that the TI transition happens at GaN/InN/GaN quantum well with 3 to 4 InN atomic layers. Since polarization fields occur in many materials, a similar mechanism may apply to other systems as well. Our approach may pave the way toward integrating controllable TIs with conventional Ge lattices or by strong Ge and p orbital hybridization in an ordered surface alloy $Ag_2 Ge$. 

We thank grants: DOE-BES (Grant No. DE-SC0001099); NSF- DGE0801627; MRSEC program (NSF- DMR11121053); NSF DMR-0906805; China 973-program 2011CB922204 and China NSF 10934007.

Financial support from EU project 2D Nanolattices.

1:03PM G18.00010 Surface band topology of Ge on Ag(111)¹, ATHANASIOS DIMOULAS, EVANGELOS GOLIAS, EVANGELIA XENOGIANNOPOLLOU, DIMITRA TSOUTSOU, POLIXRONIS TSIPAS, SIGAIVA GIAMINI, NCSR DEMOKRITOS, Athens, Greece — While compelling evidence for silicene on Ag (111) has been recently published [1], the existence of germanene remains elusive. We have performed MBE growth of (sub) monolayer Ge on single crystal Ag (111) substrates, supported by DFT calculations, with the aim to obtain germanene. RHEED data indicate a $(\sqrt{3} \times \sqrt{3}) R30^\circ$ superstructure, while in-situ ARPES reveals a rich surface band structure consisting of linearly, highly dispersive cone-like features with hexagonal and snow-flake warping clearly imaged in the constant energy contour plots $k_x-k_y$. Unlike the case of graphene-like 2D crystals where Dirac cones are expected at the K-points, here the cone-like features appear at the center (I' points) of the surface Brillouin zone similar to what is observed in topological insulators. This suggests the possibility to witness a non-trivial surface band topology triggered by intrinsic spin-orbit coupling as predicted [2] for 2D honeycomb Ge lattices or by strong Ge and p orbital hybridization in an ordered surface alloy $Ag_2 Ge$.

We found that the TI transition happens at GaN/InN/GaN quantum well with 3 to 4 InN atomic layers. Since polarization fields occur in many materials, a similar mechanism may apply to other systems as well. Our approach may pave the way toward integrating controllable TIs with conventional semiconductor devices.

1:15PM G18.00011 Polarization-driven topological insulator transition in a GaN/InN/GaN quantum well¹, M.S. MIAO, Q. YAN, C.G. VAN DE WALLE, Materials department and materials Research Lab, University of California Santa Barbara, California 93106-5050, USA, W.K. LOU, L.L. LI, K. CHANG, SKLSM, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, P. R. China — Topological insulators (TIs), a new state of quantum matter, have recently attracted significant attention, both for their fundamental research interest and for their potential device applications. Although many families of TI materials have been found, the realization of TI in conventional semiconductors remains elusive, mainly due to their sizable gaps and small spin-orbit interactions (SOI). Based on advanced first-principles calculations combined with an effective low-energy $k$-Hamiltonian, we show that the intrinsic polarization of materials can be utilized to simultaneously reduce the energy gap and enhance the SOI, driving the system to a TI state. The proposed system consists of ultrathin InN layers embedded into GaN, a layer structure that is experimentally achievable. We found that the TI transition happens at GaN/InN/GaN quantum well with 3 to 4 InN atomic layers. Since polarization fields occur in many materials, a similar mechanism may apply to other systems as well. Our approach may pave the way toward integrating controllable TIs with conventional semiconductor devices.

1:27PM G18.00012 Electronic Structure calculations in a 2D SixGe1-x alloy under an applied electric field¹, JOSE EDUARDO PADILHA, University of S˜ ao Paulo, RENATO B. PONTES, Federal University of Goiás, LEANDRO SEIXAS, ANTÔNIO J.R. DA SILVA, ADALBERTO FAZZIO, University of S˜ ao Paulo — The recent advances and promises in nanoscience and nanotechnology have been focused on hexagonal materials, mainly on carbon-based nanostructures. Recently, new candidates have been raised, where the greatest efforts are devoted to a new hexagonal and buckled material made of silicon, named Silicene. This new material presents an energy gap due to spin-orbit interaction of approximately 1.5 meV, where the measurement of quantum spin Hall effect (QSHE) can be made experimentally. Some investigations also show that the QSHE in 2D low-buckled hexagonal structures of germanium is present. Since the similarities, and at the same time the differences, between Si and Ge, over the years, have motivated a lot of investigations in these materials. In this work we performed systematic investigations on the electronic structure and band topology in both ordered and disordered SixGe1-x alloys monolayer with 2D honeycomb geometry by first-principles calculations. We show that an applied electric field can tune the gap size for both alloys. However, as a function of electric field, the disordered alloy presents a W-shaped behavior, similarly to the pure Si or Ge, whereas for the ordered alloy a V-shaped behavior is observed.

This work is supported by CAPES, CNPq and FAPESP.

1:39PM G18.00013 Reflection from surface step defect in topological insulator nanofilm, THAKSHILA M. HERATH, Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA, PRABATH HEWAGEEGANA, Department of Physics, University of Kelaniya, Kelaniya 11600, Sri Lanka, VADIM M. APALKOV, Department of Physics and Astronomy, Georgia State University, Atlanta, GA 30303, USA — Ultrathin topological insulator nanofilm with a step-like defect, which divides two regions of nanofilm with different thicknesses, is considered. Electron, propagating along the nanofilm surface, is reflected from the step. We calculate the reflectance of such electron for different parameters of the nanofilm and different parameters of the defect. We demonstrate that such system has an interesting property. Namely, the incident electron wave not only produces the reflected and transmitted waves, but also generates the mode, localized at the step-like defect. Such mode results in an enhancement of the electron density at the defect by ~20%. The strength of such enhancement depends on the parameters of the nanofilm and the height of the step.


11:15AM G19.00001 Precursor Hidden Order Fluctuations in URu2Si2¹, PETER RISEBOROUGH, Physics Department, Temple University — It has been proposed that the Hidden Order phase in URu2Si2 is a combined spin-orbit density wave, which is stabilized by the effect of the spin-flip part of the inter-orbital Hund’s rule exchange. The transition involved the nesting of bands with different orbital characters and results in a partial gapping of the Fermi-surface. Above the transition temperature, the system exhibits combined spin and orbital fluctuations whose lifetimes and amplitudes increase as the temperature is reduced towards the critical temperature. These fluctuations produces hot-spots on the Fermi-surface, modifies the electronic structures as precursor to the opening of the gap. We examine the dependence of precritical fluctuations on the transition temperature. As the critical temperature is reduced to zero, it is found that the nature of the transition changes from second-order to first-order.

¹This work was supported by the US Department of Energy, Office of Basic Energy Sciences through award DEFG02-84ER45872.
11:27AM G19.00002 Charge-2e Skyrmion condensate in a hidden order state,

CHEN-HSIUAN HSU, SUDIP CHAKRAVARTY, University of California, Los Angeles — A higher angular momentum ($l = 2$) d-density wave, a mixed triplet and a singlet, interestingly, admits skyrmionic textures. The Skyrmions carry charge $2e$ and can condense into a spin-singlet $s$-wave superconducting state. In addition, a charge current can be induced by a time-dependent inhomogeneous spin texture, leading to quantized charge pumping. The quantum phase transition between this mixed triplet $d$-density wave and skyrmionic superconducting condensate likely leads to deconfined quantum critical points. We suggest connections of this exotic state to electronic textures that are strongly correlated, such as the heavy fermion URu$_2$Si$_2$. At the very least, we provide a concrete example in which topological order and broken symmetry are intertwined, which can give rise to non-BCS superconductivity.

1Reference: arXiv:1210.0034v2. This work is supported by NSF under Grant No. DMR-1004520.

11:39AM G19.00003 Evidence for an orbital moment in the superconducting state of URu$_2$Si$_2$,

GANG LI, QIU ZHANG, DANIEL RHODES, BIN ZHENG, PALLAB GOSWAMI, National High Magnetic Field Lab, P. TOBASH, FILIP RONNING, JOE D. THOMPSON, ERIC D. BAUER, Los Alamos National Lab, LUIS BALICAS, National High Magnetic Field Lab — URu$_2$Si$_2$ was suggested to be a chiral $d$-wave superconductor with a $k_z (\pm i k_y)$ orbital component for the Cooper pair wave-function. This state breaks time-reversal symmetry due to the orbital moment associated with this pair wave-function. Here, we report torque magnetometry in URu$_2$Si$_2$ at high fields and very low temperatures revealing a change in the sign of the magnetic hysteresis for $H \parallel H_{c2}$, and for angles $15^\circ$ away from the $ab$-plane, i.e. from a clear diamagnetic response dominated by the pinning of vortices to a state with a much smaller but paramagnetic-like hysteretic response which disappears at $H_{c2}$. If diamagnetism results from screening super-currents, we conclude that this hysteretic paramagnetic response must result from super-currents circulating in the opposite sense which generate an effective moment as expected for a chiral superconductor.

3Supported by DOE-BES through award DE-SC0002613.

11:51AM G19.00004 Global k-space perspective of temperature-dependent U f-states in URu$_2$Si$_2$,

J.D. DENLINGER, Lawrence Berkeley National Lab, L. DUDY, U. Wuerzburg, Germany, J.-S. KANG, Catholic U. of Korea, J.W. ALLEN, U. of Michigan, N.P. BUTCH, U. of Maryland, M.B. MAPLE, UC San Diego — In recent years, high-resolution angle-resolved photoemission (ARPES) measurements [1] have identified a narrow band of $f$-states close to the Fermi level in URu$_2$Si$_2$ whose temperature dependent spectral weight and/or energy shifts correlate to the hidden-order transition at $17.5K$. These $f$-states have been observed close to normal emission at a few select photon energies of $\sim 6, 21$ and $30 eV$ corresponding to momentum space locations close to $Z_1$ and $Z$ points respectively. We attempt to provide a more global $k$-space context for the presence of such $f$-states and their relation to the bulk Fermi surface topology using synchrotron-based wide-angle and photon energy-dependent ARPES mapping of the electronic structure. In addition, x-ray polarization and small-spot spatial dependences are exploited to assist identification of these narrow-band $f$-states and their relation to specific U- or Si-terminations of the cleaved surface.


12:03PM G19.00005 Formation of coherent heavy fermion states at the hidden order transition in URu$_2$Si$_2$, as seen by ARPES,

SHOUVIK CHATTERJEE, Cornell University, JAN TRINCKAUF, TORBEN HANKE, Leibnitz Institute for Solid State and Materials Research, IFW Dresden, DANIEL SHAI, JOHN HARTER, Cornell University, TRAVIS WILLIAMS, GREG MACDONALD, McMaster University, JOCHEN GECK, Leibnitz Institute for Solid State and Materials Research, IFW Dresden, KYLE SHEN, Cornell University — We present high-resolution angle-resolved photoemission (ARPES) spectra that allow us to delineate the evolution of the low energy electronic structure of the heavy-fermion superconductor URu$_2$Si$_2$ across the hidden order (HO) transition. By employing a range of excitation photon energies, we are able to disentangle various features in the electronic structure which, to date, have not been clearly identified. In contrast to the conventional Kondo lattice scenario, we find that precisely at $T_{HO}$, the low energy electronic structure changes due to hybridization from incoherent and localized $f$ states to a coherent heavy fermion liquid. We also observe a sharp drop in the scattering rate upon cooling through $T_{HO}$ suggesting that the large scattering rate is caused by fluctuations in the order parameter. Our findings place clear constraints on the possible theoretical models for the HO state while clarifying a few of the apparently inconsistent observations of the previous ARPES measurements.

12:15PM G19.00006 Heavy fermion phases probed by temperature dependent tunneling spectroscopy,

ANA MALDONADO, Laboratorio de Bajas Temperaturas, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain, ISABEL GUILLÁMON, H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK, JOSE GABRIEL RODRIGO, HERMANN SUDEROW, ANA MALDONADO, Laboratorio de Bajas Temperaturas, Departamento de Fisica de la Materia Condensada, Universidad Autonoma de Madrid, 28049 Madrid, Spain, DAI AOKI, JACQUES FLOUQUET, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France — Heavy fermions offer a rich physical phenomenology at very low temperatures, exhibiting different phase transitions on cooling that determine their electronic properties. Their ground states cover many electronic interactions, such as Kondo effect, superconducting or long range magnetic ones and, eventually, their coexistence. Thus, exploring the local electronic properties of these systems using scanning tunneling microscopy/spectroscopy (STM/S) at different temperatures is essential. In this communication, tunneling spectroscopy measurements using a superconducting tip of Al in the superconducting phase of URu$_2$Si$_2$ and using one of Au in the paramagnetic and antiferromagnetic phases of, respectively, CeRu$_2$Si$_2$ and CeRh$_2$Si$_2$ will be discussed. The features found in the tunneling spectroscopy of each compound at 0.15K and their respective thermal evolution reflect the formation of different electronic ground states.


3A. Maldonado et al., Accepted in J. Phys.: Condens. Matter

12:27PM G19.00007 From hidden order to magnetic order: Optical conductivity reveals new behavior in URu$_2$Si$_2$,

JESSE THOMPSON, ERIC D. BAUER, Los Alamos National Lab, LUIS BALICAS, University of California, San Diego, NICHOLAS BUTCH, Lawrence Livermore National Lab, BRIAN MAPLE, University of California, San Diego, THOMAS TIMUSK, McMaster University — As a new generation of experimental techniques is brought to bear against the heavy-Fermion compound URu$_2$Si$_2$, striking new details about the electronic structure changes at the mysterious hidden order (HO) transition are becoming clear. Far infrared optical conductivity measurements were performed on oriented samples of URu$_2$Si$_2$ doped with both Fe and Re. While Re-doping substitutes for U atoms, Fe-doping substitutes for Si atoms across the hidden order (HO) transition. By employing a range of excitation photon energies, we are able to disentangle various features in the electronic structure which, to date, have not been clearly identified. In contrast to the conventional Kondo lattice scenario, we find that precisely at $T_{HO}$, the low energy electronic structure changes due to hybridization from incoherent and localized $f$ states to a coherent heavy fermion liquid. We also observe a sharp drop in the scattering rate upon cooling through $T_{HO}$ suggesting that the large scattering rate is caused by fluctuations in the order parameter. Our findings place clear constraints on the possible theoretical models for the HO state while clarifying a few of the apparently inconsistent observations of the previous ARPES measurements.

1This work supported by the Natural Science and Engineering Research Council of Canada and US DOE (Grant No. DE FG02-04ER46105)
12:39PM G19.00008 NMR Evidence for pseudogap in URu$_2$Si$_2$\cite{1}. KENT SHIRER, ADAM DIOGUARDI, JOHN CROCKER, NICHOLAS APROBERTS-WARREN, ABIGAIL SHOCKLEY, CHING LIN, DAVID NISSON, University of California - Davis, JASON COOLEY, Los Alamos National Laboratory, BRIAN MAPLE, University of California - San Diego, JASON HARALDSEN, MATTHIAS GRAF, Los Alamos National Laboratory, NICHOLAS CURRO, University of California - Davis — We report $^{29}$Si NMR measurements in single crystals and aligned powders of URu$_2$Si$_2$ in the hidden order and paramagnetic phases. In the paramagnetic phase, the spin lattice relaxation data reveal evidence of spin fluctuations of U moments. Furthermore, we find evidence for partial suppression of density of states below 30 K.

\textsuperscript{1}Work at UC Davis was supported by UCOP-TR01, the NNSA under the SSAA program through DOE Research Grant #DOE DE-FG52-09NA29464, and the NSF under Grant No. DMR-1005393.

12:51PM G19.00009 Spin Correlations in the Different Phases of URu$_2$Si$_2$\cite{2}, TRAVIS J. WILLIAMS, McMaster University, H. BARATH, Johns Hopkins University, Z. YAMANI, Canadian Neutron Beam Centre, NRC Chalk River, J.A. RODRIGUEZ-RIVERA, J.B. LEAO, NIST Center for Neutron Research, J.D. GARRETT, G.M. LUKE, McMaster University, W.J.L. BUYERS, Canadian Neutron Beam Centre, NRC Chalk River, C. BROHOLM, NIST Center for Neutron Research — We report a neutron scattering study of the magnetic excitation spectrum in three temperature and pressure driven phases of URu$_2$Si$_2$: the paramagnetic, ‘hidden order’ and antiferromagnetic phases. The experiment was conducted using the novel neutron scattering spectrometer MACS at the NIST Center for Neutron Research\cite{3}. Wide-angle detector coverage offers comprehensive scattering data covering an entire plane in momentum space with excellent energy resolution. The ambient pressure data show a magnetic excitation spectrum characteristic of Fermi surface nesting in the paramagnetic phase and the development of a gap in the excitation spectrum upon cooling through the $T_c = 17.5$ K phase transition. The efficiency of MACS allowed a comprehensive data set in the high-pressure phase. Throughout the (H0L) scattering plane we find qualitatively similar excitations as in the hidden order phase though with a substantial reduction in the overall spectral weight and an upward shift in energy. These data should allow a critical evaluation of recent theoretical work to understand the small and large moment phases of URu$_2$Si$_2$. \cite{1,2,3} [J.A. Rodriguez-Rivera, Meas. Sci. Technol. 19, 034023 (2008)].

1:03PM G19.00010 Phonon Behavior in the Hidden Order state of the Heavy Fermion Superconductor URu$_2$Si$_2$\cite{4}, DILLON GARDNER, CRAIG BONNOIT, Massachusetts Institute of Technology, TRAVIS WILLIAMS, GRAEUME LUKE, McMaster University, YOUNG LEE, Massachusetts Institute of Technology — The heavy fermion compound URu$_2$Si$_2$ has generated much interest after the initial discovery of coexisting superconductivity and magnetism. Subsequent measurements revealed a phase transition at $T$=17.5 K into what is referred to as the “hidden order” state. The order parameter of this state remains unknown. Anomalous behavior in both the lattice component of thermal conductivity and thermal expansion parameters suggest that the phonons may also exhibit anomalous behavior that can shed light on the nature of the Hidden Order. We presentinelastic X ray scattering measurements of lattice dynamics in both the hidden order phase and high temperature phase.

1:15PM G19.00011 Anisotropic phonon softening in URu$_2$Si$_2$, NICHOLAS BUTCH, MICHAEL MANLEY, JASON JEFFRIES, Lawrence Livermore National Laboratory, MARC JANOSCHEK, KEVIN HUANG, BRIAN MAPLE, UC San Diego, JEFFREY LYNN, NIST Center for Neutron Research — We studied the low-energy phonons of URu$_2$Si$_2$ via inelastic neutron scattering. At the wave-vectors associated with magnetic excitations, the phonons show surprisingly little modification. However, we find important temperature and direction dependence of the phonons in the basal plane. Possible ramifications for the symmetry of the hidden order will be discussed.

1:27PM G19.00012 High-magnetic field magnetostriction and thermal expansion in URu$_2$Si$_2$, V.F. CORREA, CAB-CNEA, Bariloche, Rio Negro, Argentina, S. FRANCOUAL, M. JAIME, N. HARRISON, A. LACERDA, MPA-CMMS, LANL, Los Alamos, New Mexico 87545, USA, T.P. MURPHY, E.C. PALM, S.W. TOZER, NICMFL, FSU, Tallahassee, Florida 32310, USA, P.A. SHARMA, MPA-CMMS, LANL, Los Alamos, New Mexico 87545, USA, J.A. MYDOSH, Kamerlingh Onnes Laboratory, Leiden University, NL-2300 RA Leiden, The Netherlands — We report high magnetic field (up to $\mu_0\mathcal{H} = 45$ T) $c$-axis thermal expansion and magnetostriction experiments on URu$_2$Si$_2$ single crystals. The sample length change $\Delta L(T)/L_0$, associated with the transition to the “hidden order” phase becomes increasingly discontinuous as the magnetic field is raised above 25 T. The re-entrant ordered phase III is clearly observed in both the thermal expansion $\Delta L(T)/L_0$ and magnetostriction $\Delta L(B)/L_0$ above 36 T, in good agreement with previous results. The sample length is also discontinuous at the boundaries of this phase, mainly at the upper boundary. A change in the sign of the coefficient of thermal-expansion is observed at the metамagnetic transition (B$_f$ $\approx$ 38 T) which is likely related to the existence of a quantum critical end point. See V.F. Correa et al., Phys. Rev. Lett. (in the press).

1:39PM G19.00013 Revealing the electronic structure of USb$_2$ using femtosecond optical pulses, JINGBO QI, TOMASZ DURAKIEWICZ, E. BAUER, R. BAUMBACH, K. GOFRYK, Los Alamos National Laboratory, T. KLIMCZUK, ITU Karlsruhe, P. RISEBOROUGH, Temple University, ANTOINETTE TAYLOR, ROHIT PRASANKUMAR, Los Alamos National Laboratory — USb$_2$ is a very interesting moderately heavy system, as it displays dispersive 5f bands as well as the first example of a clear kink structure in f-electron systems. This material also exhibits a renormalized zone-centered hole-like band, driven by boson-mediated interband scattering processes. Employing ultrafast optical spectroscopy, we explored the nature of the boson participating in this band renormalization, and explicitly characterized the gap structures near the Fermi surface in USb$_2$ for the first time. Our results reveal new physical properties of this material, which have not previously been unveiled by other experimental methods.

1:51PM G19.00014 Non-Fermi vs. Inhomogeneous-Fermi Liquid behaviour in UCu$_4$Ni in the context of the Kondo Disorder Model, ARIANA VALDEZ, OSCAR BERNAL, Department of Physics and Astronomy, California State University, Los Angeles, CA 90032, R.G. STEWART, J.S. KIM, Department of Physics, University of Florida, Gainesville FL 32611 — UCu$_4$Ni is a site-disordered material with diverging thermodynamic and anomalous transport properties. Local nuclear magnetic resonance (NMR) experiments in combination with bulk magnetic susceptibility measurements performed on the same samples indicate that the low-temperature divergence of $\chi$ might be due in part to the presence of paramagnetic impurities. In this contribution, we describe the magnetization in terms of a Kondo disorder model and extract a set of parameters of the distribution of Kondo temperatures, which indicate that the low-temperature side of the distribution does not have sufficient area to accommodate a non-Fermi liquid divergence. We use the same parameters to subsequently calculate the specific heat $C$ and to extrapolate to low temperatures, which allows us to compare with the known divergence of the magnetic contribution to $C/T$ below 10 K. We discuss to what extent the physics of this material is that of a non-Fermi liquid as opposed to an inhomogeneous Fermi fluid.

\textsuperscript{1}Work supported by NSF-DMR 1105380
\textsuperscript{2}Supported by MBRs RISE Program through grant GM061331.
The effects of grinding on the magnetic susceptibility of UCu$_{0.95}$Ni$_{1.05}$

Carlos Sanchez, Carmen Quen, Edith Soto, Oscar Bernal\textsuperscript{1}.

Physics and Astronomy Department, California State University, Los Angeles, CA, G.R. Stewart, Physics Department, University of Florida, Gainesville, FL — The effects of grinding on the magnetic susceptibility of UCu$_{0.95}$Ni$_{1.05}$ were studied in order to understand magnetization measurements in this material. Substantial information was recovered from these experiments, which were done at temperatures ranging from 3K to 300K and magnetic fields from 500 Oe to 4.75 kOe. For instance, a new and unexpected ferromagnetic (FM) phase transition was found at about 150 K in both ingot and powder samples. Similarly the magnetic properties of the powder seem to differ slightly from the ingot's. The powder's magnetic susceptibility $\chi_{\text{powd}}$ appears greater than the ingot's $\chi_{\text{ing}}$ at all temperatures measured, with the difference $\Delta \chi = \chi_{\text{powd}} - \chi_{\text{ing}}$ increasing with decreasing temperature. We analyze the observed $\Delta \chi$ in terms of two potential sources: impurities added to the powder during the grinding process and the effects of sample geometries in combination with the presence of a second (FM) phase in the studied material. We discuss how the measured differences might affect the study of the physics of this non-Fermi liquid/quantum critical compound.

\textsuperscript{1}Work supported by NSF-DMR 1105380

Tuesday, March 19, 2013 11:15AM - 2:15PM — Session G22 DCMP: Electronic Phenomena of Nanostructures

11:15AM G22.00001 Fermi liquid nature of the ground state of multiple-quantum dots in parallel\textsuperscript{1}, MANAS KULKARNI, Princeton University, Robert Konik, Brookhaven National Laboratory — We argue through a combination of $1/N$ diagrammatic expansion, slave boson mean field theory and the Bethe ansatz that the ground state of multiple quantum dots arranged in parallel is a singlet Fermi-liquid ground state. This conclusion is arrived at by showing the validity of Friedel Sum Rule (a fingerprint of Fermi-liquid physics) and finding that impurity entropy vanishes in the limit of zero temperature (singlet). Our conclusion is in contradiction to other studies that predict a non-Fermi liquid ground state. We discuss possible reasons for this discrepancy.

11:27AM G22.00002 Coupled collective modes in electronic systems of different dimensionalities\textsuperscript{1}, Ben Yu-Kuang Hu, The University of Akron, Euyheon Hwang, Sungkukwan University, South Korea and The University of Maryland, College Park, Sankar Das Sarma, The University of Maryland, College Park — We consider electronic collective modes in coupled systems in which the individual components have different dimensionalities. Many-body diagrammatic techniques are used to derive formal results for the screened intra- and inter-system Coulomb interaction. We specifically investigate the case of a quasi-one-dimensional quantum wire in close proximity to a two-dimensional electron gas. We evaluate the screened intra- and inter-system Coulomb interaction within the random phase approximation, and find the existence of modes which have hybrid properties characteristic of both one- and two-dimensional systems. We also investigate the spatial dependence of the coupled 1-d + 2-d collective modes within the two-dimensional electron gas, and show that the coupled modes within that layer vary from being purely two-dimensional in character far away from the quantum wire to being strongly hybridized close to the wire.

\textsuperscript{1}Supported by LPS-CMTC and US-ONR.

11:39AM G22.00003 Influence of Rashba spin-orbit interactions on the Kondo effect\textsuperscript{1}, Arturo Wong, Kevin Ingersent, U. of Florida, Mahdi Zarea, Northwestern U., Sergio Ulloa, Nancy Sandler, Ohio U. — Recent studies\textsuperscript{[1]} have pointed out that the thermodynamics of the Kondo effect are essentially unaltered by the presence of Rashba spin-orbit interactions in a host two-dimensional electron gas. However, it has also been proposed\textsuperscript{[2]} that the presence of bulk Rashba interactions induces a coupling between a magnetic impurity and conduction electrons with nonzero orbital angular momentum about the impurity site. In this work we revisit this problem using the numerical renormalization group. In agreement with previous studies, we find only minor changes in the Kondo temperature scale when the Rashba coupling is increased at fixed Fermi energy. However, for fixed band filling, increasing the spin-orbit coupling can move the Fermi energy near to a Van Hove singularity in the effective density of states, leading to an exponential enhancement of the Kondo scale. Static spin correlations confirm that the impurity couples to conduction channels of nonzero orbital angular momentum. We also explore the effects of a magnetic field applied in the plane of the host system.


11:51AM G22.00004 Spin-polarized conductance in double quantum dots: Interplay of Kondo, Zeeman and orbital effects\textsuperscript{1}, Luis Dias da Silva, Instituto de Fisica, Universidade de Sao Paulo, Edson Vernek, Instituto de Fisica, Universidade Federal de Uberlandia, Kevin Ingersent, Department of Physics, University of Florida, Nancy Sandler, Sergio Ulloa, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University — We study the effect of an external magnetic field in the Kondo regime of a double-quantum-dot system in which a strongly correlated dot is coupled to a noninteracting dot that is also connected to external leads. In zero field, the spectral function of the hanging dot has previously been shown to exhibit a split-peak structure near the Fermi level due to “Kondo resonance filtering” by the noninteracting dot. We show, using the numerical renormalization group, that application of a magnetic field leads to a subtle interplay between electronic interference, Kondo physics, and Zeeman splitting with nontrivial consequences for the spectral and transport properties. The value of the correlated-dot spectral function at the Fermi level exhibits a nonuniversal field dependence that can be explained using a generalized Friedel sum rule for a Kondo system with energy-dependent hybridization. By tuning gate voltages and the magnetic field, one can achieve complete spin polarization of the linear conductance between the leads, raising the prospect of applications of the device as a highly tunable spin filter.

\textsuperscript{1}Supported in part by NSF-Materials World Network (DMR-0710540, 1107814, 0710581, 110828) and, in Brazil, by CNPq (493299/2010-3), FAPESP (2010/20804-9) and FAPEMIG (CEX-APQ-02371-10).

12:03PM G22.00005 Controlling entanglement and spin-correlations in double quantum dots with electrical currents in the non-equilibrium regime\textsuperscript{1}, C.A. Busser, Ludwig-Maximilians-Universität, München, F. Heidrich-Meisner, FAU Erlangen-Nuremberg and LMU Munich — We study the non-equilibrium dynamics in a parallel double-quantum dot structure induced by a large bias voltage. By applying both a magnetic flux and a voltage, it is possible to generate spin-spin-correlations between the two quantum dots. The sign and absolute value of these correlations can be controlled by changing the bias voltage. Using a canonical transformation we argue that the mechanism that drives the spin-spin correlations can be understood in terms of an effective Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction that is mediated by the current. Our study is based on the Anderson-impurity model and we use time-dependent density matrix renormalization group simulations to obtain currents and spin-correlations in the non-equilibrium regime. We also perform quench in the Hamiltonian to prove the stability of the entangled state.

\textsuperscript{1}Acknowledgement: Deutsche Forschungsgemeinschaft DFG FOR912
12:15PM G22.00006 SU(4) Kondo effect in a double quantum dot . ANDREW KELLER, Stanford University, SAMI AMASHA, MIT Lincoln Laboratory, ILEANA RAU, IBM Research - Almaden, LUCAS PEETERS, Stanford University, JORDAN KATINE, HGST, HADAS SHTRIKMAN, Weizmann Institute of Science. David Goldhaber-Gordon, Stanford University — Lateral quantum dots are highly tunable experimental systems ideal for exploring the interplay of spin and charge correlations. We present studies of a parallel-coupled double quantum dot system in a GaAs/AlGaAs heterostructure. In the limit of negligible inter-dot tunneling, the conductance through both dots is enhanced at inter-dot orbital degeneracies, where the energy for an electron to be on either dot is the same. We show how at four-fold orbital and spin degeneracies, signatures in the zero-bias conductance, the temperature dependence, and the bias spectroscopy suggest an SU(4) Kondo effect may be realized, combining spin and pseudospin.

12:27PM G22.00007 What Is Measured in the Scanning Gate Microscopy of a Quantum Point Contact? . STEVEN TOMSOVIC, Department of Physics and Astronomy, P.O. Box 642814, Washington State University, Pullman, WA 99164-2814, USA, RODOLFO A. JALABERT, WOJCIECH SZEW, DIETMAR WEINMANN, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, CNRS-UdS, 23 rue du Loeoss, B.P. 43, 67034 Strasbourg Cedex 2, France — The conductance change due to a local perturbation in a phase-coherent nanostructure is calculated. The general expressions to first and second order in the perturbation are applied to the scanning gate microscopy of a two-dimensional electron gas containing a quantum point contact. The first-order correction depends on two scattering states with electrons incoming from opposite leads and is suppressed on a conductance plateau; it is significant in the step regions. On the plateaus, the dominant second-order term likewise depends on scattering states from both sides. It is always negative, exhibits fringes, and has a spatial decay consistent with experiments.

12:39PM G22.00008 Understanding Nanocontacts with atomic precision . CARLOS SABATER, MARIA JOSE CATURLA, University of Alicante, JUAN JOSE PALACIOS, University Autonoma of Madrid, CARLOS UNIETED, University of Alicante, UNIVERSITY OF ALICANTE TEAM, UNIVERSITY AUTONOMA OF MADRID TEAM — Measuring the variations of the conductance indentation experiments between two electrodes, we can obtain information on the changes in the atomic structure of the contact. We have analysed the Jump-to-Contact(JC) phenomenon which can be observed as the first contact when the two metals approach each other. Moreover, we have studied the Jump-out-of-contact(JOC) phenomenon which is the last contact before breaking the two electrodes. Secondly, we further approach the two electrodes and when the indentation depth is limited to a certain value of conductance, almost the exact behaviour in the evolution of the conductance can be obtained for hundreds of cycles of formation and rupture. That is, the same sequence of atomic configurations was followed. Both processes are rationalized using MD simulations together with DFT transport calculations, which show: a) the most probable atomic configurations in the first contact following the JC or JOC processes; b) that after repeated indentations the two metallic electrodes are shaped into tips of a reproducible structure formed through a mechanical annealing process. These results improve our understanding of atomic-sized contacts and the evolution of their structural characteristics.

12:51PM G22.00009 Emergent Localization from Many-Body Physics in Clean Quantum Point Contacts . CASPAR H. VAN DER WAL, M.J. IQBAL, E.J. KOOP, J.B. DEKKER DEKKER, J.P. DE JONG, J.H.M. VAN DER VELDE, University of Groningen, The Netherlands, D. REUTER, A.D. WIECK, Ruhr-University Bochum, Germany, R. AGUADO, Instituto de Ciencia de Materiales of Madrid, Spain, Y. MEIR, Ben-Gurion University of the Negev, Israel — Quantized conductance in quantum point contacts (QPCs) is the signature of control over electron transport at the nanoscale. As a function of channel width the conductance then increases in steps of \( G_0 = 2 e^2/h \). However, experiments often show an additional feature with a conductance plateau near zero, known as the 0.7 anomaly. This has been studied since 1995 but its full understanding is still an open problem. Spontaneous localization due to many-body effects in open QPCs, and the associated Kondo effect, has emerged as a promising theory for the 0.7 anomaly [1]. This theory work predicted that the many-body effects should give a single localized state in the 0.7 plateau, which is in agreement with experiments. We show here how to simulate the 0.7 anomaly using the many-body theory. The wave function is shown to have oscillations which are consistent with experiments.

1:03PM G22.00010 Electrolyte gating of gold point contacts . TREVOR PETCH, MENYOUNG LEE, DAVID GOLDHABER-GORDON, Stanford University — Gold point contacts are fabricated in-situ by electromigration in an ionic liquid bath. These contacts are shown to be stable at room temperature at conductances as small as 50 \( G_0 \). By electrolyte gating the contacts using a counter electrode in the ionic liquid, conductance changes of 25% are observed, corresponding to accumulation of more than one electron per gold surface atom. Double step chronocoulometry and x-ray reflectometry suggest that ion ordering in the ionic liquid near the gold interface is consistent with the observed changes in conductance.

1:15PM G22.00011 Electron energy spectra in two dimensional quantum rings consisting of two nanoelements . AVAG SAHAKYAN, RUZAN MOVSEYSYAN, The State Engineering University of Armenia, ARMEK KOCHARIAN, California State University, Los Angeles — Electron spectrum and ground state properties in two dimensional confined quantum rings with \( R_{1,2} \) radii consisting of the two different (materials) nanoelements divided by two secored finite size quantum wells with various potentials and spanning angles, is studied in the presence of transverse magnetic field. The calculated wave function shows oscillations along the radial direction which are progressing by approaching to the internal radius of the ring, \( R_2 \). Situation here is similar to the problem of fall of the particle on the attractive center. However, these oscillations are interrupted on the internal ring boundary by providing the new ground state which is sensitive to the change of magnetic flux. For shallow energy levels some energy states are undergoing changes controlled by magnetic field accompanied with the persistent current and abrupt phase transitions. Magnetization and magnetic susceptibility show characteristic two dimensional anomalous behaviors different from one found in one dimensional ring.

1:27PM G22.00012 Lateral quantization of two-dimensional electron states by embedded Ag nanocrystals\(^1\) . CHRIS VAN HAESENDONCK, KOEN SCHOUTEDEN, Laboratory of Solid-State Physics and Magnetism, KU Leuven, BE-3001 Leuven, Belgium — We show that quantization of image-potential state (IS)electrons above the surface of nanostructures can be experimentally achieved by Ag nanocrystals that appear as stacking fault tetrahedrons (SFTs) at Ag(111) surfaces. By means of cryogenic tunneling spectroscopy the \( n = 1 \) IS of the Ag(111) surface is revealed to split up in discrete energy levels, which is accompanied by the formation of pronounced standing wave patterns that directly reflect the eigenstates of the SFT surface. The IS confinement behavior is compared to that of the surface state electrons in the SFT surface and can be directly linked to the particle-in-a-box model. ISs provide a novel playground for investigating quantum size effects and defect induced scattering above nanostructured surfaces.

\(^1\)This work has been supported by the Research Foundation – Flanders (FWO, Belgium). K.S. is a postdoctoral researcher of the FWO.
1:39PM G22.00013 MoS$_2$ grain-boundary: First-principles investigations$^1$. DU Y. LE, TALAT S. RAHMAN, Department of physics, University of Central Florida, Orlando, FL 32816, USA — We present results of our first-principles electronic structure investigations, using the spin-polarized density-functional-theory, of the electronic and geometric structures of various models of grain-boundaries formed between different MoS$_2$ domains when grown as a single layer. From analysis of electronic band structures, we find, in all considered models, that the grain-boundaries exhibit metallic behavior. More interestingly, we find signatures of magnetism in the grain-boundary formed between two sulfur edges with 0% sulfur coverage. Details analysis of the geometric structures lead us to the conclusion that certain grain-boundaries undergo (2 × 1) reconstructions. We provide full details of the electronic and spin density states and charge redistribution at the domain boundaries. We make contact with recent experimental observations and discuss the modifications in the characteristics for MoS$_2$ grown on Cu(111) $^1$.

$^1$Work supported in part by DOE Grant DE-FG02-07ER15842

1:51PM G22.00014 Ab initio Simulations of charge transfer properties at Quantum Dot/TiO$_2$ Interface in Quantum Dot-Sensitized Inter-Calce Cells, XUKAI XIN, Georgia Institute of Technology, RANA BISWAS, Iowa State University, ZHIQIN LIN, Georgia Institute of Technology — Quantum dot-sensitized solar cells (QDSSCs) have emerged as a very promising solar architecture for next generation photovoltaics. The QDSSCs exhibit a remarkably fast electron transfer from the quantum dot (QD) donor to the TiO$_2$ acceptor with size quantization properties that allows for the modulation of QD band gaps to control the photoresponse and photoconversion efficiency of QDSSCs. To understand the mechanisms that underpin this rapid charge transfer, the electronic properties of CdSe and PbSe QDs on the TiO$_2$ substrate were simulated using a rigorous ab initio method. In contrast to the plane wave approaches, this method capitalized on localized orbital basis set that is computationally less intensive, and provides excellent electronic structure of the constituent systems. We consider QDs grown on TiO$_2$ without functional ligands passivating the QD surface. We find a remarkable set of electron bridging states between QDs and TiO$_2$ occurring via the strong bonding between the conduction bands of QDs and TiO$_2$. Such bridging states account for the fast adiabatic charge transfer from the QD donor to the TiO$_2$ acceptor, and may be a general feature for other strongly coupled donor/acceptor systems and nanostructured semiconductor interfaces.

2:03PM G22.00015 Effect of hydrogen passivation on the electronic structure of ionic semiconductor nanostructures, HUIXIONG DENG, National Renewable Energy Laboratory, SHU-SHEN LI, JINGBO LI, Institute of Semiconductors, Chinese Academy of Sciences, SU-HUAI WEI, National Renewable Energy Laboratory, INSTITUTE OF SEMICONDUTORS, CHINESE ACADEMY OF SCIENCES COLLABORATION — In theoretical studies of thin film and nanostructured semiconductors, pseudohydrogen (PH) is widely used to passivate the surface dangling bonds. Based on these calculations, it is often observed that passivated nanostructures, due to quantum confinement, have a larger band gap than their bulk counterparts. Using first-principles band structure theory calculation and comparing the differences between PH-passivated and real-hydrogen–passivated (RH-passivated) semiconductor surfaces and nanocrystals, we show that, unlike PH passivation that always increases the band gap with respect to the bulk value, RH passivation of the nanostructured semiconductors can either increase or decrease the band gap, depending on the ionicity of the nanocompounds. The difference between PH and RH passivations decreases when the covalency of the semiconductor increases and can be explained using a band coupling model. This observation greatly increases the tunability of nanostructured semiconductor properties, especially for wide-gap ionic semiconductors.

Tuesday, March 19, 2013 11:15AM - 2:15PM —
Session G30 DCMP: Self-Assembly 338 - Bulent Akgun, National Institute of Standards and Technology

11:15AM G30.00001 Is a hierarchical dynamics the best route to the self-assembly of a hierarchical structure? THOMAS HAXTON, STEPHEN WHITELAM, Lawrence Berkeley National Laboratory — Mimicking nature’s ability to assemble functional hierarchical materials will require understanding how to promote the self-assembly of structure on multiple length scales while avoiding kinetic traps. We use computer simulation to study the self-assembly of a simple hierarchical structure, a square lattice whose repeat unit is a tetramer. Although the target material is organized hierarchically, it self-assembles most reliably when its assembly pathway consists of the sequential addition of monomers to a single structure. Hierarchical assembly pathways via dimer and tetramer intermediates result in lower yield, because these intermediates tend to associate in ways incompatible with the target structure. In addition, assembly via trimers results in the formation of incomplete building blocks (trimers) that cannot combine to form the target crystal. We use analytic theory to relate assembly pathways to the underlying thermodynamics, identifying two principles for optimal assembly: 1) make the free energy gap between the target phase and the most stable fluid phase comparable to the thermal energy, and 2) ensure that no other dense phases (liquids or close-packed solids of monomers or oligomers) or fluids of incomplete building blocks fall within this gap.

11:27AM G30.00002 Optimized assembly and steady-state length-scale control in dissipative systems of photo-switchable colloids, ANTONIO OSORIO-VIVANCO, University of Michigan, MONICA OLVERA DE LA CRUZ, Northwestern University, SHARON GLOTZER, University of Michigan — Photo-switchable nanoparticles, such as those developed by Wei et al., can be assembled into a broad range of structures using light exposure as a control parameter. Jha et al. explored the evolution of these structures using kinetic Monte Carlo simulations. In this work, we build on these studies using Molecular Dynamics with a Langevin thermostat to, by judicious choice of exposure parameters that control the dissipative nature of the system, engineer and optimize the self-assembly pathways as well as control the length scales of the steady-state structures.

11:39AM G30.00003 Self organization of exotic oil-in-oil phases driven by tunable electrohydrodynamics, ANAND YETHIRAJ, Department of Physics & Physical Oceanography, Memorial University of Newfoundland, St. John’s, NL, Canada, ATUL VARSHNEY, SHANKAR GHOSH, S. BHATTACHARYA, Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai 400-005, India — The tuning of electrostatic interactions has helped to elucidate when coherent crystalline structures or incoherent amorphous structures form in colloidal systems. However, there is little understanding of self-organization in situations where hydrodynamic interactions are also present. We present a minimal two-component oil-in-oil model system where we can control the strength and length scale of the electrohydrodynamic interactions by tuning the amplitude and frequency of the imposed electric field. As a function of the hydrodynamic length scale, we observe a rich phenomenology of exotic structure and dynamics, from coherent cloud-like structures and chaotic droplet dynamics, to polyhedral droplet phases, to coherent droplet arrays.

11:51AM G30.00004 Novel Behavior in Self-Assembled Superparamagnetic Nanoparticle Monolayers at the Air-Water Interface, JACOB STANLEY, LEANDRA BOUCHERON, YELING DAI, Department of Physics, University of California, BINHUA LIN, MATI MERON, Argonne National Lab and University of Chicago, OLEG SHPYRKO, Department of Physics, University of California — Iron oxide nanoparticles, coated with an oleic acid ligand, have been found to form self-assembled monolayers when deposited at the air-water interface. Even for low particle densities these particles aggregate into hexagonally close-packed islands which merge into a uniform layer at higher densities. Using Grazing Incidence Small Angle X-Ray Scattering (GISAXS) we were able to measure the first through fifth order diffraction peaks. By analyzing the positions and shapes of these peaks we investigated the in-plane structure of these monolayers and characterized how the structure changes as a function of compression in a Langmuir-Blodgett trough. Since iron oxide nanoparticles are known to be super-paramagnetic, we sought to investigate the role magnetic effects may have on the interparticle interactions and ordering within the film. We performed Grazing Incidence Diffraction (GID) measurements on the film while varying an external magnetic field. We will discuss the results of our findings.

12:03PM G30.00005 Structure and dynamics of self-assembly, HENRIK VAN LEMBERICH, RICHARD JAMES, University of Minnesota — We investigate structures that are composed of many identical building blocks. Of particular interest are equilibrium structures where every building block sees the same environment - we call these “objective structures”. For example, carbon nanotubes and virus capsids are both objective structures. The dynamics of assembly is investigated through experiments and simulations. The experiment consist of a macro-scale shaker containing identical neutrally buoyant magnetic particles. We model the translation and rotation of particles using Langevin dynamics. This kind of modelling is applicable to both our experiment and to molecular assembly.

12:15PM G30.00006 How to Maximize Self-Assembly in Free Surface Films by Resonant Wave-length Excitations, SANDRA TROIAN, NAN LIU, California Institute of Technology, MC 128-95, Pasadena, CA 91125 — Application of an external force probe on self-assembly processes in thin liquid films can offer significant insight into the fundamental dynamics of pattern formation. Less appreciated is the fact that modulation of such forces can induce resonant excitation effects in linearly unstable systems. While temporal modulation is rather common, there has been less emphasis on spatial forcing as a method for corralling emergent structure formation; such studies have also been strictly limited to 2D. In this talk, we call attention to a novel 3D hydrodynamic instability in nanoscale films whose free surface is exposed to a large uniform thermal gradient. Such films spontaneously develop arrays of nanopillars whose uniformity is often compromised by nanoscale inhomogeneities in film thickness, temperature and surface defects. In this talk we focus on resonant wave-length excitations induced by spatial modulation of the external thermal field near the linear stability point. Linear stability, weakly nonlinear analysis and simulations of the full nonlinear interface equation demonstrate the existence of a spatial coherence regime leading to more rapid growth and denser packing of perfectly uniform arrays, of significance to recent advances in lithographic patterning.

12:27PM G30.00007 Analysis of pattern formation in systems with competing range interactions, VYACHESLAV R. MISKO, HAJUN ZHAO, FRANCOIS M. PEETERS, University of Antwerp — Pattern formation is governed by competing interaction. Examples include: Langmuir monolayers, colloids and gels, ferrofluids, magnetic garnet thin films, type-I superconductors, the pasta phase in neutron stars, etc. We analyzed pattern formation and identified various morphologies in a system of particles interacting through a non-monotonic potential with a competing range interaction characterized by a repulsive core (r < r_c) and an attractive tail (r > r_c), using molecular-dynamics simulations [1]. Depending on parameters, the interaction potential models the inter-particle interaction in various physical systems ranging from atoms, molecules and colloids to vortices in superconductors. We constructed a “morphology diagram” in the plane “critical radius r_c” — density n — and proposed a new approach to characterize the patterns. Namely, we elaborated a set of quantitative criteria in order to identify the different pattern types, using the radial distribution function (RDF), the local density function and the occupation factor. We also discuss the dynamics of the obtained patterns [2].


12:39PM G30.00008 Crystallographic Tailoring: Self-Assembling Complex Crystals Through Building Block Design, PABLO F. DAMASCENO, Applied Physics, MICHAEL ENGEL, Chemical Engineering Department, SHARON C. GLOTZER, Materials Science and Engineering Department, University of Michigan, Ann Arbor MI — A primary challenge for the development of bulk, scalable and high yield materials with interesting properties is the limited number of structures that can be obtained via self-assembly of nano and micrometer sized particles. To increase this variability, several suggestions have been proposed among which the exploration of new anisotropic building blocks has received much attention. Here we present the results of a systematic and extensive computational study of hard polyhedral particles [1,2] and their subsequent assembly into a diverse range of complex structures. Our results show that 1) by utilizing more complex, anisotropically designed building blocks new structures can be self-organized purely from entropy maximization principles and, 2) a predictive criteria for assembly can be formulated, allowing for specific choices of building blocks given a target structure to be self-assemble. [1] Pablo F. Damasceno, Michael Engel & Sharon C. Glotzer. ACS NANO (2012). [2] Pablo F. Damasceno, Michael Engel & Sharon C. Glotzer. SCIENCE (2012).

12:51PM G30.00009 Design Rules for the Self-Assembly of Voronoi Particles, BENJAMIN SCHULTZ, University of Michigan, Dept. of Phys, PAULO DAMASCENO, University of Michigan, Dept. of App. Phys., MICHAEL ENGEL, University of Michigan, Dept. of Chem. Eng., SHARON GLOTZER, University of Michigan, Dept. of Phys., App. Phys., Chem. Eng. — Recent theoretical advances have developed methodologies for predicting the assembly of hard, polyhedral particles. In this work, we use the Voronoi tessellation to generate polyhedral shapes that form space-filling superlattices that are isostrophic to well-known atomic crystals. We focus on the assembly of these polyhedra into crystalline superlattices with orientational and positional order. Analogous to potentials designed to stabilize crystals at zero temperature, these particles are designed to stabilize the space-filling tiling at infinite pressure. We study a set of these particles in simulation and characterize how their symmetry and other geometric features affect their assembly characteristics at finite pressure. We calculate the relative stability of competing structures for several shapes that do not assemble their target structure and discuss how features of the shape affect this stability. From our conclusions, we demonstrate how to move beyond the concept of Voronoi tessellation for the design of hard polyhedral particles targeted for self-assembly.

1:03PM G30.00010 Self-assembly of binary space-tessellating compounds, MIHIR KHADILKAR, UMANG AGARWAL, FERNANDO ESCOBEDO, Cornell University — Self-assembly of polyhedral nanoparticles and their mixtures has been a topic of interest in both experimental and simulation studies due to its potential to help engineer novel materials. Hard-core mixtures that tessellate space are particularly interesting since they are expected to form entropy-driven high-pressure ordered structures. Using Monte Carlo simulations, we study three such binary tessellating mixtures; namely, cuboctahedra + octahedra (Mixture 1), octahedra + tetrahedra (Mixture 2), and truncated cubes + octahedra (Mixture 3). We see that upon gradual compression of the isotropic system, Mixture 1 and 2 form a metastable, glassy disordered phase while Mixture 3 demixes into a disordered phase and an unusual ‘semi-crystalline’ phase where truncated cubes form a cubic lattice while the octahedra remain disordered occupying interstitial pockets. While our results identify some relations between properties of individual species and their mixtures, they also illustrate the potential of tessellating mixtures as designable materials that can lead to novel equilibrium phases or serve as entropic glass formers. Preliminary results on non-tessellating binary mixtures will also be briefly discussed to provide a broader context of the results for the tessellating cases.
characteristic power laws. The conductivity is described in terms of correlations between quantum phase slip events. We find that the universal point contact conductivity is modified by the Villain duality. The magnetic field-induced diamagnetism is treated using a variational scheme developed by Benfatto et. al (2007) and of Josephson pair tunneling between parallel superconducting films in the presence of a transverse magnetic field, modeled as a 2+1 dimensional XY model, to that of the transition states and to measure the kinetics of the transitions. Combining experimental measurements of the kinetics with a recent theory using provides reversible bonds between the spheres. Analyzing time series of clusters of 3, 4, and 6 spheres allows us to compare the free energy of rigid configurations to that of the transition states and to measure the kinetics of the transitions. Combining experimental measurements of the kinetics with a recent theory using a geometrical approach for calculating energy landscapes leads to a new understanding of how hydrodynamics effect transitions rates between energy minima.

We further demonstrate control over the particle functionalization and coating by realizing patchy and Janus colloids. We further demonstrate control over the particle functionalization and coating by realizing patchy and Janus colloids.

1:15PM G30.00011 Targeted self-assembly of complex lattices and meta materials from isotropic interactions , OSKAR LINDGREN, ERIK EDLUND, MARTIN NILSSON JACOBI, Chalmers University of Technology — I will present an analytical method for designing isotropic interactions causing particles to self-assemble into complex lattices. The method is designed as opposed to previous trial and error schemes where the interactions are modified and tested until the desired pattern self-assembles. Since a naive implementation of the design scheme generally yields interaction potentials too complicated to implement experimentally, we provide a systematical simplification scheme to minimize the interaction potentials’ complexity without changing which pattern is produced by the self-assembly process. We also prove that our suggested simplification scheme is optimal. The method has been tested using simulated systems and proven to work for a wide range of patterns, ranging from chiral 2D surfaces to 3D diamond-like crystals. The recent improvements in simplicity for the designed potentials makes experimental realization feasible. The interactions can also be designed so that the self-organizing systems obtain different material properties like directional sound propagation or stealth-like properties via the diffraction pattern.

1:27PM G30.00012 Rheology of Self-Assembling Colloidal Chains , KAZEM V. EDMOND, STEFANO SACANNA, ZACHARY D. FORBES, ANDREW D. HOLLINGSWORTH, DAVID J. PINE, New York University — We probe the rheology of self-assembling chains of “pacman” particles using a Zimm viscometer, a modified Couette apparatus. Pacman particles are microscopic spherical particles specially designed to have a spherical indentation on their surface. In the presence of a depletion, overlap between the indentation and another particle’s surface maximizes the excluded volume between the two interacting particles, resulting in a selective attraction between them. Careful tuning of the interaction strength in a suspension of particles induces the formation of long chains. Shaving this material can twist, stretch, and break the chains, causing the material to exhibit unique rheological properties.

1:39PM G30.00013 Shaping Colloids for Self-Assembly , STEFANO SACANNA, NYU, GI-RA YI, Sungkyunkwan University, DAVID PINE, NYU — The creation of a new material often starts from the design of its constituent building blocks at a smaller scale. From macromolecules to colloidal architectures, to granular systems, the interactions between basic units of matter can dictate the macroscopic behavior of the resulting engineered material and even regulate its genesis. Information can be imparted to the building blocks by altering their physical and chemical properties. In particular, the shape of building blocks plays a fundamental role at the colloidal scale, as it can govern the self-organization of particles into hierarchical structures and ultimately into the desired material. Herein we report a simple and general approach to create an entire zoo of new anisotropic colloids. Our method is based on a controlled deformation of multiphase colloidal particles that can be selectively liquidified, polymerized, dissolved and functionalized in bulk. We further demonstrate control over the particle functionalization and coating by realizing patchy and Janus colloids.

1:51PM G30.00014 Probing transition pathways of self-assembled colloidal clusters1 , REBECCA W. PERRY, Harvard University, School of Engineering and Applied Sciences, MIRANDA HOLMES-CERFON, New York University, Courant Institute of Mathematical Sciences, MICHAEL P. BRENNER, Harvard University, School of Engineering and Applied Sciences, VINOTHAN N. MANOHARAN, Harvard University, School of Engineering and Applied Sciences and the Department of Physics — Clusters of colloidal particles bound by weak interactions explore rich energy landscapes characterized by a few minima and many higher-energy, non-rigid configurations. To investigate how such systems transit through their energy landscapes, we designed a two-dimensional system that lends itself to simple observations with brightfield video microscopy. In our aqueous system, a short-range depletion interaction strongly confines the diffusion of the spherical polystyrene colloids to a shallow volume close to a glass cover slip. The same depletion interaction provides reversible bonds between the spheres. Analyzing time series of clusters of 3, 4, and 6 allows us to compare the free energy of rigid configurations to that of the transition states and to measure the kinetics of the transitions. Combining experimental measurements of the kinetics with a recent theory using a geometrical approach for calculating energy landscapes leads to a new understanding of how hydrodynamics effect transitions rates between energy minima.

We acknowledge support from the NSF Graduate Research Fellowship Program

2:03PM G30.00015 Optical assembly of thermodynamically stable colloidal clusters mediated by depletion , BHASKAR JYOTI KRISHNATREYA, STEFANO SACANNA, KAZEM EDMOND, DAVID PINE, DAVID G. GRIER, New York University — Colloidal particles with complementary shapes can self-organize into composite structures under the influence of entropic attractions mediated by depletion. What structures can form is governed by the depletion itself to simple observations with brightfield video microscopy. In our aqueous system, a short-range depletion interaction strongly confines the diffusion of the spherical polystyrene colloids to a shallow volume close to a glass cover slip. The same depletion interaction provides reversible bonds between the spheres. Analyzing time series of clusters of 3, 4, and 6 allows us to compare the free energy of rigid configurations to that of the transition states and to measure the kinetics of the transitions. Combining experimental measurements of the kinetics with a recent theory using a geometrical approach for calculating energy landscapes leads to a new understanding of how hydrodynamics effect transitions rates between energy minima.

1:15PM G30.00011 Targeted self-assembly of complex lattices and meta materials from isotropic interactions , OSKAR LINDGREN, ERIK EDLUND, MARTIN NILSSON JACOBI, Chalmers University of Technology — I will present an analytical method for designing isotropic interactions causing particles to self-assemble into complex lattices. The method is designed as opposed to previous trial and error schemes where the interactions are modified and tested until the desired pattern self-assembles. Since a naive implementation of the design scheme generally yields interaction potentials too complicated to implement experimentally, we provide a systematical simplification scheme to minimize the interaction potentials’ complexity without changing which pattern is produced by the self-assembly process. We also prove that our suggested simplification scheme is optimal. The method has been tested using simulated systems and proven to work for a wide range of patterns, ranging from chiral 2D surfaces to 3D diamond-like crystals. The recent improvements in simplicity for the designed potentials makes experimental realization feasible. The interactions can also be designed so that the self-organizing systems obtain different material properties like directional sound propagation or stealth-like properties via the diffraction pattern.

11:15AM G36.00001 c-axis resistivity, pseudogap, superconductivity and Widom line in doped Mott insulators , GIOVANNI SORDI, Institut Laue-Langevin, Grenoble, France, PATRICK SEMON, Université de Sherbrooke, K. HAULE, Rutgers University, A.-M. S. TREMBLAY, Universite de Sherbrooke and Canadian Institute for Advanced Research — Layered doped Mott insulators, such as the cuprates, show unusual temperature dependence of the resistivity. We calculate the c-axis resistivity $\rho_{c}$ for the two-dimensional Hubbard model within plaquette cellular dynamical mean-field theory. The temperature and doping dependencies of $\rho_{c}$ are controlled by the first-order transition between pseudogap and correlated metal phases from which superconductivity can emerge. On the large doping side of the transition $\rho_{c}(T)$ is metallic, while on the low-doping side $\rho_{c}(T)$ changes from metallic to semi-conducting behavior with decreasing $T$. As a function of doping, the jump in $\rho_{c}$ across the first-order transition evolves into a sharp crossover at higher temperatures. This crossover coincides with the pseudogap temperature $T^{*}$ in the single-particle density of states, the spin susceptibility and other observables. Such coincidence in crossovers is expected along the continuation of the first-order transition into the supercritical regime.

11:27AM G36.00002 C-Axis Conductivity of a Layered Superconductor in a Transverse Magnetic Field , SHIMUL AKHANJEE, ROBERT KONIK, CPMPS Dept. Brookhaven National Laboratory — We study the temperature and field dependence of Josephson pair tunneling between parallel superconducting films in the presence of a transverse magnetic field, modeled as a 2+1 dimensional XY model, transformed under the Villain duality. The magnetic field-induced diamagnetism is treated using a variational scheme developed by Benfatto et. al (2007) and the conductivity is described in terms of correlations between quantum phase slip events. We find that the universal point contact conductivity is modified by characteristic power laws.

Tuesday, March 19, 2013 11:15AM - 2:03PM  —  Session G36 DCMP: Superconductivity: Transport Properties 344 - Zhiuan Xu, Zhejiang University, China

11:15AM G36.00001 c-axis resistivity, pseudogap, superconductivity and Widom line in doped Mott insulators , GIOVANNI SORDI, Institut Laue-Langevin, Grenoble, France, PATRICK SEMON, Université de Sherbrooke, K. HAULE, Rutgers University, A.-M. S. TREMBLAY, Universite de Sherbrooke and Canadian Institute for Advanced Research — Layered doped Mott insulators, such as the cuprates, show unusual temperature dependence of the resistivity. We calculate the c-axis resistivity $\rho_{c}$ for the two-dimensional Hubbard model within plaquette cellular dynamical mean-field theory. The temperature and doping dependencies of $\rho_{c}$ are controlled by the first-order transition between pseudogap and correlated metal phases from which superconductivity can emerge. On the large doping side of the transition $\rho_{c}(T)$ is metallic, while on the low-doping side $\rho_{c}(T)$ changes from metallic to semi-conducting behavior with decreasing $T$. As a function of doping, the jump in $\rho_{c}$ across the first-order transition evolves into a sharp crossover at higher temperatures. This crossover coincides with the pseudogap temperature $T^{*}$ in the single-particle density of states, the spin susceptibility and other observables. Such coincidence in crossovers is expected along the continuation of the first-order transition into the supercritical regime. The magnetic field-induced diamagnetism is treated using a variational scheme developed by Benfatto et. al (2007) and the conductivity is described in terms of correlations between quantum phase slip events. We find that the universal point contact conductivity is modified by characteristic power laws.

11:27AM G36.00002 C-Axis Conductivity of a Layered Superconductor in a Transverse Magnetic Field , SHIMUL AKHANJEE, ROBERT KONIK, CPMPS Dept. Brookhaven National Laboratory — We study the temperature and field dependence of Josephson pair tunneling between parallel superconducting films in the presence of a transverse magnetic field, modeled as a 2+1 dimensional XY model, transformed under the Villain duality. The magnetic field-induced diamagnetism is treated using a variational scheme developed by Benfatto et. al (2007) and the conductivity is described in terms of correlations between quantum phase slip events. We find that the universal point contact conductivity is modified by characteristic power laws.
11:39AM G36.00003 Low-frequency Electronic Transport Noise in La$_2$−$\delta$Ba$_3$CuO$_4$ Nanowires$^1$.

ADAM WEIS, YIZHOU XIN, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign — In the pseudogap regime, high temperature superconductors often exhibit electronic structure, such as charge stripes. Charge stripes pinned to disorder have been predicted to contribute to low-frequency resistance fluctuations when sample dimensions are comparable to the size of stripe domains (Carlson, 2006). We are extending our previous studies of resistance fluctuations in YBa$_2$Cu$_3$O$_{6−x}$ (Bonetti, 2004; Caplan, 2010) to thin films of La-based cuprates expected to have a more stable stripe phase, particularly in the regime near 1/8-filling. We present measurements of the low-frequency electronic transport in La$_2$−$\delta$Ba$_3$CuO$_4$ nanowires fabricated by pulsed laser deposition and lithographic techniques. We discuss temperature dependence of the power spectral density and its relevance to correlated electron phases above T$_c$.

$^1$This research was supported by the DOE-DMS under grant DE-FG02-07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

11:51AM G36.00004 Hall effect and ghost critical field in disordered superconducting films

NICHOLAS BREZNAY, AHARON KAPITULNIK, Stanford University — abstract—We observe a peak in the Hall resistance occurring at a magnetic field H$^*$ in superconducting disordered thin films. Below the zero-field transition temperature Tc0, H$^*$ exactly tracks the upper critical field, Hc2, all the way to zero field. Near Tc0, H$^*$ becomes vanishingly small, while above Tc0 the peak again scales to higher fields as the temperature is further increased. Companion measurements of the fluctuation magnetoconductance at temperatures above Tc0 allow precise and independent determination of the `ghost critical field' Hgc, the field scale for suppression of fluctuating supercurrents above Tc0. We find that H$^*$ and Hgc are distinct quantities but show similar scaling above Tc0, and compare these results to similar findings in studies of the Nernst effect in thin films [A. Pourret et al. Phys. Rev. B 76, 214504, (2007)] and high-temperature superconductors [J. Chang et al. Nature Physics 8, 751 (2012)].

12:03PM G36.00005 Comparing the specific heat to the cyclotron mass in two dopings of YBCO in the underdoped regime$^1$. JONATHON KEMPER, Florida State University/NHMFL, SCOTT C. RIGGS, Stanford University, O. VAFEK, Florida State University/NHMFL, A. MIGLIORI, J.B. BETTS, B.J. RAMSHAW, R.D. MCDONALD, F.F. BALAKIREV, Los Alamos Nat’l Lab/NHMFL, R. LIANG, D.A. BOND, University of British Columbia, G.S. BOEBINGER, Florida State University/NHMFL — Two underdoped High T$_c$ superconductors, YBa$_2$Cu$_3$O$_{5.1}$ and YBa$_2$Cu$_3$O$_{6.56}$, show finite electronic specific heat even in vanishing magnetic field and temperature as well as quantum magneto-oscillations at high magnetic fields. Previous results show the high-field electronic specific heat up to 45 T to be a sum of contributions from superconducting vortices and quantum magneto-oscillations, the latter a signature of an un-gapped Fermi surface. The vortex contribution appears as a smooth square-root field dependence at high magnetic fields. Previous results show the high-field electronic specific heat up to 45 T to be a sum of contributions from superconducting vortices and quantum magneto-oscillations, the latter a signature of an un-gapped Fermi surface. The vortex contribution appears as a smooth square-root field dependence at high magnetic fields.

$^1$Work funded in part by the DOE, NSF, and State of Florida.

12:15PM G36.00006 Exfoliated Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ thin flakes for electronic transport experiments

MENYOUNG LEE, MICHAEL NEUMANN, DAVID GOLDBADER-GORDON, Stanford University, LUKE SANDILANDS, KENNETH BURCH, University of Toronto, ZHIJUN XU, ALINA YANG, GENDA GU, Brookhaven National Lab — Bismuth-based cuprates are the model high-temperature superconductors of choice for experimental probes that are spectroscopic and sensitive to the surface (STM, ARPES), while studies of transport properties have typically focused on rare-earth element-based compounds. We will first discuss preparation methods for and characterization of tape-exfoliated single crystal Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ thin flakes. In addition, data from electronic transport measurements, aimed at observing a modulation of critical temperature and an insulator to superconductor transition as a function of hole density in the compound, will be presented.

12:27PM G36.00007 Nonlinear transport properties of La$_2$CuO$_4$/ La$_2$−$\delta$Sr$_3$ CuO$_4$ heterostructures in the resistive state

BO WEN, ROMAN YAKOBOV, M.P. SARACHIK, SERGEY VITKALOV, Physics Department, City College of the City University of New York, New York 10031, USA, A. BOLLINGER, I. BOZOVIC, Brookhaven National Laboratory, USA, A. SERGEEV, SUNY Research Foundation, SUNY at Buffalo, Buffalo, NY14226, USA — We report measurements of the nonlinear transport properties of oxide heterojunctions La$_2$CuO$_4$/La$_2$−$\delta$Sr$_3$ CuO$_4$ in the vicinity of the superconducting transition. The transition occurs over a wide temperature range (7-15K) and shifts to lower temperatures in the presence of a magnetic field, as expected. Strongly nonlinear behavior is observed for the Y−$\delta$ characteristic. At low bias currents the nonlinearity has a non-thermal origin close to the transition temperature and is strongly sensitive to magnetic fields. Above the middle of the superconducting transition the nonlinear behavior is consistent instead with electron heating with a value of electron-phonon thermal conductance of $\sim 10^{-6}$ W/K per square micron, which is significantly smaller than the thermal conductance of Nb and NbN ultrathin superconducting films. Our results indicate that this novel low-dimensional superconducting material shows great promise for substantial enhancement of direct detection and wide band mixing of radiation.

$^1$Work was supported by National Science Foundation (ECCS-1128459).

12:39PM G36.00008 Tuning the static spin stripe phase and superconductivity in La$_{2−x}$Ba$_x$CuO$_4$ ($x = 1/8$) by hydrostatic pressure

ZURAB GUGUCHIA, Physik-Institut der Universität Zurich, ALEXANDER SHENGELAYA, Department of Physics, Tbilisi State University, ALEXANDER MAISURADZE, Physik-Institut der Universität Zurich, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, GIORGi GHAMBASHIDZE, Department of Physics, Tbilisi State University, EKATERINA POMJAKUSHINA, KAZIMIERZ CONDER, Laboratory for Developments and Methods, Paul Scherrer Institute, HUGO KELLER, Physik-Institut der Universität Zurich — Muon spin rotation ($\mu$SR) and magnetization measurements were performed in stripe-stabilized La$_{1.875}$Ba$_{0.125}$CuO$_4$ as a function of pressure up to $p \approx 2.25$ GPa. At ambient pressure this system exhibits static spin stripe order below $T^{\text{SO}} \approx 30$ K. Zero-field $\mu$SR experiments indicate that the volume fraction $\omega$ of static spin-stripe order significantly decreases with increasing $p$, while the size of the ordered moment and the ordering temperature remain constant. The magnetization measurements show that the sample exhibits a tiny superconducting (SC) volume fraction at ambient pressure. However, by the application of pressure the SC phase volume increases proportionally to the non-magnetic volume fraction ($1-\omega$). These results indicate that in La$_{1.875}$Ba$_{0.125}$CuO$_4$ magnetism and superconductivity occur in mutually exclusive spatial regions.
of Texas at Austin

describing the mechanical properties of our samples. The microhardness values decreased with increasing Nd doping and applied load. Finally, the Hays-Kendall approach was determined as the most successful model. Furthermore, XRD and SEM measurements were analyzed for superconducting properties of (Sm123) \(_x\) (Nd123) \(_{1-x}\) superconducting samples which were fabricated by the solid state reaction method and annealed at 840°C for 72 h. For the comparison, an undoped sample was produced to the same conditions. The effects of Nd addition on structural and micromechanical properties were systematically investigated. The volume fraction, lattice parameters, crystal structure and grain size of the samples were characterized using the X-ray diffractometer and Scanning Electron Microscope. In addition, this study includes determination of the activation energy of Nd in the Bi-2212 system using the magnetoresistivity measurements. And also, we were investigated the mechanical properties for all samples using the Vickers microhardness measurements. Microhardness values of the samples decrease with increasing adding and applied load. The Vickers hardness of the samples studied, exhibits the typical indentation size effect (ISE).

1:03PM G36.00010 Resistivity of Sr\(_2\)RuO\(_3\) under uniaxial stress. DANILO BRODSKY, CLIFFORD HICKS, ANDREW P. MACKENZIE, University of St. Andrews — We report high precision resistivity measurements on single crystals of Sr\(_2\)RuO\(_3\) under in-plane uniaxial stress. A specially built probe enables the stress to be varied continuously whilst the sample is at low temperature. The needle-like shape of the samples ensures that the strain is homogeneous in the region probed. We compare results for different directions of applied stress relative to the crystal axes.

1:15PM G36.00011 Circuit influence on electron transport in hybrid superconductor—normal-metal nanostructures. VLADIMIR BUBANJA, Measurement Standards Laboratory of New Zealand, Industrial Research Ltd, Wellington, New Zealand, SHUICHI IWABUCHI, Department of Physics, Nara Women's University, Nara, Japan — We study the effects of the circuit impedance on transport properties of hybrid structures consisting of a superconductor tunnel-coupled to two normal-metal electrodes. At subgap conditions (i.e. at low voltages and temperatures with respect to the superconducting energy gap) the dominant transport mechanism of Cooper pairs is by Andreev reflection. We derive the analytic expressions for the direct and crossed Andreev current, and the elastic cotunneling current. The results can be used for improving the accuracy of hybrid devices employed in electrical metrology and for noise measurements in quantum information processing.

1:27PM G36.00012 Micro-mechanical and Structural Properties and Activation Energy Calculation of Nd2O3 Added Bi\(_2\)Sr\(_2\)Ca\(_1\)Cu\(_2\)O\(_y\) Superconducting System. OZGUR OZTURK, ELIF ASIKUZUN, MURAT COSKUNYUREK, SEYDANUR KAYA, Kastamonu University, Department of Physics 37100 Kastamonu-Turkey, MUSTAFA YILMAZLAR, Faculty of Education, Sakarya University 54300 Hendek, Sakarya-Turkey, GURCAN YILDIRIM, CABIR TERZIOGLU, Abant Izzet Bayaz University, Department of Physics 14280 Bolu-Turkey. — Nd added Bi-2212 superconducting samples with \(x = 0, 0.001, 0.005, 0.01, 0.05\) and 0.1 were prepared by conventional solid state reaction method and annealed at 840°C for 72 h. The experimental data of a number of single crystals which have the different crystal structure and different chemical bonding inside the polycrystallined samples were analyzed with the ISE models, the sample encountering with resistance and elastic deformation was observed as well as plastic deformation. The microhardness values on different surfaces of materials were calculated by using Meyer Law, PSR (proportional specimen resistance), modified PRS (MPSR) and Hays–Kendall (HK) approach. The results showed that the Hays-Kendall approach was determined as the most successful model. Furthermore, XRD and SEM measurements were analyzed for superconducting properties of (Sm123) \(_{1-x}\) (Nd123) \(_x\) superconducting system. The results showed that while Nd123 concentration is increasing, microhardness values at the minimum load and averaged plateau region of load.

1:39PM G36.00013 Analysis of Indentation Size Effect (ISE) Behavior in Low-Load Vickers Microhardness Testing of (Sm123)\(_{1-x}\) (Nd123)\(_x\) Superconductor System. SUKRU CELIK, R.T.E.U., Department of Physics, Rize, Turkey, OZGUR OZTURK, 2Kastamonu University, Department of Physics, Kastamonu, Turkey, ELYAAN COSKUN, R.T.E.U., Department of Physics, Rize, Turkey, ELIF ASIKUZUN, 2Kastamonu University, Department of Physics 37100 Kastamonu, Turkey, KEMAL OZTURK, K.T.U., Department of Physics, Trabzon, Turkey, CABIR TERZIOGLU, A.I.B.U., Department of Physics, Bolu, Turkey — Indentation size effect (ISE) for (Sm123)\(_{1-x}\) (Nd123)\(_x\) superconducting systems were investigated with the solid state reaction technique for values of \(x = 0.00, 0.05, 0.10, 0.20\), and 0.30 by analyzing the theoretical models. When the experimental data of a number of single crystals which have the different crystal structure and different chemical bonding inside the polycrystallined samples were analyzed with the ISE models, the sample encountering with resistance and elastic deformation was observed as well as plastic deformation. The microhardness values on different surfaces of materials were calculated by using Meyer Law, PSR model, MPSR model, EDP (Elastic / Plastic Deformation model) model and the Hays-Kendall (HK) approach. The results showed that the Hays-Kendall approach was determined as the most successful model. Furthermore, XRD and SEM measurements were analyzed for superconducting properties of (Sm123)\(_{1-x}\) (Nd123)\(_x\) superconductor system. The results showed that while Nd123 concentration is increasing, microhardness values at the minimum load and averaged plateau region of load.

1:51PM G36.00014 Investigation of Indentation Size Effect (ISE) of Bi\(_2\)Sr\(_2\)CaNd\(_x\)Cu\(_2\)O\(_y\) Superconducting System using Vickers Microhardness Test Method. ELIF ASIKUZUN, OZGUR OZTURK, SEYDANUR KAYA, MURAT COSKUNYUREK, Kastamonu University, Department of Physics, Kastamonu, Turkey, NEVIN SOYLU, AHMET VARILCI, CABIR TERZIOGLU, Abant Izzet Bayaz University, Department of Physics, Bolu, Turkey — In this work, the effects of Nd doping on the structural and mechanical properties of the samples were analyzed. Nd\(_2\)O\(_3\) doped Bi-2212 superconductors were obtained using solid state reaction method. Microhardness measurements were made to analyze the mechanical properties. XRD and SEM measurements were done for determination of crystal structure and surface morphology and calculation of the lattice parameters. The Vickers microhardness was calculated for undoped and doped samples. The experimental results of the microhardness measurements were analyzed using Kick’s Law, PSR (proportional specimen resistance), modified PRS (MPSR) and Hays–Kendall (HK) approach. The microhardness values of the samples decreased with increasing Nd doping and applied load. Finally, the Hays-Kendall (HK) approach was determined as the most successful model describing the mechanical properties of our samples.

Tuesday, March 19, 2013 2:30PM - 5:30PM –
Session J1 DCMP GMAG: Invited Session: Buckley Prize Session Ballroom I - Allan MacDonald, University of Texas at Austin
2:30PM J1.00001 Oliver E. Buckley Condensed Matter Prize Lecture: Transfer of spin momentum between magnets: its genesis and prospect. JOHN SLONCZEWSKI, Retired — Consider two nanoscopic monodomain magnets connected by a spacer that is composed of a non-magnetic metal or a tunnel barrier. Any externally applied electric current flowing through these three layers contributes tiny pseudo-torques to both magnetic moments (J.S. 1989). Such a weak spin-transfer torque (STT) may counteract and overcome a comparably small torque caused by viscous dissipation (L. Berger 1996; J.S. 1996). Any initial motion (e. g. excited by ambient temperature) of one moment (or both), may grow in amplitude and culminate in steady precession or a transient switch to a new direction of static equilibrium. In a memory element, the STT effect writes 0 or 1 in a magnetic-tunnel junction. Indeed, worldwide developments of memory arrays and radio-frequency oscillators utilizing current-driven STT today enjoy a nine-digit dollar commitment. But the fact that transfer of each half-unit of spin momentum $h/4\pi$ through a barrier requires the transfer of at least one unit of electric charge limits its efficiency. Arguably, STT should also arise from the flow of external heat, in either direction, between an insulating magnet, of ferrite or garnet (e. g. YIG) composition, and a metallic spacer (J.S. 2010). Whenever s-d exchange annihilates a hot magnon at the insulator/metal-spacee interface, it transfers one unit $h/2\pi$ of spin momentum to the spacer. Conduction electrons within the spacer will transport this spin momentum to the second current without requiring an electric current. Such a thermagnonic method, modestly powered by a Joule-effect heater, can substantially increase the efficiency of STT. Support for this prediction comes from (1) an estimate of the sd-exchange coefficient from data on spin relaxation in magnetically dilute (Cu,Ag,Au)Mn alloys; (2) a DFT computation (J. Xiao et al 2010); and (3) most persuasively, data from spin pumping driven across a YIG/Au interface by ferromagnetic resonance (B. Heinrich et al 2011; C. Burrowes et al 2012).

3:06PM J1.00002 Oliver E. Buckley Condensed Matter Prize Lecture: S-d Exchange, Spin Accumulation, And The Roots Of Spintronics , LUC BERGER, Carnegie Mellon University, Physics Dept. — The success of spintronics in metals such as nickel, cobalt, Ni-Fe and Ni-Co is based on the existence of high-mobility spin-up 4s electrons at the Fermi level, which carry most of the current. The spin-up Fermi level is located above the top of the 3d band. This basic fact, first recognized by Mott in 1936, was confirmed by the Hall-effect measurements of Pugh et al (1950-1965), and by data of deviation from Matthiessen’s rule by Campbell, Fert and Jaoul (1967-1977). In order to explain giant magnetoresistance and the existence of the spin-transfer torque, an interaction is needed which couples 4s conduction electrons to magnetic 3d electrons. This is the s-d exchange interaction, introduced by Vonsovski in 1946 and Zener in 1951. Theories of Gilbert damping, based on s-d exchange, were soon developed (Turov (1955), Mitchell (1957)). But a serious problem was caused by the existence of a momentum gap between spin-up and spin-down Fermi surfaces, which prevents spin switching from happening at low T. The problem can be solved if local defects exist which act as extra sources of momentum. One such source is spin-flip scattering (Turov (1961), Heinrich, Freitova and Kambersky (1967)). A second one is the presence of an interface (Slonczewski (1996), Berger (1996)). Spin accumulation is another concept of importance to spintronics. It represents an imbalance between spin-up and spin-down Fermi levels. Introduced by Aronov in 1976, it was developed by Johnson and Slisbee (1985-1993) and by Valet and Fert (1993). It is the hidden agent through which the current “pumps” energy into many spintronics devices. In semiconductor lasers, the same role is played by the difference between conduction-band and valence-band Fermi levels.

3:42PM J1.00003 From point contacts to spin-transfer torque1, MAXIM TSOI, University of Texas at Austin — Point contacts - nanoscale electrical contacts between conductors - have been around for decades and proved to be unique experimental tools for studying the electronic transport properties of metals. Following the theoretical prediction of spin-transfer torque (STT) by John Slonczewski [1] and Luc Berger [2], point contacts were instrumental for the first experimental demonstration of STT in spin-valve multilayers [3], thanks to extremely high current densities routinely produced in such contacts. In this talk I will briefly review the point-contact technique and its contributions to the field of current-induced control over magnetic nanostructures.


4:18PM J1.00004 to be determined, DANIEL RALPH, Cornell Univ — No abstract available.

4:54PM J1.00005 The Spin Torque Lego - from spin torque nano-devices to advanced computing architectures1, JULIE GROLLIER, CNRS/Thales laboratory, Palaiseau, France — Spin transfer torque (STT), predicted in 1996 [1], and first observed around 2000, brought spintronic devices to the realm of active elements. A whole class of new devices, based on the combined effects of STT for writing and Giant Magneto-Resistance or Tunnel Magneto-Resistance for reading has emerged. The second generation of MRAMs, based on spin torque writing : the STT-RAM, is under industrial development and should be out on the market in three years. But spin torque devices are not limited to binary memories. We will rapidly present how the spin torque effect also allows to implement non-linear nano-oscillators, spin-wave emitters, controlled stochastic devices and microwave nano-detectors. What is extremely interesting is that all these functionalities can be obtained using the same materials, the exact same stack, simply by changing the device geometry and its bias conditions. So these different devices can be seen as Lego bricks, each brick with its own functionality. During this talk, I will show how spin torque can be engineered to build new bricks, such as the Spintronic Memristor, an artificial magnetic nano-synapse. I will then give hints on how to assemble these bricks in order to build novel types of computing architectures, with a special focus on neuromorphic circuits.


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Tuesday, March 19, 2013 2:30PM - 5:30PM –
Session J2 DCMP: Invited Session: Topological States and Plasmonics in Graphene Ballroom II - Qian Niu, University of Texas at Austin

2:30PM J2.00001 Topological insulator gap in graphene with heavy adatoms. RUQIYAN WU1, University of California, Irvine — It is important to search an effective approach to expand the spin-orbit coupling gap of graphene for the realization of the two-dimensional topological insulator (TI) state. We found that heavy In or TI adatoms may dramatically enhance the gap to detectable values of order 7 or 20 meV, large enough for the realization of quantum spin Hall effect in experimental conditions. However, In and TI atoms may easily coalesce on graphene due to their weak binding energies and shallow segregation barriers. We proposed a new way to produce a two-dimensional spin-orbit coupling gap using the impurity bands that are mediated by graphene. First principles calculations predict that the gaps generated by osmium and iridium exceed 200 meV over a broad range of adatom coverage. The position of the Fermi level can be manipulated by using external electric field and co-adsorbates. The mechanism at work is expected to be rather general and may open the door to designing new TI phases in many materials.

1 Co-Authors: J. Hu, J. Alicea, and M. Franz
3:06PM J2.00002 Engineering topological states in graphene systems , ZHENHUA QIAO 1, Department of Physics, The University of Texas at Austin, Austin, Texas, USA — In this talk, I will introduce our recent progress on engineering various topological states in graphene systems. The presentation includes two parts: (i) We show that in monolayer graphene, Rashba spin-orbit coupling (SOC) together with Zeeman field can open a nontrivial bulk gap to host the quantum anomalous-Hall effect [1]. We further show that this can be realized via doping magnetic metal atoms on graphene [2,3]. In Bernal stacking bilayer graphene, an interlayer potential difference breaks the inversion symmetry and opens a bulk gap to support the quantum valley-Hall effect. We find that Rashba SOC can induce a topological phase transition from the quantum valley-Hall effect to a Z2 topological insulator [4]. When the Zeeman field is further considered, a rich variety of topological phases emerge. (ii) When the mass term (e.g., sublattice potential in monolayer graphene, or interlayer potential difference in bilayer graphene) varies spatially, topologically protected 1D kink states arise along zero lines. We demonstrate that such 1D kink state exhibits zero bend resistance for arbitrary turns in its propagating path [5]. We further point out that similar kink states can be tailored in graphene nanorods in boron nitride sheets [6]. When the kink current experiences a crossing junction composed of four zero lines, we find the splitting of the 1D kink state at the bifurcation point obeys an explicit law of current partition [7].

References:
[7] Z.H. Qiao et al., to be submitted.

1 Collaborators: Shengyuan A. Yang, Wanxiang Feng, Jun Ding, Jeil Jung, Wang-Kong Tse, Chuangwei Lin, Hua Jiang, Haiwen Liu, Junren Shi, Jian Wang, Yuqiu Yao, Allan H. MacDonald, and Qian Niu

3:42PM J2.00003 Giant Rashba effect and spin polarization of Dirac fermions in graphene , OLIVER RADER, Helmholtz-Zentrum Berlin — Graphene in spintronics has so far meant a material with low spin-orbit coupling which could be used as high-performance spin current leads. If the spin-orbit interaction could be enhanced by an external effect, the material could serve also as an active element in a spintronics device such as the Das-Datta spin effect field transistors. We show that by intercalation of Au under graphene grown on Ni(111), a Rashba-type spin-orbit splitting of ~100 meV can be created in a wide energy range while the Dirac cone is preserved and becomes slightly p-doped. We discuss different superstructures of Au under the graphene which are observed in the experiment. Ab initio calculations indicate that a sharp graphene-Au interface at the equilibrium distance accounts for only ~10 meV spin-orbit splitting and enhancement can occur due to Au atoms in the hollow position that get closer to graphene while preserving the sublattice symmetry. For the system graphene/Ir(111) we observe a large splitting of the Dirac cone as well. The large lattice mismatch of this system allows us to investigate properties of the pseudospin that are related to the structure of minigaps that occur at the zone boundary of the superstructure. We also report on the giant Rashba splitting of an Ir(111) surface state which persists underneath the graphene. Finally, we re-investigate with p(1×1) graphene/Ni(111) and Co(0001) typical examples where the sublattice symmetry breaking by the substrate is believed to lead to a large band gap at the Dirac point. We show that this is not the case and the Dirac point of graphene stays instead intact, and we discuss implications of this finding.

Supported by SPP 1459 of the Deutsche Forschungsgemeinschaft.

4:18PM J2.00004 Infrared nano-imaging and nano-spectroscopy of graphene plasmons , ZHENG LI, University of California, San Diego — Graphene plasmons, which are collective oscillations of Dirac fermions in graphene, are of broad interests in both fundamental research and technological applications. In this talk, we present first nano-imaging and nano-spectroscopy studies of graphene plasmons using scattering-type scanning near-field optical microscope—a unique technique allowing efficient excitation and high-resolution imaging of graphene plasmons. With this technique, we were able to show that common graphene/SiO2/Si back-gated structure support propagating surface plasmons in the infrared frequencies. The observed plasmons are highly confined surfaces modes with a wavelength around 200nm that are conveniently tunable by the back gate voltages [Nature 487, 82–85 (2012)]. In addition, we performed nano-spectroscopy of graphene over a broad range of mid-infrared frequencies. Our spectroscopy results provide evidence of strong coupling between graphene plasmons and SiO2 optical phonons [Nano Lett. 11(11), 4701-4705 (2011)]. Finally, we were able to map and characterize various types of line defects inside CVD graphene film by exploring real space patterns of propagating surface plasmons. These line defects, including cracks, wrinkles, and even grain boundaries, trigger distinct plasmonic features due to plasmon interference. Further modeling and analysis unveiled unique electronic properties associated with these line defects.

4:54PM J2.00005 Quantum Anomalous Hall Effects and Topological Phase Transitions in Silicene , MOTOKIBO EZAWA, Department of Applied Physics, University of Tokyo — Silicene is a monolayer of silicon atoms forming a two-dimensional honeycomb lattice, which is experimentally manufactured this year. The low energy theory is described by Dirac electrons, but they are massive due to a relatively large spin-orbit interaction. I will explain the following properties of silicene: 1) The band structure is controllable by applying an electric field [1]. Silicon undergoes a phase transition from a topological insulator to a band insulator by applying external electric field [1]. 2) The topological phase transition can be detected experimentally by way of diamagnetism [7]. 3) There is a novel circular dichroism and spinvalley selection rules by way of photon absorption [6]. 4) SiCene shows a quantum anomalous Hall effects when ferromagnet is attached onto silicone [3]. 5) SiCene shows a photo-induced quantum Hall effects when we apply strong laser onto silicone [8]. 6) Single Dirac cone state emerges when we apply photo-irradiation and electric field, where the gap is open at the K point and closed at the K’ point [8].

References:

Tuesday, March 19, 2013 2:30PM - 5:30PM –
Session J3 DCMP GSNP: Invited Session: Colloidal Carbon Nanotubes
Ballroom III - Erik K. Hobbie,
North Dakota State University
2:30PM J3.00001 Soft Materials Approaches to Carbon Nanotubes: from Gels to Composites

MOHAMMAD ISLAM, Carnegie Mellon University — Carbon nanotubes combine low density with exceptional mechanical, electrical and optical properties. Unfortunately, these nanoscale properties have not been retained in bulk structures. I will describe surface modification assisted self-assembly of single wall carbon nanotube into macroscopic nanotube networks - hydrogels and aerogels. The nanotube networks are ultra-lightweight, electrically conducting and thermally insulating. The shapes and sizes of these nanotube networks are readily tunable and is a tremendous strength of our fabrication method. The interesting properties and structure of these nanotube networks make them suitable for diverse applications. For example, we have used these networks as scaffolds to enhance elastic modulus of polymers by 36,000%. The porous nanotube networks also show high capactiance, and can be impregnated with catalysts nanoparticles at high loading, which can then be simultaneously used as electrodes and catalysts supports in electrochemical cells. A weakness of the nanotube networks is their fragility – but we have recently developed a method to transform these inelastic networks into superelastic materials by coating them with between one and five layers of graphene nanoplates.

3:06PM J3.00002 Connectedness percolation of carbon nanotube dispersions: impact of interactions, polydispersity and external fields

PAUL VAN DER SCHOOT, Department of Applied Physics, Eindhoven University of Technology — There is considerable industrial interest in novel flexible, transparent electrodes for electro-optical applications, in part because of dwindling natural reserves of indium, a component of transparent electrodes used, e.g., in LCD display technology. For this purpose, frantic research is currently being conducted worldwide into polymeric composites containing electrically conducting inorganic and metallic nanowires, carbon nanotubes, graphite flakes, graphene, and so on. One of the objectives is to get as high as possible a conduction for as low as possible a nanoparticle loading but progress is slow. Unclar is why, e.g., carbon nanotubes dispersed in plastic matrix materials can have such widely diverging electrical percolation thresholds, even when their mean physical dimensions and other characteristics seem very similar. In our attempt to shed light on this, we apply continuous space connectedness percolation theory to collections of anisometric particles with arbitrary polydispersity in length, width and levels of conduction between them. We find that the percolation threshold is extremely sensitive to even quite modest degrees of polydispersity and of alignment induced in the processing of the fluid composites before they set and become the final solid product. We find that the way polydispersity influences the percolation threshold depends on whether or not the length and width distributions are coupled or not. Finally, we provide an explanation why composites with graphene filler seems to have a larger percolation threshold than those with carbon nanotubes.

3:42PM J3.00003 Fluid Phases of Carbon Nanotubes and Graphene

MATTEO PASQUALI, Department of Chemical & Biomolecular Engineering and Chemistry, The Smalley Institute for Nanoscale Science and Technology, Rice University — Nanoscale carbon— including Carbon Nanotubes (CNTs) as well as graphene, i.e., graphite in its single layered form—has remarkable electrical, thermal, and mechanical properties, more so than previously known polymer molecules or colloidal particles. Realizing these properties in applications requires understanding and controlling the behavior of fluid phases of CNTs and graphene. Biological and environmental applications are likely to require dilute phases of CNTs and graphene; material processing, e.g., production of coatings and fibers, will require more concentrated phases. Fluid processing is one of the most important fronts of applied research in CNTs and graphene. Nano-carbon fluids are almost considered an oxymoron because dispersing or dissolving CNTs and graphene into fluid phases is exceedingly difficult. This talk reviews advances in understanding and controlling fluid phases of CNTs and graphene, with specific focus on single-object properties and true solutions. The dynamics of individual CNTs can be studied by fluorescence microscopy, revealing that their translational and rotational motion and bending stiffness can be described well by the semiflexible chain model. Even at low concentrations (few parts per million), CNTs form complex fluid phases with intriguing properties. In strong acids, CNTs as well as graphene dissolve spontaneously. At low concentration, these fluids can be used for making transparent, conducting films and coatings. In crowded environments, CNTs reapeate like stiff polymers. At sufficiently high concentrations, CNTs and graphene form liquid crystals that can be spun into well-aligned, macroscopic fibers. Like in polymeric systems, the properties of macroscopic CNT materials depend on the length (molecular weight) of the constituent CNT macromolecules.

4:18PM J3.00004 Field-assisted assembly and orientational order of colloidal ellipsoids

MICHAEL SOLOMON, University of Michigan — Colloidal particles with anisotropy in shape and interactions can potentially be assembled into colloidal crystalline solids with unusual structure and geometry. Field-assisted assembly is a means to produce structures that are otherwise difficult to achieve by equilibrium self-assembly. Here we show, by means of confocal microscopy direct visualization, how controlled application of electric fields can improve general prospects for assembly of any anisotropic colloid. By studying the model case of ellipsoidal colloidal rods, we find that applied fields can be designed which produce liquid crystal phases of colloids in a simple, versatile manner. By directly visualizing the assembled particles in three dimensions we learn that the quality of orientational order achieved is comparable to that of materials such as liquid crystalline polymers. We understand the results in terms of the underlying electrokinetics of the system as well as connect the observed field-induced orientational order to the equilibrium isotropic-nematic transition predicted for rods with prolate spheroidal shape. Specifically, the applied field generates a force that is balanced by a gradient in osmotic pressure generated by the density dependence of the rod suspension. If the field strength is sufficiently large, the resultant osmotic pressure produces a phase transition. We discuss how the required field conditions for assembly can be tailored based on the shape and size of the anisotropic building block.

4:54PM J3.00005 DNA-wrapped Carbon nanotubes as a model rod-like colloid system

MING ZHENG, National Institute of Standards and Technology — Single-wall carbon nanotubes (SWCNTs) exhibit many fascinating physical behavior as the result of their quasi one-dimensional crystalline structures. SWCNTs can be dispersed into rod-like colloid particles by a few small molecules and polymers, among which the most one effect is single-stranded DNA (Nature Materials 2, 338, 2003). The structure of a DNA-SWCNT hybrid is controlled by both the sequence of the wrapping DNA, and the atomic configuration, or chirality, of the SWCNT (Science 302, 1545, 2003). This has been exploited by us to purify single-chirality SWCNTs from synthetic mixtures via liquid chromatography (Nature 460, 250, 2009; JACS 133, 12998, 2011). DNA-SWCNTs have well-defined surface structures, tunable aspect-ratios, and ultra-small diameters. These attributes provide unique advantages to the DNA-SWCNT colloid system in probing inter-particle interactions in crowded and high salt environment (ACS Nano 5, 8258, 2011). In this talk, I will present some recent observations we made on DNA-SWCNT clustering that shed new light on the Hofmeister effect.

Tuesday, March 19, 2013 2:30PM - 5:30PM
Session J12 DCMP: Topological Insulators: Magnetic Transport and Weak Localization

2:30PM J12.00001 ABSTRACT WITHDRAWN
2:42PM J12.00002 Transport Signatures of the Quantum Anomalous Hall Effect in 3D Topological Insulators 1, BRIAN DELLABETTA, TAYLOR HUGHES, MATTHEW GILBERT, University of Illinois at Urbana-Champaign — The unique physics of spin-orbit coupled topological insulators (TIs) exposed to magnetic moments leads to a quantized conductance known as the quantum anomalous Hall effect (QAHE). While magnetic disorder has been experimentally shown to open a gap in the surface states of TIs, no clear transport signatures of the QAHE have been observed in 3-dimensional TIs. We perform 3D real space calculations using the Non-Equilibrium Green’s Function Formalism to show that topological insulators in proximity to arrays of ferromagnets offer a unique environment in which to study this phenomenon. We show that ferromagnetic domain walls on patterned surfaces manifest chiral surface modes with quantized currents that can be altered by changing the configuration of the magnetic arrays. We compare topologically trivial and nontrivial models to show a qualitative difference in the induced transport flow based on ferromagnet orientation, and propose a variety of experimental configurations which yield transport signatures of the QAHE.

1We acknowledge support from the AFOSR under grant FA9550-10-1-0459.


2:54PM J12.00003 Singular spin response of topological insulators in ac magnetic fields 1, HAIMING DENG, LUKAS ZHAO, INNA KORZHOVSKA, ZHIYI CHEN, LIA KRUSIN-ELBAUM, City College of New York — Orbital magnetic susceptibility in weak magnetic fields has several contributions whose physical origin is not simple in contrast to the clear Landau diamagnetism of free electrons. Experimentally, anomalous magnetism has been observed in graphite, and bismuth and Bi-Sb alloys, both of which are narrow gap semimetals. Here we report on the identification of a singular response in ac magnetic susceptibility — a suppression of diamagnetism at magnetic fields that appears ubiquitous in all topological insulators (SbBi2Se3, PbBi2Se3) we have studied. We observe two distinct contributions to this effect: a broader one that typically disappears around 40-50 K and is likely related to edges, and a divergent-like one (in the $H \rightarrow 0$ limit) that is robust up to room temperature and is likely related to the bulk. The frequency dependence and the dependence on the Fermi level of these effects will be discussed in the context of separation of orbital and spin effects.

1Supported in part by NSF-DMR-1122594.

3:06PM J12.00004 Magnetoresistance in thin Bi2Te3 layers contacted by Indium (In) superconducting electrodes, ZHUO WANG, RAMESH MANI, Georgia State University — Topological Insulators (TIs) are materials that insulate in the bulk but conduct electricity on their surfaces, which topologically protected by time-reversal symmetry. Transport measurements of topological insulators in the proximity of a superconductor are theoretically predicted to be a significant method to detect Majorana Fermions. Our experiment studied the interplay between superconductivity and TI surface states below the critical temperature of a type-I superconductor. Here, we used the four terminal lock-in technique to study the transport properties of Bi2Te3 specimens contacted by Indium superconducting electrodes, while sweeping perpendicular magnetic field, at T < 4.2 K. The results indicate a sharp suppression of the longitudinal resistance at weak magnetic fields, below the critical temperature of Indium. What’s more exciting is that the interaction between superconductivity and TI surface states induces resistance enhancement at T ≤ 2.8K, well below the critical temperature of Indium, in the absence of a magnetic field.

3:18PM J12.00005 ABSTRACT WITHDRAWN

3:30PM J12.00006 Magneto-optical Studies of Bi2Te3 Flakes, LI-CHUN TUNG, University of North Dakota, WENLONG YU, ZHIGANG JIANG, Georgia Institute of Technology, DIMITRY SMIRNOV, 1National High Magnetic Field Laboratory-Tallahasseee — Magneto-transmittance spectroscopy is used to probe the magnetic-field induced excitations in topological insulator-Bi2Te3. Bi2Te3 single crystals are repeatedly exfoliated on scotch tape until the sample flakes are sufficiently thin and become permeable in the infrared frequency range. The sample with the underlying tape is placed in a 4K cryostat and the magneto-optical properties of Bi2Te3 are investigated by a broadband Fourier-Transform infrared spectrometer (Bruker 66) using light-pipe optics. The magneto-transmittance data of the sample on the tape and the bare tape up to 35T are collected and analyzed as a stacked multilayer. The average conductivity of the sample flakes at different magnetic fields is evaluated and several magnetic-field dependent features are revealed. These features coincide with the cyclotron resonance energy of the bulk band electrons and potentially linked to the surface state electrons. Implications of these results will be discussed in the presentation.

3:42PM J12.00007 Spin-orbit scattering in quantum diffusion of massive Dirac fermions, WENYU SHAN, Wean Hall 6424, Carnegie Mellon University, 5000 Forbes Ave, Pittsburgh — We theoretically study the effects of spin-orbit scattering on weak (anti-)localization in two-dimensional massive Dirac systems. We clarify that weak anti-localization and localization of a single massive Dirac cone come from the diffusion of a singlet Cooperon in the massless limit and one of triplet Cooperons in the large-mass limit, respectively. Spin-orbit scattering behaves like random magnetic scattering to the triplet Cooperon, and suppresses the weak localization in the large-mass regime, different from conventional systems where spin-orbit scattering leads to a crossover from weak localization to antilocalization. This behavior suggests an experiment to detect the weak localization of bulk subbands in topological insulator thin films, in which an enhancement of "weak anti-localization" is expected after doping heavy-element impurities. Finally, we compare the conventional electron and Dirac fermion systems in the quantum diffusion transport under ordinary, spin-orbit, and magnetic scattering.

3:54PM J12.00008 Transport properties of SnPbTe topological crystalline insulator films 1, BADIH A. ASSAF, Dept. of Physics, Northeastern University, FERMAT KATMIS, Francis Bitter Magnet Lab, Dept of Physics, MIT, PENG WEI, Francis Bitter Magnet Lab, MIT, JAGADEESH S. MOODERA, Francis Bitter Magnet Lab, Dept of Physics, MIT, DON HEIMAN, Dept. of Physics, Northeastern University — A new phase of topological insulators, the topological crystalline insulator, has been recently predicted to arise in band-inverted Sn-Pb chalcogenides, where the topological surface states are protected by crystal symmetry instead of spin-orbit coupling [1]. We grew epitaxial thin films of SnTe and Sn1−xPbxTe by MBE and sputtering on (100) and (111) surfaces of BaF2 and Si. We report on magnetotransport measurements on SnTe films having hole densities ranging between 10^{16} and 10^{18} cm^{-2} and mobilities up to 200 cm^{2}/Vs. Weak antilocalization is observed in all films, allowing us to study the behavior of the phase coherence length versus temperature in an attempt to shed light on the dimensionality of the transport as a function of the Fermi level. Some evidence of 2D transport is found in low carrier density films. [1]T. H. Hsieh et al. Nature Communication 3, 982 (2012).

1Work supported by NSF-DMR-0907007, NSF-DMR-0504158, ONR N00014-09-1-0177 and NSF-DMR-0819762 (CMSE initiative 2).

4:06PM J12.00009 ABSTRACT WITHDRAWN
4:18PM J12.00010 Kondo resistance minimum in topological insulators, JIE WANG, DIMITRIE CULCER, ICQD, University of Science and Technology of China — We present a theory of the Kondo resistance minimum applicable to topological insulators (TI) and spin-orbit coupled semiconductors in the high-temperature limit, defined as $T > T_K$, the Kondo temperature. We derive the $T$-matrix for a general strongly spin-orbit coupled system, including the many-body Kondo scattering terms. The physics is qualitatively different from the well-known case of metals due to the interplay of impurity degrees of freedom with the spin-orbit induced spin-momentum locking of the conduction electrons. TI have a single Fermi surface, while in spin-orbit coupled semiconductors scattering between the two spin-split Fermi surfaces must be taken into account. We determine the resistance minimum and Kondo temperature, and comment briefly on Kondo screening and Kondo singlet formation in the presence of strong spin-orbit coupling.

4:30PM J12.00011 Competing weak localization and weak antilocalization in ultrathin topological insulators. MURONG LANG, LIANG HE, XUFENG KOU, PRAIMEY UPADHYAYA, YABIN FAN, UCLLA, HAO CHU, NAI-CHANG YEH, California Institute of Technology, KANG WANG, UCLA — We demonstrate the evidence of a surface gap opening in $\langle Bi_{0.75}Sb_{0.25}\rangle_2Te_3$ samples for film thickness below 6 quintuple layers, through magnetotransport and scanning tunneling spectroscopy measurements. By tuning Fermi level position relative to the gap, the striking crossover between weak antilocalization and weak localization is observed in nonmagnetic 4 and 5 QL films at low field region, a characteristic feature of quantum interferences competition, possibly owing to the change of net Berry phase. Furthermore, when the Fermi level is swept into the surface gap, the overall unitary behaviors are revealed at higher magnetic field, which are in contrast to the pure WAL signals obtained in thicker films. Besides, the surface gap of ultrathin film is also determined by low temperature STS measurements. Our findings show an exotic phenomenon characterizing the gapped TI surface states and point to the future realization of quantum spin Hall effect and dissipationless TI-based applications.

4:42PM J12.00012 Weak anti-localization in ultrathin Sb(111) films, S. CAIRNS, N. MCCLOHON, C. ROBISON, J. KEAY, C.K. GASPE, K.S. WICKRAMASINGHE, T.D. MISHIMA, M.B. SANTOS, S.Q. MURPHY, University of Oklahoma, Norman — We report the first studies of localization in ultrathin Sb films. Sb is a topological semi-metal with a negative bandgap of 180meV, however it is anticipated that in ultra-thin films, quantum confinement will open the bulk gap, such that transport is dominated by the topological surface states. We have studied the magneto-transport of nominally 4.5nm thick films of Sb(111) grown via molecular beam epitaxy at a temperature of 300$^\circ$C on nearly lattice matched epilayers. The longitudinal response is consistent with that of a single conducting channel with a phase breaking length of $\sim$200nm at 1.8K. Scanning electron microscopy shows that the Sb growth proceeded by a Volmer-Weber (islanding) process resulting in disordered films. More recent growths performed at lower temperature have yielded significantly less resistive, smoother and thinner films for which transport measurements are ongoing.

4:54PM J12.00013 Weak-Localization-Like Magnetoresistance on a Topological Insulator - Ferromagnetic Insulator Interface, QI YANG, MERAV DOLEV, LI ZHANG, Stanford University, JINFENG ZHAO, University of California, Davis, MIN LIU, Stanford University, SUBHASH RISBUD, University of California, Davis, ALEXANDER PALEVSKI, Tel Aviv University, Isreal, AHARON KAPITULNIK, Stanford University — In this talk, we will present measurements on the interface between a topological insulator (TI) and a ferromagnetic insulator (FI). The results provide a likely indication for gap opening in the FI surface states by its proximity to the FI. While above the Curie temperature ($T_C$) of the FI we observed weak-antilocalization-like positive magnetoresistance as ubiquitously in TIs, below $T_C$ an unusual weak-localization-like negative magnetoresistance was seen at low magnetic fields, which has never been observed in TIs without any magnetic doping. Such proximity introduced gap-opening and resulting massive Dirac fermions will hopefully lead to realization of many intriguing phenomena such as the quantum anomalous Hall effect and the inverse spin-galvanic effect.

5:06PM J12.00014 Weak Localization and Antilocalization in Topological Insulator Thin Films with Coherent Bulk-Surface Coupling, ION GARATE, LEONID GLAZMAN, Yale University — We evaluate quantum corrections to conductivity in an electrically gated thin film of a three-dimensional (3D) topological insulator (TI). We derive approximate analytical expressions for the low-field magnetoresistance as a function of bulk doping and bulk-surface tunneling rate. Our results reveal parameter regimes for both weak localization and weak antilocalization, and include diffusive Weyl semimetals as a special case.

5:18PM J12.00015 Coherent Topological Transport on the Surface of Bi$_2$Se$_3$, DOHUN KIM, PAUL SYERS, Department of Physics, University of Maryland, NICHOLAS P. BUTCH, Condensed Matter and Materials Division, Lawrence Livermore National Laboratory, JOHNPIERRE PAGLIONE, MICHAEL S. FUHRER, Department of Physics, University of Maryland — We report weak anti-localization (WAL) measurements in gate-tuned, bulk insulating Bi$_2$Se$_3$ thin crystals with thicknesses varying between 5 and 17 nm. The gate-voltage dependent WAL behavior shows systematic variation as a function of crystal thickness. For the thickest samples, we observe two decoupled surfaces exhibiting perfect WAL as expected for the symplectic class. As the films are made thinner, we observe a gate-voltage tuned crossover from two decoupled surfaces to a single coherently coupled 2D system exhibiting WAL. The observed crossover is governed by competition between the phase coherence time and inter-surface tunneling time associated with the hybridization gap. In contrast to classical transport in which the signature of the hybridization gap appears only in the ultrathin limit (< 3nm), phase coherent transport is extraordinarily sensitive to sub-meV coupling between top and bottom topological surfaces, and the surfaces of a TI film may be coherently coupled even for thicknesses as large as 12 nm. On further thinning, the WAL behavior is suppressed altogether at small carrier density, which we associate with the opening of a sizable gap on order the Fermi energy and destruction of topological protection.
2:30PM J18.00001 Correlated effects in topological phase transitions. HSIANG-HSUAN HUNG, Department of Physics, The University of Texas at Austin, Austin, TX, 78712, USA, LEI WANG, Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland, ZHENG-CHENG GU, Institute for Quantum Information, California Institute of Technology, Pasadena, California 91125, USA, GREGORY A. FIELTE, Department of Physics, The University of Texas at Austin, Austin, TX, 78712, USA — Correlation effects in topological phases have been a central topic of interest, yet elusive in experiment. In this talk, we present the results of a numerical study beyond mean-field theory of a phase transition between a two-dimensional Z2 topological insulator phase and a trivial insulator that is driven by correlation effects. In addition to the Z2 invariant, we find that certain features of the single-particle Green’s functions (simpler to compute than the full Z2 invariant) carry important information that are strongly indicative of a non-trivial Z2 topological character. We observe that the fluctuations originating from correlations tend to move the topological phase transition boundary to larger values of interactions.

2:42PM J18.00002 Topological insulators of interacting bosons in two dimensions: Classification, effective field theory and microscopic construction, YUAN-MING LU, ASHVIN VISHWANATH, University of California, Berkeley — While topological insulators of non-interacting fermions have been extensively studied, we know very little about topological insulators of bosons, whose realization necessitates strong interaction. In this work we apply Chern-Simons effective theory to classify and characterize interacting bosonic topological insulators in two spatial dimensions. These topological phases have a unique ground state on any closed manifold and no fractional excitations: yet they feature gapless edge states which are often protected by a symmetry. Examples include a bosonic analog of chiral superconductors, bosonic integer quantum Hall states (with Hall conductance quantized to even integers) and bosonic analog of the quantum spin Hall state. We show that these topological phases can be constructed in various ways: such as in arrays of coupled one-dimensional quantum wires. Our formulation also naturally applies to topological insulators of two-dimensional interacting fermions.

2:54PM J18.00003 Topological parity invariant in interacting two-dimensional systems from quantum Monte Carlo, THOMAS C. LANG, Department of Physics, Boston University, VICTOR GURARIE, ANDREW M. ESSIN, Department of Physics, University of Colorado, STEFAN WESSEL, Institute for Theoretical Solid State Physics, RWTH Aachen University — We report results on calculating the parity invariant from Green’s functions in quantum Monte Carlo simulations of strongly interacting systems. The topological invariant is used to study the trivial- to topological-insulator transitions in the Kane-Mele-Hubbard model with an explicit bond dimerization. We explore accessibility and behavior of this invariant within quantum Monte Carlo simulations.

3:06PM J18.00004 Rotating spin density wave and inverse spin pumping in quantum spin Hall edges, QINGLEI MENG, TAYLOR HUGHES, SMITHA VISHVESHWARA, University of Illinois Urbana-Champaign — We explore interaction effects in quantum spin Hall (QSH) edges in the presence of a finite bias voltage. Using bosonization techniques, we show that repulsive interactions give rise to a spin density wave phase in which the transverse magnetization exhibits spatial rotation. The effect of a finite bias voltage on this phase is to give the rotation a temporal variation. Using spin transfer torque methods, we show that the system can induce an inverse spin pumping effect in which the magnetic moment of a ferromagnet placed in its proximity can be made to rotate. We demonstrate that this device is equivalent to an electric inductor and in principle can also emit microwave radiation, thus providing a unique way of probing QSH properties.

3:18PM J18.00005 Theory of correlated topological insulators with broken axial spin symmetry, STEPHAN RACHEL, Dresden University of Technology, JOHANNES REUTHER, Caltech, RONNY THOMALE, EPFL Lausanne — The two-dimensional Hubbard model defined for topological band structures exhibiting a quantum spin Hall effect poses fundamental challenges in terms of phenomenological characterization and microscopic classification. We consider weak, moderate, and strong interactions and argue that the resulting phase diagrams depend on the microscopic details of the spin orbit interactions which give rise to the non-trivial topology. In particular, it turns out that there is a crucial difference between models with broken and with conserved axial spin symmetry. These results suggest that there is a general framework for correlated 2D topological insulators with broken axial spin symmetry.

3:30PM J18.00006 ABSTRACT WITHDRAWN —

3:42PM J18.00007 Band geometry of fractional topological insulators, RAHUL ROY, University of California, Los Angeles — Recent numerical simulations of flat band models with interactions which show clear evidence of fractionalized topological phases in the absence of a net magnetic field have generated a great deal of interest. We provide an explanation for these observations by showing that the physics of these systems is the same as that of conventional fractional quantum Hall phases in the lowest Landau level under certain ideal conditions which can be specified in terms of the Berry curvature and the Fubini study metric of the topological band. In particular, we show that when these ideal conditions hold, the density operators projected to the topological band obey the celebrated $W_{\infty}$ algebra. Our approach provides a quantitative way of testing the suitability of topological bands for hosting fractionalized phases.

3:54PM J18.00008 An effective theory of two-dimensional fractional topological insulators, PRERADG NIKOLIC, George Mason University — A generic spin-orbit coupling in 2D electron systems can be represented by an SU(2) gauge field with a non-trivial SU(2) flux. This makes it possible to stabilize novel non-Abelian incompressible quantum liquids by appropriate interactions (perhaps useful in quantum computing). We will discuss a generalization of the Chern-Simons Lagrangian to an arbitrary SU(N) symmetry group that describes such liquids. This effective field theory contains a Landau-Ginzburg part, which identifies the low energy fluctuations near any putative second-order quantum phase transition between conventional phases. Whenever an incompressible quantum liquid intervenes in such a phase transition, the fractional statistics of its quasiparticles is governed by the topological term of this theory and determined by the low energy dynamics. Commuting external gauge fields reduce the topological term to a Chern-Simons or BF form appropriate for fractional quantum (spin) Hall states, but the generic non-commuting gauge fields are expected to yield new classifiable topological orders without a quantum Hall analogue. We will discuss the possible non-Abelian fractional states in topological insulator quantum wells shaped by the Rashba spin-orbit coupling.

3:54PM J18.00008 An effective theory of two-dimensional fractional topological insulators, PRERADG NIKOLIC, George Mason University — A generic spin-orbit coupling in 2D electron systems can be represented by an SU(2) gauge field with a non-trivial SU(2) flux. This makes it possible to stabilize novel non-Abelian incompressible quantum liquids by appropriate interactions (perhaps useful in quantum computing). We will discuss a generalization of the Chern-Simons Lagrangian to an arbitrary SU(N) symmetry group that describes such liquids. This effective field theory contains a Landau-Ginzburg part, which identifies the low energy fluctuations near any putative second-order quantum phase transition between conventional phases. Whenever an incompressible quantum liquid intervenes in such a phase transition, the fractional statistics of its quasiparticles is governed by the topological term of this theory and determined by the low energy dynamics. Commuting external gauge fields reduce the topological term to a Chern-Simons or BF form appropriate for fractional quantum (spin) Hall states, but the generic non-commuting gauge fields are expected to yield new classifiable topological orders without a quantum Hall analogue. We will discuss the possible non-Abelian fractional states in topological insulator quantum wells shaped by the Rashba spin-orbit coupling.

1Supported by ONR, NIST and DOE (Institute for Quantum Matter at Johns Hopkins University)

4:06PM J18.00009 Exactly soluble lattice models for abelian topological phases, CHIEN-HUNG LIN, MICHAEL LEVIN, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742, USA — We construct exactly soluble bosonic lattice models that realize a large class of abelian topological phases. These models are a generalization of the “string-net” models of Ref. [1], but unlike the original construction, we find that our models can realize phases with broken time reversal symmetry. We analyze the braiding statistics of the quasiparticle excitations and show that they are described by nonchiral $U(1) \times U(1) \times \cdots \times U(1)$ Chern-Simons theories (i.e. equal numbers of left and right moving edge modes).

4:18PM J18.00010 Topological Phases in gapped edges of fractionalized systems. FRANK PÖLLMANN, JOHANNES MOTRUK, Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany, EREZ BERG, Weizmann Institute of Science, Rehovot 76100, Israel, ARI TURNER, University of Amsterdam, 1090 GL Amsterdam, The Netherlands — We present an extension of the classification scheme for topological phases in interacting one-dimensional fermionic systems to parafermionic chains. We find that the parafermions support both topological as well as symmetry broken phases in which the parafermions condense. In a series of recent works an experimental way of creating parafermions had been proposed: they can arise on the edge of a two-dimensional fractional topological insulator when coupled to superconducting and ferromagnetic domains. The low-energy edge degrees of freedom are described by a chain of coupled parafermions. As a concrete example of our classification we consider the \( \nu = 1/3 \) fractional topological insulator for which we calculate the phase diagram and study the entanglement spectra. We furthermore discuss a concrete physical realization which allows us to tune between the different topological phases.

4:30PM J18.00011 Quantum Geometry of the “Fuzzy-Lattice” Hubbard Model and the Fractional Chern Insulator. SAGAR VIJAY, F.D.M. HALDANE, Princeton University — Recent studies of interacting particles on tight-binding lattices with broken time-reversal symmetry reveal “zero-field” fractional quantum Hall (FQH) phases (fractional Chern insulators, FCI). In a partially-filled Landau level, the non-commutative guiding-centers are the residual degrees of freedom, requiring a “quantum geometry” Hilbert-space description (a real-space Schrödinger description can only apply in the “classical geometry” of unprojected coordinates). The continuum description does not apply on a lattice, where we describe emergence of the FCI from a non-commutative quantum lattice geometry. We define a “fuzzy lattice” by projecting a one-particle bandstructure (with more than one orbital per unit cell) into a single band, and then renormalize the orbital on each site to unit weight. The resulting overcomplete basis of local states is analogous to a basis of more than one coherent state per flux quantum in a Landau level. The overlap matrix characterizes “quantum geometry” on the “fuzzy lattice”, defining a “quantum distance” measure and Berry fluxes through elementary lattice triangles. We study quantum geometry at transitions between topologically-distinct instances of a fuzzy lattice, as well as \( N \)-body states with local Hubbard interactions.

4:42PM J18.00012 Series of Abelian and Non-Abelian States in C\( >1 \) Fractional Chern Insulators. ANTOINE STERYDIUK, CÉCILE REPELLIN, Laboratoire Pierre Aigrain, ENS and CNRS, BODGAN BERNEVIG, Department of Physics, Princeton University, NICOLAS REGNAULT, Department of Physics, Princeton university; Laboratoire Pierre Aigrain, ENS and CNRS — We report the observation of a new series of abelian and non-abelian topological states in fractional Chern insulators (FCI). The states appear at bosonic filling \( n_{\text{B}} = k/(C+1) \) \( k, C \) integers in a wide variety of lattice models, in fractionally filled bands of Chern numbers \( C \geq 1 \) subject to on-site Hubbard interactions. We show strong evidence that the \( k = 1 \) series is abelian while the \( k > 1 \) series is non-abelian. The energy spectrum at both ground-state filling and upon the addition of quasiholes shows a low-lying manifold of states whose total degeneracy and counting matches, at the appropriate size, of the Fractional Quantum Hall (FQH) SU(C) (color) singlet \( k \)-clustered states (including Halperin, non-abelian spin singlet (NASS) states and their generalizations). The ground-state moments are correctly predicted by the FQH to FCI lattice folding. However, the counting of FCI states also matches that of a spinless FQH series, preventing a clear identification just from the energy spectrum. The entanglement spectrum lends support to the identification of our states as SU(C) color-singlets but offers new anomalies in the counting for \( C > 1 \), possibly related to dislocations that call for the development of new counting rules of these topological states.

4:54PM J18.00013 Rydberg-Atom Quantum Simulation and Chern Number Characterization of a Topological Mott Insulator. ALEXANDRE DAUPHIN, Université libre de Bruxelles - Université Complutense, MARKUS MUELLER, MIGUEL-ANGEL MARTIN-DELGADO, Universidad Complutense — In this talk we consider a system of spinless fermions with nearest and next-to-nearest neighbor repulsive Hubbard interactions on a honeycomb lattice within the mean-field treatment, and propose and analyze a realistic scheme for analog quantum simulation of this model with cold atoms in a two-dimensional hexagonal optical lattice. Besides a semi-metallic and a charge-density-wave ordered phase, the system exhibits a quantum anomalous Hall phase, which is generated dynamically, i.e. purely as a result of the repulsive fermionic interactions and in the absence of any external gauge fields. We establish the topological nature of this dynamically created Mott insulating phase by the numerical calculation of a Chern number, and study the possibility of coexistence of this phase with the other phases characterized by local order parameters. Based on the knowledge of the mean-field phase diagram, we then discuss in detail how the interacting Hamiltonian can be engineered effectively by state-of-the-art experimental techniques for laser-dressing of cold fermionic ground-state atoms with electronically excited Rydberg states that exhibit strong dipolar interactions.

5:06PM J18.00014 Spin-orbit interactions in a helical Luttinger liquid with a Kondo impurity. ERIK ERIKKSSON, University of Gothenburg — We study the transport properties of a helical Luttinger liquid with a Kondo impurity and spin-orbit interactions. Such a system, which may be realized at the edge of a quantum spin Hall insulator with a gate-induced electric field, provides a mechanism to electrically control the conductance. A Rashba spin-orbit interaction may even change the nature of the Kondo screening [Eriksson et al., Phys. Rev. B 86, 161103(R) (2012)]. Considering other types of spin-orbit interactions, together with an extended non-equilibrium analysis, we further improve the understanding of these phenomena.

5:18PM J18.00015 Manipulating Majorana Fermions in Quantum Nanowires with Broken Inversion Symmetry. ALEJANDRO M. LOBOS, JQI and CMTC, Department of Physics, University of Maryland, XIONG-JUN LIU, JQI and CMTC, Department of Physics, University of Maryland, and Institute of Advanced Study, Hong Kong University of Science & Technology, Hong Kong — We study a Majorana-carrying quantum wire, driven into a trivial phase by breaking the spatial inversion symmetry with a tilted external magnetic field. Interestingly, we predict that a supercurrent applied in the proximate superconductor is able to restore the topological phase and therefore the Majorana end-states. Using Abelian bosonization, we further confirm this result in the presence of electron-electron interactions and show an insightful connection of this phenomenon to the physics of a one-dimensional doped Mott-insulator. The present results have important applications in e.g., realizing a supercurrent assisted braiding of Majorana fermions, which proves highly useful in topological quantum computation with realistic Majorana networks.

The authors acknowledge support from JQI-NSF-PPCN, Microsoft-Q, and DARPA-QuEST.

2:30PM J19.00001 Quantum criticality of YbBiPt  
G.M. SCHMIEDESHOFF, Occidental College, E.D. MUN, S.L. BUD’KO, C. MARTIN, H. KIM, M.A. TANATAR, R. PROZOROV, Ames Laboratory and Iowa State University, J.-H. PARK, T. MURPHY, National High Magnetic Field Laboratory, Florida State University, N. DILLELY, Quantum Design, P.C. CANFIELD, Ames Laboratory and Iowa State University — YbBiPt is a stoichiometric heavy fermion compound with an enormous Sommerfeld coefficient and a magnetic ground state that can be suppressed by fields of about 4 kOe. We will present and discuss recent thermodynamic and transport measurements, and the evidence for field induced quantum criticality in this material. Work at Ames Laboratory was supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358. The National High Magnetic Field Laboratory was supported by the US National Science Foundation, the State of Florida and the US Department of Energy. Work at Occidental College was supported by the National Science Foundation under DMR-1006118.

2:42PM J19.00002 ABSTRACT WITHDRAWN

2:54PM J19.00003 The High-Field Fermi Surface of YbRh$_2$Si$_2$  
AARON SUTTON, PATRICK M.C. ROURKE, Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7, VALENTIN TAUFOUR, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France, ALIX MCCOLLAM, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, Netherlands, GERARD LADERTOT, GEORG KNEBEL, JACQUES FLOQUET, INAC, SPSMS, CEA Grenoble, 38054 Grenoble, France, STEPHEN R. JULIAN, Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario, Canada M5S 1A7 — We report the culmination of our de Haas-van Alphen (dHvA) oscillation rotation studies on the heavy Fermion material YbRh$_2$Si$_2$. Past measurements included rotations in the a-b and a-c planes and resulted in the observation of a previously unobserved frequency attributed to the so-called J-sheet of the Fermi surface. While the purpose of these measurements was to determine whether or not the high field Fermi surface resembled a small or large Fermi surface, the measurements have highlighted the need for more advanced band structure calculations in order to determine its nature. In our latest measurements we completed our study by rotating from the (110) direction towards the c-axis. The experiment was successful in elucidating a new aspect of the Fermi surface, and though qualitative agreement with rudimentary band structure calculations was observed, the measurement has reinforced the need for a more comprehensive theoretical understanding of the material.

3:06PM J19.00004 CePt$_3$In$_7$: Focused Ion Beam Sample Preparation for Quantum Oscillation Measurements under High Pressure  
JAKOB KANTER, P. MOLL, Laboratory for Solid State Physics, ETH Zurich, Switzerland, S. FRIEDEMANN, P. ALIREZA, M. SUTHERLAND, S. GOH, Cavendish Laboratory, University of Cambridge, Cambridge, UK, F. RNONNING, E.D. BAUER, Los Alamos National Laboratory, Los Alamos, New Mexico, USA, B. BATLOGG, Laboratory for Solid State Physics, ETH Zurich, Switzerland — Electronic transport measurements under high pressures face several experimental challenges due to confined sample space and high forces acting on contacts and leads. As a result conventional preparation methods are often limited in the number of possible leads and usually do not allow for sample structuring. The Focused Ion Beam (FIB) enables sample contacting and structuring down to a sub-micrometre scale, making the measurement of several samples with complex shapes on a single anvil feasible. This talk will discuss Shubnikov-de Haas measurements of FIB prepared CePt$_3$In$_7$ samples under high pressures. CePt$_3$In$_7$: belongs to the $T_mM_{13}I_{3m+2n}$ heavy fermion family. Compared to the CeMn$_7$ members of this group, the structure of CePt$_3$In$_7$ has a more pronounced two dimensional character, but also exhibits an antiferromagnetically ordered as well as a superconducting phase. We have studied the changes of the quasiparticle masses for the various orbits as function of pressure approaching the quantum critical point.

3:18PM J19.00005 A THz spectroscopy study of the field-induced quantum phase transition in the heavy fermion antiferromagnet CeCu$_2$Ge$_2$  
GRACE BOSSE, C.M. MORRIS, Johns Hopkins University, Y. LI, J. ECKSTEIN, University of Illinois at Urbana-Champaign, N.P. ARMITAGE, Johns Hopkins University — We report time domain THz spectroscopy data of a thin film of the heavy fermion compound CeCu$_2$Ge$_2$ in the presence of a magnetic field. It has been shown that it is possible to tune the antiferromagnetic long-range order of CeCu$_2$Ge$_2$ towards a quantum critical point using magnetic field as a tuning parameter. Measurements to obtain the frequency dependent complex conductivity as a function of temperature and field were taken down to temperatures below the onset of magnetic order and fields as high as 7 T. The effects of the quantum critical fluctuations on the frequency dependent scattering rate and mass renormalization, which are obtained using an extended Drude model analysis, will be discussed.

3:30PM J19.00006 Quantum Criticality in high purity specimens of CeRh$_3$Ge$_7$ and Ce$_3$Pt$_7$Si$_5$  
ERIC D. BAUER, RYAN E. BAUMBACH, XIN LU, Los Alamos National Laboratory, ROSS D. MCDONALD, Los Alamos National Laboratory, National High Magnetic Field Laboratory, FILIP RONNING, JOE D. THOMPSON, Los Alamos National Laboratory — We report results for high purity specimens of the heavy fermion antiferromagnets CeRh$_3$Ge$_7$, and Ce$_3$Pt$_7$Si$_5$, which have similar ordering temperatures: $T_N = 5.5$ K and 6.3 K, respectively, and belong to the same family of materials that includes the pressure-induced superconductor CeNi$_3$Ge$_3$. Our measurements show that the antiferromagnetic state is suppressed to zero temperature at similar magnetic fields ($H_c = 23$ T and 36 T, respectively) suggesting comparable magnetic energy scales in these compounds. In contrast, while the pressure needed to access a quantum critical point (QCP) in Ce$_3$Rh$_7$Ge$_7$ is extremely low ($P_c < 5$ kbar), the Néel temperature for Ce$_3$Pt$_7$Si$_5$ is insensitive to pressures up to 15 kbar. This result implies that although these compounds are markedly similar, the mechanism that drives the QCP in Ce$_3$Rh$_7$Ge$_7$ is not present in Ce$_3$Pt$_7$Si$_5$. Our measurements show that the quantum criticality is suppressed by fields as high as 36 T. The effects of the quantum critical fluctuations on the frequency dependent scattering rate and mass renormalization, which are obtained using an extended Drude model analysis, will be discussed.

3:42PM J19.00007 Magnetic cluster glass formation in Ni-V close to the disordered ferromagnetic quantum phase transition  
RUIZHE WANG, SARA UBAID-KASSIS, ALMUT SCHROEDER, Kent State University, P.J. BAKER, F.L. PRATT, ISIS, S.J. BLUNDELL, T. LANCASTER, I. FRANKE, J.S. MOELLER, Oxford University, THOMAS VOJTA, Missouri University of Science and Technology — The d-metal alloy Ni$_{1-x}$V$_x$ undergoes a quantum phase transition from a ferromagnetic ground state to a paramagnetic ground state as the vanadium concentration $x$ is increased. We present magnetization, ac-susceptibility and muon-spin relaxation data at several vanadium concentrations below and above the critical concentration $x_c \approx 11\%$ where the onset of ferromagnetic order is suppressed. Below $x_c$, Ni$_{1-x}$V$_x$ is characterized as a strongly disordered ferromagnet since the muon data reveal a broad magnetic field distribution. Above $x_c$, the temperature dependence of the magnetic susceptibility is best described in terms of a magnetic quantum Griffiths phase. At the lowest temperatures, we identify a magnetic cluster glass phase which masks the actual ferromagnetic quantum critical point. We study how this cluster glass is formed (i) by lowering the temperature from the quantum Griffiths phase and (ii) by increasing the vanadium concentration starting from the disordered ferromagnet. The onset of the cluster glass phase is recognized by a change of the magnetic dynamics revealed through susceptibility and muon-spin relaxation measurements.

1Part of this work supported by NSF DMR 0306766 and OBR 440653.
3:54PM J19.00008 Anisotropic transport and magnetic properties, and magnetic-field tuned ground states of CeZn$_2$\textsuperscript{1}, H. HODOVANETS, S. L. BUD’KO, M. G. KIM, D.K. PRATT, A. KREYSSIG, A.I. GOLDMAN, P.C. CANFIELD, Ames Laboratory and Department of Physics, Iowa State University, Ames, IA — We have studied the electrical, magnetic, and thermal properties of single crystals of CeZn$_2$ by the means of magnetization, resistivity, heat capacity, and thermoelectric power. The compound exhibits an antiferromagnetic long-range order below 2.0 K. The zero-field temperature dependent resistivity of CeZn$_2$ is similar to that of other strongly correlated, Kondo lattice, compounds. $T_N$ is suppressed with the applied magnetic field and disappears for $H \approx 4.5$ kOe ($H//\text{[110]}$) and $H \approx 120$ kOe ($H//\text{[001]}$). Temperature-dependent resistivity for $H//\text{[110]}$ shows sub-linear behavior up to 2.5 K for $H=45$ kOe, followed by Fermi liquid behavior for limited range of temperatures ($T < 1.1$ K) and fields (47.5 kOe $\leq H \leq 50$ kOe). The $H$ vs. $T$ phase diagrams for $H//\text{[110]}$ and $H//\text{[001]}$ will be discussed.

\textsuperscript{1}Supported by the Department of Energy, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

4:06PM J19.00009 Electrical resistivity of CeZn$_2$ under pressure\textsuperscript{1}, VALENTIN TAUFOUR, Department of Physics and Astronomy, Iowa State University, Ames, 50011, U.S.A, STELLA K. KIM, HAHYOA HODOVANETS, SERGEY L. BUD’KO, PAUL C. CANFIELD, Ames Laboratory, U.S. DOE, Iowa State University, Ames, Iowa 50011, U.S.A — In most Ce-based intermetallic compounds, the magnetic exchange is assumed to be due to the RKKY interaction. This interaction competes with the Kondo interaction, leading to the suppression of the magnetic order and the possibility of field and/or pressure induced quantum criticality. In order to study this competition in CeZn$_2$, a compound that orders antiferromagnetically below $T_N = 2$ K, we performed electrical resistivity measurements on a single crystal of CeZn$_2$ under pressure up to 5 GPa in a Bridgman pressure cell modified to use a liquid pressure transmitting medium (1.1 mixture of n-pentane: iso-pentane). $\Delta \rho(T)$ slightly increases and approaches a broad maximum in the studied pressure range. At ambient pressure, the antiferromagnetic order is suppressed by a magnetic field along the [1,1,0] direction of the tetragonal crystal structure. The temperature versus magnetic field phase diagram at 5 GPa will be compared to the one at ambient pressure.

\textsuperscript{1}This work was supported by AFOSR-MURI grant FA9550-09-1-0603 (V. Taufour and P. C. Canfield) and by US DOE under the Contract No. DE-AC02-07CH11358 (S. K. Kim, H. Hodovanets and S. L. Bud’ko).

4:18PM J19.00010 Magnetic structures of R$_2$CoGa$_6$ (R = Gd, Tb and Dy) and evolution of the magnetic structures along the series of intermetallic compounds with R = Gd - Tm, CARLOS GILES, JOSE RENATO MADERGAN, Argonne National Laboratory, CRIS ADRIANO, University of Illinois at Chicago, RAFAEL VESCOVI, PASCOAL PAGLIUSO, University of Campinas — In this work we have determined the magnetic structure of R$_2$CoGa$_6$ (R = Gd, Tb and Dy) intermetallic compounds using X-ray resonant magnetic scattering in order to study the evolution of the anisotropic magnetic properties along the series for R = Gd-Tm. The three compounds have a commensurate antiferromagnetic structure with a magnetic propagation vector (1/2 1/2 1/2) with Neel temperatures of 21.0, 27.5 and 15.2 K for R = Gd, Tb and Dy, respectively. The critical exponent $\beta$ obtained from the temperature dependence of the integrated intensity of the resonant magnetic peaks suggest a 3D magnetism for the three compounds. The energy line shapes at the $L_2$ and $L_3$ edges of the magnetic peaks for these compounds present a purely dipolar character as demonstrated by comparison to first principle calculations. Comparing the simulated and integrated intensities corrected for absorption, we conclude that the magnetic moment direction is in the ab-plane for Gd$_2$CoGa$_6$ compound and parallel to the c-axis for the Tb$_2$CoGa$_6$ and Dy$_2$CoGa$_6$ compounds. This information is used to discuss the evolution of the magnetic structure of R$_2$CoGa$_6$ series for R = Gd-Tm where both the direction of the ordered moment and the ordering temperature evolution along the series can be explained through the competition between the indirect Ruderman-Kittel- Kasuya-Yoshida exchange interaction and crystalline electric field effects.

4:30PM J19.00011 Electronic structure and Fermi surface topology in PuIn3 and PuSn3, CHENG-CHING WANG, Theoretical Division, Los Alamos National Laboratory, MATTTHW JONES, University at Buffalo, SUNY, JIAN-XIN ZHU, Theoretical Division, Los Alamos National Laboratory — The itinerant-to-localized crossover of the 5f electrons that occurs near plutonium in the actinide series is one of the most challenging issues in condensed matter physics, while the highest superconductivity across the whole f-electron systems emerges in PuCoGe. These novel behaviors are indicative of strong electronic correlations effects. Electronic band structure calculations serve as the first step for better understanding of these correlation effects. The compounds PuIn3 and PuSn3 crystallize into cubic AuCu3-type structure and have an actinide-actinide distance far above the Hill limit, making the 5f-ligand hybridization the dominant mechanism for Pu 5f -electron delocalization. With their simple crystallographic structure and rich magnetic and electronic properties, these two compounds provide a particularly convenient and systematic way to study the delocalization-localization crossover of Pu 5f electrons. It is particularly encouraging that PuIn3 is the first Pu-based compound in which the de-Haas van-Alphen effect has been observed. In this talk, we present a systematic study of electronic structure calculations of PuIn3 and PuSn3 in the framework of density functional theory with the generalized gradient approximation.

4:42PM J19.00012 Quantum Criticality in the strongly correlated 3d electron system YFe$_2$Al$_{10}$, LIUSUOU WU, KEESSEONG PARK, Stony Brook University, MONIKA GAMZA, Brookhaven National Lab, MOOSUNG KIM, Stony Brook University, MEIGAN ARONSON, Brookhaven National Lab & Stony Brook University — A remarkable behavior in quantum critical systems is the critical scaling near the quantum critical point (QCP), where Fermi liquid (FL) physics usually breaks down. This kind of behavior has been observed in many f electron based heavy fermion (HF) systems. We have measured the magnetization and specific heat of the 3d-electron metal YFe$_2$Al$_{10}$, non-FL behavior with strong divergence in magnetic susceptibility ($\gamma \sim T^{-\gamma}, \gamma = 1.4$) and specific heat ($C_m//T=\log T$) were observed, and this suggested YFe$_2$Al$_{10}$ may locate close to a ferromagnetic QCP. What attracts us most is the unusual scaling of magnetic susceptibility ($d\chi/dT=B^{-\gamma}\psi(T/B^3)$) and specific heat ($\Delta C_m/T=\psi(T/B^3)$), which was observed over a range more than three decades in $T/B^3$. The overall scaling behaviors mapped well with the assumption that a FL phase was resumed as the system was tuned far from the QCP, where all the critical fluctuation was suppressed. Based on the scaling analysis, a possible form of the critical free energy will also be discussed.

4:54PM J19.00013 Terahertz conductivity of MnSi thin films, J. STEVEN DODGE, LALEH MOHTASHEMI, AMIR FARAHANI, Simon Fraser University, ERIC KARHU, THEODORE MONCHESKY, Dalhousie University — We present measurements of the low-frequency optical conductivity of MnSi thin films, using time-domain terahertz spectroscopy. At low temperatures and low frequencies, we extract the DC resistivity, scattering life time and plasma frequency from a Drude fit. We obtain a value of $\sigma_{dc} \approx 1.0$ eV, which can be used to estimate the renormalization coefficient through comparison with band theory. At higher temperatures, deviations from Drude behavior are observed, suggesting a loss of quasi-particle coherence. In the region of low temperatures and high frequencies, we see evidence for a crossover to the anomalous power law dependence observed by Mena et al.\textsuperscript{1} As the temperature increases, the anomalous frequency dependence becomes more pronounced, and the plasma frequency inferred from a Drude fit decreases dramatically. Above $T \approx 50$ K, $\sigma_{dc}(\omega)$ develops a negative slope that is inconsistent with both a Drude model and the anomalous power law observed earlier,\textsuperscript{1} indicating a sharp pseudogap in the conductivity spectrum.

2:30PM J22.00001 Temperature dependence of highly homogeneous excitonic spectra of site-controlled pyramidal quantum dots. VALENTINA TRONCALE1, 2, ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL), LABORATORY OF PHYSICS OF NANOSTRUCTURES, CH-1015 LAUSANNE, EMANUELE PELUCCHI, TYNDALL NATIONAL INSTITUTE, CORK, IRELAND, ALOK RUDRA, ELI KAPON, ECOLE POLYTECHNIQUE FEDERALE DE LAUSANNE (EPFL), LABORATORY OF PHYSICS OF NANOSTRUCTURES, CH-1015 LAUSANNE, LABORATORY OF PHYSICS OF NANOSTRUCTURES, EPFL, CH-1015 LAUSANNE TEAM — Site-controlled pyramidal quantum dots grown by MOVPE on patterned GaAs substrates offer many advantages such as emission wavelength, heterostructure tailoring and higher symmetry for efficient photon entanglement. We address the temperature dependence of X, 2X, X+, X− exciton linewidths, providing insight on exciton-phonon interaction in this system. The investigated structures consist of GaAs/AlGaAs pyramidal QDs, positioned on ZnMg centers, characterized using non-resonant micro-photoluminescence at low temperatures. PL spectra of individual QDs are highly reproducible, showing transitions excitons with inhomogeneous broadening as low as 2 meV, caused by slight thickness/composition fluctuations. Interferometric T-dependent linewidth measurements of the four excitonic transitions revealed values at T=0 K smaller than previously reported but larger than the estimated exciton radiative lifetime. We conclude that even at T=0 K the exciton decoherence time in GaAs QDs is not completely governed by a radiative lifetime and discuss this effect.

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2:42PM J22.00002 Carrier Dynamics in Site-Controlled InGaN/GaN Quantum Dots1, 2, TYLER HILL, LEI ZHANG, HUI DENG, University of Michigan Physics, CHU-HSIANG TENG, BRANDON DEMORY, PEI-CHENG KU, University of Michigan EECS — We investigate the individual micro-photoluminescence and time resolved photoluminescence properties of several hundred site-controlled InGaN/GaN quantum dots fabricated “top down” by plasma etching. The optical properties of semiconductor quantum dots can be very inhomogeneous due to small fluctuations in dot size, compositions, growth conditions, or doping levels. Controlled variation of growth conditions combined with the knowledge of experimental uncertainties in the semiconductor properties allows for a statistical analysis to obtain quantitative correlations between the optical properties of the quantum dots and the growth conditions or structural properties. We find that, with an indium fraction of 10-15%, quantum dots with diameters smaller than 33 nm show markedly different carrier dynamics than those with a diameter larger than 60nm: 1) Fluctuations in indium mole fraction or monolayer fluctuations in the InGaN layer have a more significant effect on photoluminescence than changing dot diameter; 2) Non-radiative decay related to surface recombination is the dominant decay channel in the system; 3) Increasing surface to volume ratio helps suppress the internal quantum efficiency of multi-exciton states, leading to more strongly antibunched photon sources.

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Tuesday, March 19, 2013 2:30PM - 5:30PM — Session J22 DCMP: Optical Properties and Interactions in Quantum Dots and Wells 324 - Michael Scheinber, University of California, Merced

5:06PM J19.00014 Effect of Nd Substitution on PrOsSb12 Investigated by μSR Experiments1, 2, P.-C. HO, B. SOMSANUK, Physics/CSU-Fresno, D. E. MACLAUGHLIN, Physics/UC Riverside, M. B. MAPLE, UC San Diego, L. SHU, Physics/Fudan U, China, O. O. BERNAL, Physics/CSU-Los Angeles, T. YANAGISAWA, Physics/Hokkaido U, Japan — The pseudo ternary system Pr1−xNdxOsSb12 has been used as a model system to investigate the effect of ferromagnetism (FM) on the unconventional superconductivity (SC) and quantum critical behavior of PrOsSb12 [1]. SC in this system disappears near a critical concentration xcr,1 ≈ 0.58 and FM appears above xcr,2 ≈ 0.33 [1,2]. The new μSR measurements have been performed on samples with x = 0.25, 0.75, and 1. For x = 1 and 0.75, the estimated frozen moments agree with the Nd3+ CEF ground state moment. For x = 0.25, neither time reversal symmetry breaking nor evidence of freezing of Nd3+ spins was observed in zero-field μSR measurements, the behavior of which is very different than what is observed for x = 0.45 − 0.55 [2]. In the SC state, an unexpected linear T dependence of the Gaussian relaxation rate was also found in the transverse field μSR data for x = 0.25, which is different than the plateau in PrOsSb12 below 1.3K [3]. [1] Ho, et al., PRB 83, 024511 (2011).[2] Ho, et al., 2010 APS March Meeting, A38.00005 (2010). [3] MacLaughlin et al., PRL 105, 019701 (2010).

5:24PM J22.00003 Narrow optical line width from site-controlled InGaAs quantum dots. LILY YANG, NRC Postdoc Residing at the Naval Research Laboratory (NRL), MICHAEL YAKES, NRL, TIMOTHY SWEENEY, NRC Postdoc Residing at NRL, SAMUEL CARTER, CHULSOO KIM, NRL, MINJIN KIM, Sotera, ALLAN BRACKER, DANIEL GAMMON, NRL — The incorporation of self-assembled quantum dots (QDs) in systematically scalable quantum devices requires a method of nucleating dots with nanometer-scale spatial accuracy while preserving their narrow optical line width. We have developed a semiconductor lithography, wet etching, and molecular beam epitaxial (MBE) growth to deterministically position InGaAs QDs with spectrometer limited photoluminescence line widths. Our technique takes advantage of the anisotropy in GaAs growth to evolve an etched pattern of holes and lines into faceted structures in which dots nucleate. Using this technique, we were able to grow a buffer layer of pure GaAs up to 90 nm in thickness between the processed surface and the dot nucleation surface, effectively separating the QDs from unavoidable residual defects and impurities on the patterned surface that broaden their optical line widths. Additionally, we demonstrate control over the number of dots nucleating per site, from single to a chain of several, by varying the dimensions of the original pattern. Our dots are grown in a Schottky diode structure. Their PL spectrum shows discrete charging transitions, with narrow linewidths near the spectrometer’s resolution limit of 20 micro eV.

3:06PM J22.00004 Eliminating the fine structure splitting of excitons in self-assembled InAs/GaAs quantum dots via combined stresses. LIXIN HE, JIANPING WANG, University of Science and Technology of China, MING GONG, Washington State University, G.-C. GUO, University of Science and Technology of China — Eliminating the fine structure splitting (FSS) of excitons in self-assembled quantum dots (QDs) is essential to the generation of high quality entangled photon pairs. We show by a extended two-level model that the FSS of excitons in a general self-assembled InGaAs/GaAs QD can be fully suppressed via combined stresses along the [110] and [010] directions. The results of the model Hamiltonian are confirmed by atomic empirical pseudopotential calculations. For all the QDs we calculated, the FSS can be tuned to be vanishingly small (< 0.1 μeV), which is sufficient small for high quality entangled photon emission.
3:18PM J22.00005 Rabi-Kondo correlated state in a laser-driven quantum dot. MOSHE GOLDSMITH, Yale University, BJOERN SIBERSKI, ETH Zurich, MARKUS HANL, ANDREAS WEICHELBAUM, LMU Munich, HAKAN TURECI, Princeton University, LEONID GLAZMAN, Yale University, JAN VON DELFT, LMU Munich, ATAC IMAMOGLU, ETH Zurich — Spin exchange between a single-electron charged quantum dot and itinerant electrons leads to the emergence of Kondo screening. When the quantum dot is driven resonantly by a weak laser light, the resulting emission spectrum serves as a direct probe of these correlations. In the opposite limit of vanishing exchange interaction and strong laser drive, the quantum dot exhibits coherent Rabi oscillations between the single-spin and optically excited states at the “bare” frequency $\Omega$. Here we show that the interplay between strong exchange and non-perturbative laser coupling leads to the formation of a new non-equilibrium quantum-correlated state, featuring a second screening cloud. We elucidate the signatures of that state in the spectrum of luminescence. The spectrum consists of a delta-function peak at the laser light frequency ($\Omega$) and a broad peak red-shifted by the renormalized Rabi frequency $\Omega^\ast \sim \Omega^{2/3}$. The shape of the broad peak carries detailed information about the spin screening cloud.

3:30PM J22.00006 Adiabatic rapid passage in single InGaAs quantum dots: Towards a method of “incoherent control”. PETER BRERETTON 1, MEGAN STANLEY, ALEXANDRA GRAHAM, BARBARA VAN HATTEM, PIERRE CORFDIR, AMOP Group, University of Cambridge, ISOBEL HOUGHTON, Bristol University, YANWEN WU, University of Texas Austin, MARK HOPKINSON, University of Sheffield, RICHARD PHILLIPS, AMOP Group, University of Cambridge — Adiabatic rapid passage (ARP) using frequency-swept optical pulses was shown to invert an InGaAs quantum dot from the ground state to the neutral exciton state [1,2]. As in atomic systems, ARP couples the confined electronic states of a quantum dot to a pulse that sweeps through resonance. If the sweep rate is slow with respect to the instantaneous Rabi frequency but faster than any decay rates, the dressed state is the quantum state that would adiabatically switch from one bare state to the other. Damping of the ARP inversion suggests confirmation of theoretical predictions of the effect of phonon-assisted dephasing [3]. ARP allows a train of chirped pulses to control the population state of a quantum dot without the need for locking the relative phase of the pulses. Each pulse pair will effectively drive the state vector through a $2\pi$ rotation on the Bloch sphere, regardless of the relative phase. Initial work toward this method of “incoherent control” is presented, showing an enhancement of the photocurrent under excitation with two chirped pulses separated by greater than the electron tunneling time. [1] Y. Wu, et al, PRL 106, 067401 (2011). [2] C.-M. Simon, et al PRL, 106, 166801 (2011). [3] A. Debnath, et al PRB, 86, 161304 (2012).

3:42PM J22.00007 Investigation of exciton states under two color optical excitation in quantum dot molecules. RAMANA THOTA, ERIC STINAFF, Department of Physics and Astronomy, and Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio 45701-2979, USA, ALLAN BRACKER, DAN GAMMON, Naval Research Laboratory, Washington, DC 20375, USA — It has been shown that vertically stacked InAs quantum dots may form quantum dot molecules (QDMs) where the tunneling of the carriers results in molecular wavefunction formation. These states are potentially useful for the preparation and manipulation of entangled spins, necessary components for quantum information processing. It has also been previously shown that certain charged exciton states can be created optically resulting in a straightforward method for optical spin initialization. We will present a study of optical charge state creation in vertically stacked In$_x$Ga$_{1-x}$As quantum dots grown by molecular beam epitaxy. This includes using a two color micro-photoluminescence experiment where we tune one laser through the states associated with the quantum dot (resonant excitation) and keep the other laser fixed with its excitation at the energy of the wetting layer (non-resonant excitation). This technique may result in a method for enhancement of various charged and neutral exciton states. In particular we have investigated the doubly charged exciton state, where the ground state is two spins in a known configuration, as well as biexciton enhancement, possibly useful for generating entangled photon pairs.

3:54PM J22.00008 Coulomb interaction signatures in self-assembled lateral quantum dot molecules. XIRAN ZHOU, University of Delaware, JIHOON LEE, Kwangwoon University, South Korea, GREGORY SALAMO, University of Arkansas, MIQUEL ROYO, JUAN CLIMENTE, Universitat Jaume I, Spain, MATTHEW DOTY, University of Delaware — Lateral quantum dot molecules (LQDMs) consist of at least two closely spaced InGaAs quantum dots arranged along axes perpendicular to the growth direction. Coherent interactions between neighboring QDs can lead to the formation of delocalized states with unique and useful properties. LQDMs provide an opportunity for independent control of both coupling and charge occupancy, and are thus of interest for prototype devices that use the QDs as bit registers. The experimental evidence for the existence of delocalized states and inter-dot tunneling in LQDMs, limited by the large center-to-center distance and weak tunneling strength, has been indirect. We use photoluminescence spectroscopy to investigate the ground state of single LQDMs. We apply a voltage along the growth direction that allows us to control the total charge occupancy of the quantum dot molecule. Using a combination of computational modeling and experimental analysis, we assign the observed discrete spectral lines to specific charge distributions. We explain the dynamic processes that lead to these charge configurations through electrical injection and optical generation. Our systematic analysis provides experimental evidence of inter-dot tunneling of electrons as predicted in previous theoretical work.

4:06PM J22.00009 Study of optical and electronic properties of self-assembled InAs/GaAs quantum rings. GABRIEL LINARES, Instituto de Física “Luis Rivera Terrazas,” Mexico, Puebla, SAMAR ALSOLAMY, Department of Physics and Astronomy, Ohio University, Athens, Ohio - 45701, MORGAN WARE, YURIY MAZUR, ZHIMING WANG, JIHOON LEE, GREG SALAMO, Institute for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas, ERIC STINAFF, Department of Physics and Astronomy, Ohio University, Athens, Ohio - 45701, LILIA MEZZA-MONTES, Instituto de Física “Luis Rivera Terrazas,” Mexico, Puebla — We will present a theoretical study of the properties of self-assembled InAs/GaAs quantum rings. These nanostructures are grown by metal droplet epitaxy and do not follow the traditional strain driven growth model. For certain growth conditions, two quantum dots are formed on the ring structure which then, in a sense, acts as a wetting layer. A ‘wetting layer’ of 2D InAs is assembled InAs/GaAs quantum rings. These nanostructures are grown by metal droplet epitaxy and do not follow the traditional strain driven growth model. The work at Yale University is supported by the Simons Foundation and by NSF DMR Grant No. 1206612.

The work at Yale University is supported by the Simons Foundation and by NSF DMR Grant No. 1206612.

Now at U.S. Naval Research Laboratory.

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Partially supported by Grant CB/2009/133516-CONACyT, Mexico.
4:18PM J22.00010 Luminescence studies of pairs of quantum dots formed on quantum rings by droplet epitaxy , SAMAR ALSOLAMY, Department of Physics & Astronomy, Ohio University, Athens, OH, MORGAN WARE, YURIY MAZUR, ZHIMING WANG, JHOON LEE, GREC SALAMO, Instituto for Nanoscience and Engineering, University of Arkansas, Fayetteville, Arkansas, G. LINARES, LILIA MEZA-MONTES, Instituto de Física “Luis Rivera Terrazas”, Mexico, Puebla, ERIC STINAFF, Department of Physics & Astronomy, Ohio University, Athens, OH — The use of metal droplet epitaxy may provide a novel method of growing laterally coupled nanostructures. We will present optical studies of InAs/GaAs nanostructures which result in twin quantum dots (QD) formed on a quantum ring (QR). Previous studies have investigated the coupling between vertically grown quantum dot pairs. Here we have used photoluminescence (PL) and photoluminescence excitation (PLE) to examine the possibility of energy transfer and coupling between quantum dot pairs in a single InGaAs quantum ring grown by droplet epitaxy. Power dependent photoluminescence spectra reveals a few peaks at low power, which are identified with emission from the ground state of the individual dots. As the power is increased we observe multi-exciton and excited state emission. We then perform PLE, tuning the excitation laser energy continuously from the high energy ring emission down to the individual dot states. We have observed resonant PLE emission in the QR/QD structures both at high energy and when resonant with the identified ground states of one of the QDs which may indicate energy transfer and/or coupling between the dots.

4:30PM J22.00011 Coulomb Enhancement of Superfluorescence Bursts from the Fermi Edge in Highly-Excited Quantum Wells , J.HEE KIM, TIM NOE, Dep. of Electrical and Computer Engineering, Rice University, STEPHEN A. MCGILL, National High Magnetic Field Laboratory, Florida State University, YONGRUI WANG, ALEKSANDER K. WÓJCIK, ALEXEY A. BELYANIN, Dep. of Physics and Astronomy, Texas A&M University, JUNICHIRO KONO, Dep. of Electrical and Computer Engineering, Rice University — Superfluorescence (SF) is a many-body process in which an ensemble of excited doppes spontaneously develops macroscopic coherence and abruptly decays by producing a burst of coherent radiation. We have recently reported the first observation of SF from semiconductor quantum wells in the presence of a strong perpendicular magnetic field [1]. Here, we report on results of our systematic magnetic field dependent studies of light emission from high-density electron-hole systems with gain. We observed SF pulses even at 0 Tesla when the excitation is high and the temperature is low. The SF radiation at 0 Tesla shows a continuous band of emission in time-resolved photoluminescence images, i.e., the photon energy of the emitted light changes continuously with time. We interpret this phenomenon in terms of Coulomb enhancement of gain near the Fermi energy in a high-density electron-hole system. In addition, we demonstrate that the delay between the pump pulse and the SF pulse is strongly dependent on temperature. Finally, the delay is longer for a lower-energy Landau level at a given magnetic field, i.e., the SF bursts proceed in a sequential manner from higher to lower Landau levels.


4:42PM J22.00012 Comparative Study on Intersubband Absorption in AlGaN/GaN and AlInN/GaN Heterostructures Grown on Low-Defect Substrates , COLIN EDMUNDS, LIANG TANG, JIAYI SHAO, DONGHUI LI, GEOFF COMPTON, MANUEL IFRAIN, OANA MALIS, Purdue University, ANDREW GRIER, ZORAN IKONIC, PAUL HARRISON, University of Leeds, DIMITRI ZAKHAROV, Brookhaven National Laboratory — Intersubband (ISB) devices utilizing III-nitrides have attracted attention for near- and far-infrared electronic and optical applications. However, the lattice mismatch between GaN and commonly used substrates results in a high defect density that hinders the vertical transport required for these devices. Moreover, devices in the literature utilize AlGaN/GaN heterostructures for which there is no lattice-matched alloy composition. Due to this lattice mismatch, AlGaN is not ideal for the development of complex devices such as quantum cascade lasers that often require active-region thicknesses on the order of microns for efficient operation. Fortunately, exact lattice matching occurs in AlInN/GaN heterostructures at roughly 18% In composition. To investigate the challenges of lattice-matched nitrides, we presents a comparative study of ISB absorption in high-quality AlGaN/GaN and near lattice-matched AlInN/GaN heterostructures grown by molecular-beam epitaxy on low-defect free-standing GaN substrates. Experimental measurements of transition energy, integrated absorbance and linewidth were compared to theoretical predictions that included many-body effects, interface roughness and calculations of the transition lifetime.

4:54PM J22.00013 Coulomb correlation effects and density dependence of radiative recombination rates in polar AlGaN quantum wells , GREG RUPPER, SERGEY RUDIN, U.S. Army Research Laboratory, FRANCESCO BERTAZZI, Politecnico di Torino, Torino, Italy, GREGG HARVEY, MICHAEL WRABACK, U.S. Army Research Laboratory — AlGaN narrow quantum wells are important elements of deep-ultraviolet light emitting devices. The electron-hole radiative recombination rates are important characteristics of these nanostructures. In this work we evaluated their dependence on carrier density and lattice temperature and compared our theoretical results with the experimentally determined radiative lifetimes in the c-plane grown AlGaN quantum wells. The bands were determined in the k·p approximation for a strained c-plane wurtzite quantum well and polarization fields were included in the model. In order to account for Coulomb correlations at relatively high densities of photo-excited electron-hole plasma and arbitrary temperature, we employed real-time Green’s function formalism with self-energies evaluated in the self-consistent T-matrix approximation. The luminescence spectrum was obtained from the susceptibility by summing over scattering in-plane directions and polarization states. The recombination coefficient was obtained from the integrated photo-luminescence. The density dependence of the radiative recombination rate shows effects of strong screening of the polarization electric field at high photo-excitation density.

5:06PM J22.00014 Second quantum state transitions in GaAs/AlGaAs Bragg MQW photonic crystal probed by Optical Reflectance and Electroreflectance , YUECHAO CHEN, Z. LIU, M.L. NAKARMI, Department of Physics, Graduate Center and Brooklyn College - CUNY, V.V. CHALDYSHEV, Ioffe Physico-Technical Institute, St. Petersburg, Russia — The use of metal droplet epitaxy may provide a novel method of growing laterally coupled nanostructures. We will present optical studies of InAs/GaAs nanostructures which result in twin quantum dots (QD) formed on a quantum ring (QR). Previous studies have investigated the coupling between vertically grown quantum dot pairs. Here we have used photoluminescence (PL) and photoluminescence excitation (PLE) to examine the possibility of energy transfer and coupling between quantum dot pairs in a single InGaAs quantum ring grown by droplet epitaxy. Power dependent photoluminescence spectra reveals a few peaks at low power, which are identified with emission from the ground state of the individual dots. As the power is increased we observe multi-exciton and excited state emission. We then perform PLE, tuning the excitation laser energy continuously from the high energy ring emission down to the individual dot states. We have observed resonant PLE emission in the QR/QD structures both at high energy and when resonant with the identified ground states of one of the QDs which may indicate energy transfer and/or coupling between the dots.

5:18PM J22.00015 Equipspaced level in the quantum well calculated for seven semiconductor ternary alloys conduction band , ARTHUR EJERE, Department of Physics, University of Benin, Benin city, Nigeria, GODFREY AKPOJO-TOR, Theoretical and Computational Condensed Matter Physics, Physics Department, Delta State University, Abraka, Nigeria — A model of equipspaced-level conduction band in semiconductor quantum well (QW) nanostructures is derived. The procedure starts with the effective-mass Schrödinger equation, with the local conduction-band edge as the potential experienced by an electron in the QW. Then the effective-mass Schrödinger equation with linear harmonic potential is made to coincide with it . In this study, an attempt has been made to model some semiconductor ternary alloys (AlxBe1-xGa) using this procedure, thereby adding to the varieties of QW nanostructures designs in existence. Two models are derived, one with a confining potential that may be realized by appropriate grading of the semiconductor alloy and the other with a non-confining potential where the electron effective-mass tends to zero as z tends to infinity \[m(z → ∞) → 0\]. This latter type of model is not realizable.
2:30PM J23.00001 Unconventional Transport of Spin Bipolarons on an Antiferromagnetic buckled hexagonal lattice of half-filled d-band Mn$^{2+}$ ions \(^1\), VERNER THORSMOLLE, ALEXANDER IGNATOV, MARIA PEZZOLI, KRISTJAN HAULE, DAVID KOLCHMEYER, ALEXANDER LEE, Rutgers, The State University of New Jersey, JACK SIMONSON, MEIGAN ARONSON, Stony Brook University, GIRSH BLUMBERG, Rutgers, The State University of New Jersey — Infrared reflection and transmission over a broad temperature range (10-300 K) have been measured on the anisotropic single-crystal Cu$_3$(SeO$_3$)$_2$Cl, KUN WOO KIM, California Institute of Technology, JAVIER JUNQUERA, Universidad de Cantabria, Spain

\(^1\)Supported by the US DOE through contract DE-FG02-02ER45984 at UF.

2:42PM J23.00002 Infrared evidence for multiple structural transitions in single crystal Cu$_3$(SeO$_3$)$_2$Cl, KEVIN H. MILLER, Department of Physics, University of Florida, HELMUTH BERGER, Institute of Physics of Complex Matter, Ecole Polytechnique Federale de Lausanne, DAVID B. TANNER, Department of Physics, University of Florida — Infrared reflection and transmission over a broad temperature range (10-300 K) have been measured on the anisotropic single-crystal Cu$_3$(SeO$_3$)$_2$Cl. Two distinct space groups have previously been reported for Cu$_3$(SeO$_3$)$_2$Cl at 300 K (monoclinic C2/m and triclinic P1bar). Comparing the number of observed infrared active phonons with group theoretical predictions points towards the existence of the triclinic structure at 300 K; however, an impurity-rich monoclinic structure cannot be ruled out. New phonon modes are observed upon cooling below 90 K, and again upon cooling below 40 K. The latter temperature range corresponds to the onset of long range magnetic order in the material. The structural and magnetic properties of Cu$_3$(SeO$_3$)$_2$Cl will be discussed in terms of our infrared spectra, group theoretical predictions, and comparisons to related compounds.

2:54PM J23.00003 Optical spectroscopy and Fermi Surface studies of the Rashba spin-splitting compound BiTeI, CATALIN MARTIN, K.H. MILLER, S. BUVAEV, A.F. HEBARD, University of Florida, Gainesville, Florida, 32611, USA, E.D. MUN, V. ZAPF, National High Magnetic Field Laboratory, Los Alamos, NM, 87545, USA, H. BERGER, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland, D.B. TANNER, University of Florida, Gainesville, Florida, 32611, USA — We measured the temperature dependent optical reflectivity $\rho$(\omega) and Shubnikov-de Haas oscillations in samples of BiTeI with different carrier concentrations. The electronic excitation spectrum, although consistent with Rashba spin-splitting of the bulk electronic bands, reveals additional features: a low energy excitation band and a larger number of phonons than expected from crystal structure. Some of the vibrational modes have strongly asymmetric line-shape. The period of quantum oscillations scales remarkably well with the component of magnetic field along the crystallographic c-axis and is rapidly suppressed when the field is tilted from this axis. We discuss our results in connection with possible charge accumulation at the surface of BiTeI.

3:06PM J23.00004 Enhancement of charge and spin orders in a photoexcited one-dimensional strongly correlated system, HANTAO LU, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan, SHIGETOSHI SOTA, Computational Materials Science Research Team, RIKEN AICS, Kobe, Hyogo 650-0047, Japan, HIROAKI MATSUEDA, Sendai National College of Technology, Sendai, 989-3128, Japan, JANEZ BONCA, J. Stefan Institute, SI-1000 Ljubljana, Slovenia, TAKAMI TOHYAMA, Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto, 606-8502, Japan — By using the time-dependent Lanczos method, the nonequilibrium processes of the half-filled one-dimensional extended Hubbard model, driven by a transient laser pulse, is investigated. In the case of large on-site Coulomb interactions, there are two phases separated by a first order quantum phase transition, i.e., spin-density-wave (SDW) and charge-density-wave (CDW) phases, which are characterized by algebraic decay of spin correlations and a long-range (staggered) charge order, respectively. When the system is subjected to the irradiation of a laser pulse, from the SDW side near the phase boundary, with proper laser frequency and strength, a sustainable charge order enhancement can be realized while local spin correlations remain. Analogously, from the CDW side, the suppression of long-range charge order is accompanied with a local spin correlation enhancement. We analyze the conditions and investigate possible mechanisms of the emerging order enhancements. In off-resonance region, more extended recovery of spin correlations which may come from nonlinear effect is also observed.

3:18PM J23.00005 Computational study of novel half metallic compounds, ZHIJIAN WU, JING WANG, Changchun Institute of Applied Chemistry — Half-metallic (HM) materials are metallic for one spin direction while at the same time semiconducting for the other spin direction \(^1\). The unique feature of HM material is that it has an integer spin magnetic moment. For a carefully selected material, the integer can be zero (compensated). Besides ferromagnetic (FM) parallel spin arrangements, ferrimagnetic or even antiferromagnetic (AFM) alignments are also possible. In particular, half-metallic antiferromagnet (HM-AFM) possesses no macroscopic magnetization, yet their carriers are fully spin-polarized. In this work, half metallic compounds have been predicted by using the first principles, such as NiMoO$_3$ \(^2\).


3:30PM J23.00006 A non-perturbative general expression for the conductance through a leaky chiral edge mode, KUN WOO KIM, California Institute of Technology, ALEXANDRA JUNCK, Freie Universitt Berlin, ISRAEL KLICH, University of Virginia, GIL REFAEL, California Institute of Technology — Chiral edge modes of topological insulators and Hall states exhibit non-trivial behavior of conductance in the presence of impurities or additional channels. We will present a simple formula for the conductance through a chiral edge mode coupled to a disordered bulk. For a given coupling matrix between the chiral mode and bulk modes, and a Green function matrix of bulk modes in real space, the renormalized Green function of the chiral mode is expressed in a closed form ratios of determinants. We will conclude with examples of how the formula could be applied to describe the behavior of a chiral mode coupled to different types of bulk systems.
3:42PM J23.00007 Generalization of the Peierls phase for gauge-invariant Green functions.
SYLVIA D. SWIECICKI, J.E. SIPE, University of Toronto — Solids in time-varying fields can be characterized with the non-equilibrium Green function formalism. If the interaction is described through potentials, the identification of sum rules is necessary to remove unphysical divergences that can appear in low frequency response calculations. For isolated atoms divergences are avoided by moving to a gauge-invariant Hamiltonian with the Power-Zienau-Woolley transformation. For solids, a gauge-invariant Green function formalism was proposed by Levanda and Fleurov in the generalization of the Peierls phase they introduced they consider only straight lines in spacetime. We extend this work to arbitrary paths in spacetime and show that the results for isolated atoms can be derived as a special case. More general applications are considered.

1W. Healy, Non-relativistic quantum electrodynamics (1982)

3:54PM J23.00008 Evolution of the Coherent State and the Electronic Structure in the Kondo Insulator SmB\textsubscript{6}\textsuperscript{1}. XIAOHANG ZHANG, Center for Nanophysics & Advanced Materials, University of Maryland, College Park and National Institute of Standards and Technology, N.P. BUTCH, Lawrence Livermore National Laboratory, P. SYERS, S. ZIEMAK, R.L. GREENE. J. PAGLIONE, Center for Nanophysics & Advanced Materials and Department of Physics, University of Maryland, College Park — As an exemplary Kondo insulator, SmB\textsubscript{6} has been studied for several decades; however, direct evidence for the development of the Kondo coherent state and the evolution of the electronic structure in the material has not been obtained due to the rather complicated electronic and thermal transport behavior. Recently, these open questions attracted increasing attention as the emergence of a time-reversal invariant topological surface state in the Kondo insulator has been suggested [1]. Here, we use the quasiparticle tunneling spectroscopy technique to directly investigate the temperature dependence of the electronic states in SmB\textsubscript{6}. As a signature of the Kondo screening effect in the material, a Fano-like resonance line shape is observed in the tunneling spectroscopy at temperatures below ∼ 100 K. We further demonstrate that inter-ion correlation has to be taken into account [2] in order to precisely describe the observed asymmetric tunneling conductance at low temperatures. Our quasiparticle tunneling spectroscopy results also provide important implications for the predicted nontrivial topology in the Kondo insulator.

1Dzero et al., PRL 104, 106408 (2010); 2Maltseva et al., PRL 103, 206402 (2009)

4:06PM J23.00009 Intervalley scattering and localization behaviors of group-VI transition metal dichalcogenides.
HAIZHOU LU, WANG YAO, The University of Hong Kong, DI XIAO, Carnegie Mellon University, SHUN-QING SHEN, The University of Hong Kong — We study the quantum diffusive transport of multi-valley massive Dirac cones coupled by intervalley spin-orbit scattering. We show that the intervalley spin-orbit scattering and intravalley spin-conserved scattering can be distinguished from the quantum conductivity that corrects the semiclassical Drude conductivity, due to their distinct symmetries and localization trends. In immediate practice, it allows transport measurements to estimate the intervalley scattering rate in hole-doped monolayers of group-VI transition metal dichalcogenides (e.g., molybdenum dichalcogenides and tungsten dichalcogenides), an ideal class of materials for valleytronics applications. The results can be generalized to a large class of multi-valley massive Dirac systems where time-reversal symmetry demands opposite spins in opposite valleys.

4:18PM J23.00010 The structural origin of energy band gap in ultraviolet borates.
ZHESHUAI LIN, RAN HE, Technical Institute of Physics and Chemistry, Chinese Academy of Sciences — Borate crystals have been intensively studied for their broad significant application in nonlinear optics materials, fluorescent materials, and laser crystals, especially in the ultraviolet (UV) spectral region (photon energy larger than 6.2 eV). However, due to the structural complexity the mechanism determining the energy band gap in the UV borates still hides in clouds. In this work, the structural origins of the energy band gaps in UV borates are systematically studied by ab initio methods and modeling considerations. Through analyzing the electronic band structures, we find that the top of valence bands in UV borates are dominant from the orbitals on oxygen. These orbitals construct the non-bonding states which determine the energy band gaps and their magnitudes depend on the local environments around oxygen atoms. Accordingly, the UV borates are categorized into three structural types, and in each type the ideal energy band gaps by removing the non-bonding states are almost the same. Moreover, a modified Bond Valence Sum method is adopted to parameterize the local environment around oxygen atoms, and the good agreement between the calculated and experimental energy band gaps within the accuracy of 0.3 eV can be achieved in UV borates.

4:30PM J23.00011 Electron Transport in Edge Metal-Insulator-Metal Tunnel Junctions Modulated by Underlying Ferroelectric Polarization Switching.
KIBO PARK, YOUNGJEUN JONG, SUNGCHUL JUNG, HAN BYUL JIN, Ulsan National Institute of Science and Technology, Ulsan 689-798, South Korea. JAE-HYEON GO, Hallym University, Chuncheon Gangwondo 200-702, South Korea, SOON-YONG KWON, Ulsan National Institute of Science and Technology, Ulsan 689-798, South Korea, NAM KIM, Korea Research Institute of Standards and Science, Daejeon 305-340, South Korea — The electron energy band profile in an Edge Metal-Insulator-Metal tunnel junction (EMIM) on a Insulator/Ferroelectric thin film was calculated by performing finite-element electrostatic modeling. It is found that the energy band profile in the EMIM junction alters significantly near the underlying Insulator/Ferroelectric layer depending on the polarization direction of ferroelectric layer. The energy band profile shows pinch-off when the interface bound charge at Insulator/Ferroelectric interface is negative while it shows a valley-like shape when the interface bound charge is positive. The change in the energy band profile depending on ferroelectric polarization is confirmed to result in a significant change of electron tunneling current by using WKB method. It is believed that this switching of electron tunneling resistance in the EMIM junction opens up a new way to develop non-volatile ferroelectric memory devices using non-destructive read-out.

1NRF(2010-0004370) funded by MEST in Korea

MELANIE COLE, ERIC NGO, MATHEW IVILL, S. GARY HIRSCH, CLIFF HUBBARD, RYAN TOONEN, WENDY SARNEY, US Army Research Laboratory, WMRD, INTEGRATED ELECTROMAGNETIC MATERIALS RESEARCH GROUP COLLABORATION — Voltage control of magnetism in magnetic/ferroelectric bilayers has been most recently demonstrated in ultrathin metallic magnetic films through an electric field induced spin polarized charge screening effect. Voltage-controlled magnetism in magnetic/ferroelectric multilayers would provide a unique opportunity for integrating voltage-tunable RF/microwave magnetic devices on integrated circuits. It has been theoretically predicted that the voltage-control of magnetism in ferromagnetic/ferroelectric heterostructures can be significantly enhanced by utilizing high-K dielectrics. The critical challenge is how to enhance the permittivity of the ferroelectric film while maintaining low loss and low leakage characteristics and accomplishing this in an affordable manner by employing industry standard processing methods and large area low cost substrates. In this work we demonstrate the achievement of high-K, low loss and low leakage BST films utilizing optimized sputtered SrTiO\textsubscript{3} buffer layers combined with a MOSD grown Mg-doped Ba\textsubscript{0.6}Sr\textsubscript{0.4}TiO\textsubscript{3} overgrowth film on affordable large area substrates. Results of this research serves to promote enhanced EM coupling to enable a new class of charge mediated integratable voltage control multiferroic devices exploiting the converse ME effect.
Perovskites

Secondly, these changes are most marked for x < 0.2. Thus, we provide a comprehensive picture of the electronic structure evolution in the conduction band in these materials as a function of the Mn content.

Thermodynamic stability of radiogenic Ba in CsAlSi$_2$O$_6$ pollucite

We have used first-principles density functional total energy calculations to evaluate the thermodynamic stability of pollucite with Ba replacing Cs at regular lattice sites with respect to the precipitation of Ba, Cs or their oxides. We included small clusters of substitutional Ba$_x$Cs$_{1-x}$ as well as localized complexes of BaO$_x$Cs$_{1-x}$, with compensating electron donor defects, specifically Cs vacancies and interstitial oxygen. We conclude that Cs-Ba pollucite is thermodynamically stable against precipitation of Cs or its oxide, but that partial precipitation of Ba or BaO may be thermodynamically favored under some conditions. Even this change may be kinetically limited, however.

Metal-induced gap states in ferroelectric capacitors and its relationship with complex band structures

These MIGs can be actually regarded as Bloch functions with an associated complex wave vector. Usually only real values of the wave vectors are discussed in text books, since infinite periodicity is assumed and, in that situation, wave functions growing exponentially in any direction would not be physically valid. However, localized wave functions with an exponential decay are indeed perfectly valid solution of the Schrödinger equation in the presence of defects, surfaces or interfaces. For this reason, properties of MIGs have been typically discussed in terms of the complex band structure of bulk materials. The probable dependence on the interface particulars has been rarely taken into account explicitly due to the difficulties to include them into the model or simulations. We aim to characterize from first-principles simulations the MIGs in realistic ferroelectric capacitors and their connection with the complex band structure of the ferroelectric material. We emphasize the influence of the real interface beyond the complex band structure of bulk materials.

Footnotes:
1 Fuel Cycle Research and Development, U.S. Department of Energy Waste Form Campaign
2 Financial support provided by MICINN Grant FIS2009-12721-C04-02, and by the European Union Grant No. CP-FP 228989-2 “OxIDes”. Computer resources provided by the RES.

Tuesday, March 19, 2013 2:30PM - 5:18PM
Session J28 DCMP: Liquid Crystals I

2:30PM J28.00001 2D Brownian motion of inclusions in low pressure environment on freely suspended liquid crystal film

We report 2D Brownian motion experiment of drops in different air pressure. In equilibrium, they form minimal surfaces like soap films. However, shape transformations of closed smectic membranes that change the surface area involve the formation and motion of molecular layer dislocations. These processes are slow compared to the capillary wave dynamics, therefore the effective surface tension is zero like in vesicles. Freely floating smectic bubbles are prepared from collapsing catenoid films and their dynamics is studied with optical high-speed imaging. Experiments are performed under normal gravity and in microgravity during parabolic flights.

2:42PM J28.00002 Between soap bubbles and vesicles: The dynamics of freely floating smectic bubbles

This work is supported by NASA Grant No. NAGNNX07AE48G, NSF MRSEC DMR 0820579, and NSF DMR 0606528.
2:54PM J28.00003 Critical Behavior of A Non-polar Smectic Liquid Crystal via Optical Birefringence Measurements. MEHMET CAN CETINKAYA, SELEN ERKAN, SEVTAP YILDIZ, HALUK OZBEK, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey. ITU LIQUID CRYSTALS LABORATORY TEAM — We present high sensitivity and high temperature resolution experimental data on the temperature dependence of the optical birefringence in the nematic and smectic A phases of nonpolar monolayer smectogen 4-butylloxyphenyl-4'-decyloxybenzoate liquid crystal by using a rotating-analyzer technique. We have used the birefringence data to probe the temperature behavior of the nematic order parameter S(T) in the vicinity of both the nematic-isotropic (N-I) and the nematic-smectic A (N-SmA) transitions. The critical behavior of S(T) at the N-I transition has been discussed in detail by extracting S(T) from the birefringence data [1-3]. We have tested the validity of the scaling relation \( \lambda = 1 - \alpha \) between the critical exponent \( \lambda \) describing the limiting behavior of the nematic order parameter and the specific heat capacity exponent \( \alpha \). We have shown that the temperature derivative of the nematic order parameter \( S(T) \) near the N-SmA transition has the same power law behavior as the specific heat capacity [4,5].

1Work supported by the Research Fund of Istanbul Technical University under Grants No.32936, No. 34824, No. 34254, and No. 34412.

3:06PM J28.00004 Statistical mechanics of bend flexoelectricity and the twist-bend phase in bent-core liquid crystals. SHAIKH SHAMID, SUBAS DHAKAL, JONATHAN SELINGER, Kent State University — We develop a Landau theory for bend flexoelectricity in a liquid crystals of bent-core molecules. In the nematic phase of the model, the bend flexoelectric coefficient increases as we reduce the temperature, and it diverges at the nematic to polar phase transition. At this critical point, there is a second order transition from high-temperature uniform nematic phase to low-temperature nonuniform phase composed of twist-bend or splay-bend deformations. To test the predictions of Landau theory, we perform Monte Carlo simulations to find the behavior as a function of temperature, applied electric field and interaction parameters, and to determine the orientational distribution of the mesogenic molecules.

2This work was supported in part by an allocation of computing time from the Ohio Supercomputer Center.

3This work was supported in part by an allocation of computing time from the Ohio Supercomputer Center.

3:18PM J28.00005 Imaging helical nano-filament and modulated smectic phases of bent shaped liquid crystals by cryo-TEM. CIUYU ZHANG, Kent State University, HANS SAWADE, I.N. Stranski Institute, TU Berlin, WOLFGANG WEISSFLOG, Martin Luther University Halle-Wittenberg, ANTAL JAKLI, Kent State University — Recently we showed that cryo-TEM can be used to visualize smectic layers of thermotropic liquid crystals. Here we describe cryo-TEM studies of the nanofilaments (B4 phase) and the modulated smectic layers (B7 phase) of various bent shaped liquid crystal compounds. In the B4 phase a periodic array of about 15 nm wide bands of parallel stripes, separated by a distance equal to the layer spacing, appear with a periodicity of about 120 nm corresponding to the half pitch of the nanofilaments. As cryo-TEM shows only layers that are parallel to the electron beam, these results indicate grains of straight layers twisted along the filament axis compose the nano-filaments. In the B7 phase cryo-TEM not only can visualize the smectic layers, but also the periodic modulation indicating defects with less dense molecular packing. In addition we observe a labyrinth structure with curvature radii in the 150 nm ranges. These results yield information complementary to freeze fracture TEM and X-ray observations.

3:30PM J28.00006 Wide temperature range and hysteresis free blue phase liquid crystals doped with bent-core compound. JIE XIANG, OLEG TWIEG, OLEG LAVRENTOVICH, Kent State University — We explore an approach to widen the temperature range of the liquid crystalline blue phases based on mixtures of calamitic (rod-like) and bent-core mesogens. The calamitic component has a relatively low value of the bend elastic constant that is further reduced by adding the bent-core component. The mixtures exhibit the blue phase state in a wide temperature range, about 5°C in the regime of heating and 40°C (including the room temperature) upon cooling. We present a phenomenological model to illustrate the link between the temperature range of the blue phase and the bend elastic constant that is based on Kleman’s model of double twist in liquid crystals. We also study the electro-optic properties of the mixtures. The electrooptic switching is reversible in the upper temperature range of the blue phase, but once the temperature decreases below a certain level, the electrooptic switching shows a hysteresis associated with phase separation of the components. The work was supported by NSF grant DMR 1122878.

3:42PM J28.00007 Piezoelectric properties of polymers containing bent-shape liquid crystal molecules. N. DIORIO, M. VARGA, Kent State University, A. CARIF, J.E. PUSKAS, University of Akron, K. FODOR-CSORBA, Hungarian Academy of Sciences, S. SPRUNT, J.T. GLEESON, A. JAKLI, Kent State University — Recently, bent-core liquid crystal elastomers have shown to exhibit large values of flexoelectricity as many 3 orders of magnitude larger than liquid crystal elastomers containing rod-shaped molecules. These unusual high responses are attributed to have piezoelectric origin. Motivated by this, in this study, two bent-core liquid crystals were used to make various types of materials; low molecular weight bent-core nematic fluid, side chain bent-core liquid crystal polymer, low molecular liquid crystal dispersed in a polyisobutylen-based thermoplastic elastomer, and side-chain bent-core elastomers. Liquid crystal elastomers combine elasticity and flexibility inherent to rubbers and the optical and electrical properties of liquid crystals, and are promising materials for applications such as electro-optics, flexible electronics and actuator technologies for biomedical applications. Most conventional liquid crystal elastomers have rod-shaped liquid crystal molecules chemically attached to a crosslinked polymer network. Converse piezoelectric responses were measured by a Mirau interferometer and the direct piezoelectric signals were studied by home-made device where the stress is provided by an audio speaker. The results will be analyzed in terms of ferroelectric clusters of the materials in the nematic phase and will be compared with other piezoelectric materials.

3Supported by Grants NSF-DMR -0964765 and NSF-DMR -0804878.

3:54PM J28.00008 SAXS studies of short-range order in the nematic phase of reduced symmetry mesogens. S. CHAKRABORTY, Department of Physics, Kent State University, N. DIORIO, C. ZHANG, Chemical Physics Interdisciplinary Program and Liquid Crystal Institute, Kent State University, R. BRECKON, R. TWIEG, Department of Chemistry, Kent State University, J. GLEESON, Department of Physics, Kent State University — Recently, we proposed a model based on persistent, nano-scale smectic-C-like domains (“smectic clusters”) to explain the features present in the small angle x-ray diffraction patterns from certain bent-core nematic liquid crystals (which do not possess an underlying smectic phase). We report on new results from a wider range of nematics formed by reduced-symmetry molecules – including laterally-branched (“Y”-shaped) mesogens and “H” shaped dimers – that also lack a low temperature smectic phase. We find that our model, extended to incorporate the notion of staggered molecular arrangements, is successful in reproducing the SAXS patterns and reveals variation in the temperature-dependence of cluster size among different systems. Supported by NSF DMR-0964765.
4:06PM J28.00009 Local orientation and temperature effects of a liquid crystal in contact with a nanoparticle\textsuperscript{1} JEFFERSON WARD TAYLOR, University of Maryland, College Park, MD, LYNN K. KURIHARA, Naval Research Laboratory, Washington, DC, LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD — We have studied the effects on the orientation of the liquid crystal in the immediate vicinity of a nanoparticle. We have observed a “halo” surrounding the nanoparticle, when studying the effects of the nanoparticle on the liquid crystal with the AFM. We believe this halo has an effect on the ordering of the liquid crystal in the immediate vicinity of the nanoparticle. We have also observed a short range order peak in the X-ray scattering signal, which is also associated with the effects on the liquid crystal in the immediate vicinity of the nanoparticle. The value of the coherence length of this peak is close to the value of the molecular spacing or very close of the liquid crystal in the X-ray scattering experiment for all nanocomposites studied. This coherence length does not change as a function of temperature, when the temperature is changed and goes through the SmA-nematic transition temperature. The peak and its coherence length persist into the nematic phase.

\textsuperscript{1}Supported by NSF-DMR-0906433.

4:18PM J28.00010 Electro-optical Characteristics of Carbon Nanotupe Doped Polar Smeic Liquid Crystal\textsuperscript{1} ILKNUR KOSEOGLU, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey, MEHMET CAN CETINKAYA, Piri Reis University, 34970, Tuzla, Istanbul, Turkey, HALUK OZBEK, SEVTAP YILDIZ, Department of Physics, Istanbul Technical University, 34469, Maslak, Istanbul, Turkey, ITU LIQUID CRYSTAL LAB TEAM — We present the results of electro-optical characteristics of the liquid crystal octylcyanobiphenyl (8CB) doped with well-dispersed multiwall carbon nanotubes (MWCNT) under an AC driving voltage. 8CB-MWCNT composites were prepared by following the procedures in literature \textsuperscript{1-4}. Polarized optical microscopy (POM) has been performed to check the homogenous dispersion of 8CB-MWCNT composite. We compare threshold voltages and switching behavior of pure 8CB and 8CB doped with MWCNTs which have surfaces of untreated and treated with carboxyl functional group. Threshold voltages have been determined from optical transmission-driving voltage curves at various temperatures. While the pure 8CB switches from a bright state through some intensity oscillations to the dark state, a drastic change has been observed in the transmission curves for 8CB-MWCNT composites, namely hysteric behavior has been detected. For 8CB-MWCNT composites we have observed that the first cycle for the transmission-voltage curves shows the highest amount of loop area, which gradually decreases through the following cycles, then reaching saturation. Notice that the number cycle at which the saturation is reached depend on temperature \textsuperscript{5}.

\textsuperscript{1}Supported by the Research Fund of Istanbul Technical University under Grants No.32936, No. 34824, No. 34254, and No. 34412.

4:30PM J28.00011 Effect of quantum dots on the isotropic to nematic and nematic to smectic-A phase transitions in nano composites\textsuperscript{1} PARVATHALU KALAKONDA, GERMANO S. IANNACCHIONE, WPI — Modulated Differential Scanning Calorimetry (MDSC) is used to investigate the weakly first-order isotropic to nematic (I-N) and the continuous nemat to smectic-A (N-SmA) phase transitions of the liquid crystal octylcyanobiphenyl (8CB) doped with well-dispersed quantum dots (QdS) as a function of Qd concentrations. Thermal scans were performed for all samples having Qd (CdS) weight percent from $\phi_w = 0.3$ to 3 wt\% first on cooling and then heating under near-equilibrium conditions. The I-N transitions heat capacity peak first grows then decreases in magnitude with increasing $\phi_w$, leaving a maximum at $\phi_w = 0.3\%$. The N-SmA heat capacity peak remains bulk-like for all samples. Both transitions temperatures shift lower monotonically by 3 K for $\phi_w = 0.3\%$. The enthalpy of both transitions evolve in a nontrivial way, generally decreasing with increasing $\phi_w$. These results are discussed in terms of the predominate disordering effects of the Qds.

\textsuperscript{1}Supported by NSF-MRSEC Grant DMR-0820579 and NSF Grant DMR-1006870.

4:42PM J28.00012 Towards an optical nano-laboratory in a liquid crystal defect, PAUL ACKERMAN, University of Colorado at Boulder, National Renewable Energy Laboratory, Renewable and Sustainable Energy Institute, IVAN SIMALYUKH, University of Colorado at Boulder, JAVO VAN DE LAGEMAAT, National Renewable Energy Laboratory — Probing photonic effects due to nanoscale interactions between colloids such as quantum dots and rod and anisotropic plasmonic metal nanoparticles is of great interest for applications in third-generation solar cells, optical metamaterials, and nanonanotubes. Liquid crystal (LC) structures and defects stabilized by chirality, confinement, and/or presence of colloidal microparticles can enable trapping and well-defined alignment of anisotropic semiconductor, plasmonic, and other nanoparticles with respect to the far-field director and each other. Minimization of the free energy due to LC defects provides a rich environment for precisely controlled experiments with individual and small groups of nanoparticles in the LC. This presentation will discuss characterization of trapping and alignment of various nanoparticles by LC defects and also photonic experiments performed on a single-particle level for metal and semiconductor quantum nanoparticles entrapped by these defects. This work was supported by the Division of Chemical Sciences, Geosciences, and Biosciences, Office of Basic Energy Sciences of the US Department of Energy under Contract No. DE-AC36-08GO28308 with the National Renewable Energy Laboratory (J.v.d.L. and J.S.E.).

4:54PM J28.00013 Interaction of discotics and nanoparticles\textsuperscript{1} LUZ J. MARTINEZ-MIRANDA, University of Maryland, College Park, MD, EDUARDO A. SOTO-BUSTAMANTE, Universidad de Chile, Santiago, Chile — We mixed a discotic, and 5 nm nanoparticles of ZnO up to a percentage weight of 30 – 35%, by heating them together, past the isotropic transition temperature. At that point, we mixed them together, and allowed them to cool to room temperature. We then prepared a sample for Xray study, by taking a small amount of the crystallites formed and placing them in a glass slide. We prepared a sample of the pure discotic to compare to the mixture. We found that the addition of the nanoparticle results in an enhancement of the axis in the direction parallel to the glass slide, with an intensity approximately six times that of the discotic alone and a correlation length approximately 1.3 times better. The role of the nanoparticle is very similar to the alignment role of a flat surface observed on discotics.

\textsuperscript{1}Supported by a Fulbright Specialists Fellowship

5:06PM J28.00014 High resolution synchrotron X-ray studies of lyotropic liquid crystal phases of monolayer Zirconium Phosphate nanosheet\textsuperscript{1} YUE SHI, YONGQIANG SHEN, NOEL CLARK, Department of Physics, Liquid Crystal Materials Research Center, University of Colorado-Boulder, CO 80309, USA, MIN SHUAI, ZHENGDONG CHENG, McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX 77843, USA — Aqueous suspensions of monolayer zirconium phosphate nanosheets (ZrP-NS) form various lyotropic liquid crystal phases. An interesting stripe pattern can be observed in a range of nanosheet concentrations when the suspensions were confined between flat surfaces. The stripe patterns were stable while slow evaporation of the solvent and were well-preserved even when the suspensions dried out. A high resolution synchrotron X-ray study gives detailed investigations of ZrPNS lyotropic phases at different concentrations.

\textsuperscript{1}Supported by NSF MRSEC Grant DMR-0820579 and NSF Grant DMR-1006870.

Tuesday, March 19, 2013 2:30PM - 5:30PM – Session J34 DPOLY DCMP DBGIO: Focus Session: Charged Colloids with Short-Range Attractions

342 - Frank Schreiber, Institut fuer Angewandte Physik, Universitaet Tuebingen
3:06PM J34.00002 Concentrated dispersions of therapeutic proteins, THOMAS TRUSKETT, The University of Texas at Austin — In this talk, recent experiments characterizing highly concentrated dispersions of therapeutic proteins, which are of interest for at-home treatment of disease via subcutaneous injection, are discussed. In particular, evidence for protein nanocluster formation in these systems is explored. The roles of dispersion composition, pH, and experimental pathway are elucidated for several protein systems. Observed correlations between nanocluster properties, solution viscosity, and protein stability/activity, as well as prospective theoretical explanations for these behaviors, are highlighted.

3:42PM J34.00003 Transition from monomeric phase to dynamic cluster phase in lysozyme protein solutions, YUN LIU, University of Delaware/National Institute of Standards and Technology, PETER FALUS, LIONEL PORCAR, Institute Laue-Langevin, EMILIANO FRATINI, University of Florence, WEI-REN CHEN, Oak Ridge National Laboratory, ANTONIO FARAOUE, University of Maryland/National Institute of Standards and Technology, KUNLUN HONG, Oak Ridge National Laboratory, PIERO BAGLIONI, University of Florence — Intermediate range order (IRO) has been recently observed in lysozyme solution that is caused by a combination of a short-range attraction and long-range repulsion. At very high concentration, there is observed cluster formation in lysozyme solutions that is one type of IRO structures. Here, we investigate the temperature effect on the dynamic cluster formation and identify the transition concentration from a monomeric protein phase to a cluster phase. The normalized short-time self-diffusion coefficient is not affected by changing attraction strength at the concentration of about 10% mass fraction, indicating that the system is still dominated by monomeric protein phase. However, at high concentrations, the average self-diffusion coefficient is sensitive to the change of short-range attraction strength, which is interpreted due to the growth of the size of dynamic clusters in solution. The transition concentration from dominating monomeric phase to dynamic cluster phase is estimated to be around 14% mass fraction.

3:54PM J34.00004 Langevin Dynamics Simulation of DNA Condensation Induced by Nanoparticles in Confinement, GUO-JUN LIAO, Department of Physics, National Taiwan University, Taipei, 10087, Taiwan, R.O.C., YENG-LONG CHENG, Institute of Physics, Academia Sinica, Taipei, 11529, Taiwan, R.O.C. — We study nanoparticle-induced DNA condensation in a confined suspension of dilute DNA molecules and ideal nanoparticles (NPs) with Langevin dynamics simulation. DNA condensation has been observed in a solution of dilute DNA molecules (persistence length $\lambda_p \approx 50$ nm) and high concentration of electrostatically neutral NPs (diameter $d \approx 5$ to 35 nm) in recent experimental measurements. It is believed that NPs entropically induce an attraction between DNA segments. For NPs much smaller than $\lambda_p$, a DNA molecule can be considered as a chain of connected rods, and the NP-induced depletion attraction between DNA segments can be regarded as rod-rod attraction. Thus, the strength of the depletion volume $\approx 5$ to 35 nm) in recent experimental measurements. DNA size decreases monotonically as $d$ increases, while non-monotonic dependence happens for $d/\lambda_p \approx 5$, due to the competition between DNA-DNA, DNA-NP, and NP-wall interactions.

4:06PM J34.00005 Small-Angle Neutron Scattering and Neutron Spin Echo Characterization of Monoclonal Antibody Self-Associations at High Concentrations, ERIC YEARLEY, MacroGenics, Inc., ISIDRO (DAN) ZARRAGA, Genentech, Inc., PAUL (DOUG) GODFRIN, University of Delaware, TATIANA PEREVOZCHIKOVA, National Institute of Standards and Technology, NORMAN WAGNER, University of Delaware, YUN LIU, University of Delaware/National Institute of Standards and Technology — Concentrated therapeutic protein formulations offer numerous delivery and stability challenges. In particular, it has been found that several therapeutic proteins exhibit a large increase in viscosity as a function of concentration that may be dependent on the protein-protein interactions. Small-Angle Neutron Scattering (SANS) and Neutron Spin Echo (NSE) investigations have been performed to probe the protein-protein interactions and diffusive properties of highly concentrated MAbs. The SANS data demonstrate that the inter-particle interactions for a highly viscous MAAb at high concentrations (MAb1) are highly attractive, anisotropic and change significantly with concentration while the viscosity and interactions do not differ considerably for MAb2. The NSE results furthermore indicate that MAb1 and MAb2 show promising concentration dependencies of dynamics at high Q that are correlated to the translational motion of the proteins. Finally, it has also been revealed that the individual MAb1 proteins form small clusters at high concentrations in contrast to the MAb2 proteins, which are well-dispersed. It is proposed that the formation of these clusters is the primary cause of the dramatic increase in viscosity of MAb1 in crowded or concentrated environments.

4:18PM J34.00006 The Structural Properties and Stability of Monoclonal Antibodies at Freezing Conditions, TATIANA PEREVOZCHIKOVA, University of Delaware/NIST, ISIDRO ZARRAGA, THOMAS SCHERER, Genentech, Inc., NORMAN WAGNER, University of Delaware, YUN LIU, University of Delaware/NIST — Monoclonal Antibodies (MAb) have become a crucial therapeutic agent in a number of anti-cancer treatments. Due to the inherent unstable state of proteins in an aqueous formulation, a freeze-drying method has been developed to maintain long-term stability of biotherapeutics. The microstructural changes in Mabs during freezing, however, remain not fully described, and it was proposed that the formed morphology of freeze-drying samples could affect the final product quality after reconstitution. Furthermore, it is well known that proteins tend to aggregate during the freezing process if a careful freezing procedure is not formulated. Small Angle Neutron Scattering (SANS) is a powerful tool to investigate the structural properties and interactions of Mabs during various stages of lyophilization in situ. Here we present the SANS results of freeze-thaw studies on two MAbs at several different freezing temperatures. While the chosen proteins share a significant sequence homology, their freezing properties are found to be strikingly distinctive. We also show the effect of excipients, concentration and quenching speed on the final morphology of the frozen samples. These findings provide critical information for more effective lyophilization schemes for therapeutic proteins, as well as increase our understanding on structural properties of proteins under cryogenic conditions.

4:30PM J34.00007 Shear-Dependent Interactions in Rheology Modifier (RM)-Latex Suspensions, TIRTHA CHATTERJEE, ALAN I. NAKATANI, Analytical Sciences, The Dow Chemical Company, ANTONY K. VANDYK, Dow Coatings Materials, The Dow Chemical Company — Paint viscosity, under shear is governed by its shear-induced structure which in turn controls the application properties. The micro and macroscopic structure of the RM-latex combinations under shear is central to understand paint application behavior. Using in-situ shear-small-angle neutron scattering (shear-SANS) the RM-latex structure has been studied. All studies reported here are performed on acrylic-based latex with different hydrophilically modified ethoxylated urethane (HEUR) RM varying in their hydrophobe density/chain. At a quiescent condition, latex and RM form a spherical core-shell structure, with latex particles being the core and adsorbed RMs on the surface forming the shell. The shell thickness decreases with increasing RM hydrophobe density/chain. Under shear, the solvent (D2O/H2O) is squeezed out (hydrodynamic squeezing) from the swollen RM chains and the shell structure becomes denser and anisotropic due to differing degrees of compression along the flow and vorticity directions. An effective shear-dependent latex-RM hydrodynamic volume fraction has been calculated using SANS structural data. High shear viscosity calculated on the basis of effective hydrodynamic volume using existing models do not match with the experimental data. This suggests the existence of RM molecule mediated interactions even at high shear rate.
4:42PM J34.00008 Multi-body effects in Charged Colloids - Polyelectrolyte systems, VICTOR PRYAMITSYN, VENKAT GANESAN, University of Texas at Austin — Multibody effects upon the electrostatic interaction between particles, polyelectrolyte molecules and monovalent ions were analyzed within Poisson-Boltzmann approximation. The numerical self-consistent field (SCF) theory for a polymer - nanoparticles systems was developed for a mixture of quenched polyelectrolytes and charged and uncharged particles and the pseudo-spectral method was used to solve polymer SCF equations in three dimensions within the Grand Canonical Ensemble for polymer and ions. A calculation of the free energies of a single particle and of two particles in polyelectrolyte solutions allowed us to calculate respectively the particle interaction energy and particle-particle interactions as a function of the properties of solution, polymer-particle interaction and particle size. By explicitly calculating the free energy of three particles after subtraction of the contributions from two-body interaction allowed us to calculate effective contribution of 3-body particle-particle interactions in polyelectrolyte -particles systems. We have found that the polyelectrolyte mediated two body interactions are repulsive for the larger particle-particle distances and lower polymer concentrations. Interestingly, such an electrostatic repulsion exists even if particles have

4:54PM J34.00009 A density functional approach to model highly charged spherical colloids in electrolyte mixtures, BHARAT MEDASANI, ZAVENT OVANESYAN, MARCELO MARUCHO, University of Texas at San Antonio — We present a classical density functional (DFT) approach to study ion size asymmetry, ion-ion correlation and solvent excluded volume within the mean spherical approximation. The present DFT approach is able to describe macro-ions in electrolytes comprising neutral hard sphere mimicking water molecules and ions with dissimilar valence and realistic sizes and densities. We applied the theory to study spherical electric double layers and obtained results in good agreement with simulations. We calculated ion profiles, integrated charge, mean electrostatic potential, ionic coordination number, zeta potential, and inverse differential capacity at different conditions. For higher surface charge on macromolecule, charge inversion is noticed and when the counter-ions are bigger than co-ions, surface charge amplification is observed. Layering and screening effects are more pronounced when water molecules are explicitly considered. This work has potential applications in bio-electrostatics and colloidal engineering.

5:06PM J34.00010 Measuring inter-nucleosome interactions and the roles of histone tails, STEVEN HOWELL, George Washington University, KURT ANDRESEN, Gettysburg College, ISABEL JIMENEZ-USECHE, CHONGLI YUAN, Purdue University, XIANGYUN QIU, George Washington University — Nucleosome is the first level of genome organization and regulation in eukaryotes, where negatively charged DNA is wrapped around positively charged histone proteins. Being a DNA-protein complex of biological origin, nucleosome is also a model multi-phasic nanoparticle with heterogeneous charge distributions and nanoscale-like flexibility of the subunits of the histone proteins. In solutions of nucleosomes, electrostatic forces dominate inter-nucleosome interactions at long range while specific contacts, in particular the flexible histone tails, guides short range interactions. We have thus quantified how the ions from salts (KCl, MgCl2) modulate the inter-nucleosome pair potential by modeling the total small angle x-ray scattering profiles. We additionally elucidated the individual role of the charged tails of histones H3 and H4. We found that measured effective changes at low salt concentrations are about 1/5th of theoretically predicted renormalized charges and that H4 tail deletion suppresses the attraction at high salt concentrations to a larger extent than H3 tail deletion.

5:18PM J34.00011 Multivalent Colloids through DNA Patchy Particles, YUFENG WANG, YU WANG, Molecular Design Institute and Department of Chemistry, New York University, DANA BREED, The Dow Chemical Company, VINOTHAN MANOHARAN, School of Engineering and Applied Sciences; Department of Physics, Harvard University, LANG FENG, ANDREW HOLLINGSWORTH, Center for Soft Matter Research and Department of Physics, New York University, MARCUS WECK, Molecular Design Institute and Department of Chemistry, New York University, DAVID PINÉ, Center for Soft Matter Research and Department of Physics, New York University — We demonstrate a general method for creating the colloidal analogs of atoms with multiple valences: colloidal particles with chemically functionalized patches that can form highly directional specific bonds. The valences of these “colloidal atoms” possess all the common symmetries characteristic of hybridized atomic orbitals, including sp, sp2, sp3, spd, spd2, and spd3. The chemical functionality of the patches is programmable and specific using DNA with single-stranded sticky ends, thereby creating colloidal atoms from which different kinds of “colloidal molecules” can be assembled, including the colloidal analogs of carbon dioxide and tetrahedrally coordinated methane. The bonds between these new colloidal atoms are highly directional and fully reversible with temperature.

This work is partially supported by the MRSEC Program of the National Science Foundation under Award Number DMR-0820341. Additional financial support was provided by the National Science Foundation (Che-0911460).

Tuesday, March 19, 2013 2:30PM - 5:30PM — Session J35 DCMP: Superconductivity: Vortices II 343 -

2:30PM J35.00001 Doubling of the Critical Current Density of 2G-YBCO Coated Conductors through proton irradiation, ULRICH WELP, YING JIA, WAI-KWONG WOK, Materials Science Division, Argonne National Laboratory, MARTY RUPICH, STEVEN FLESHLER, American Superconductor Corporation, Devens, MA, ASFGHAR KAYANI, Western Michigan University, Kalamazoo, MI — We report on magnetization and transport measurements of the critical current density of commercial 2G YBCO coated conductors before and after proton irradiation. The samples were irradiated along the c-axis with 4 MeV protons to a fluence of 1.5x1016 p/cm². We find that at temperatures below 50 K, proton irradiation increases Jc by a factor of 2 in low fields and increases up to 2.5 in fields of 7 T. At 77 K, proton irradiation is less effective in enhancing the critical current. Doubling of Jc in fields of several Tesla and at temperatures below 50 K will be highly beneficial for applications of coated conductors in rotating machinery, generators and magnet coils. — Work supported by the US DoE-BES funded Energy Frontier Research Center (YJ), and by Department of Energy, Office of Science, Office of Basic Energy Sciences (UW, WKK), under Contract No. DE-AC02-06CH11357.

2:42PM J35.00002 Vortex dynamics in Co-doped and K-doped BaFe2As2 with point defects, TOSHIHITO TAEN, TAKAIRO OHORI, FUMIAKI ONTAKE, YASUYUKI NAKAJIMA, TSUYOSHI TANEGAI, Department of Applied Physics, The University of Tokyo, KUNIHIRO KIHOU, SHIGEYUKI ISHIDA, HIROSHI EISAKI, National Institute of Advanced Industrial Science and Technology (AIST), HISASHI KITAMURA, Radiation Measurement Research Section, National Institute of Radiological Sciences — The discovery of iron-based superconductors urges scientists and engineers to study not only superconducting mechanism but also possible applications. In view of this situation, it is important to study vortex dynamics for understanding fundamental properties as well as for suggesting a suitable fabrication process in this system. In particular, the interaction between vortices and defects attract tremendous attention, which is because this interaction is responsible for finite critical current density Jc. The interaction changes with dimensionality and morphology of defects. In cuprate superconductors, vortex manifold shows vortex glass phase with point defects and Bose glass phase with columnar defects. Besides, in both cases, Jc shows pronounced enhancement compared with that in a pristine sample. We have already reported the enhancement of Jc by the introduction of point or columnar defects in the case of Ba2−xKxFe2−yCo2yAs2 crystal. In this talk, we show the results in proton-irradiated BaFe2As2 with electron- or hole-doping. The quantitative analysis reveals the doubling of pinning potential without changing the glassy exponent in Co-doped compounds, in addition to 2.5 times enhancement of Jc. Similar effects are observed in K-doped crystals.
2:54PM J35.00003 Fundamentals of free flux flow: proposed studies1, J.A. ALEXANDER, O. GAFAROV, A.A. GAPUD, University of South Alabama, J.Z. WU, University of Kansas — Although much is known about free flux flow (FFF) in superconductors – in which pinning is insignificant compared to interactions between quantized vortices – there still remain questions concerning fundamental dynamics. Building on our previous work in correlating FFF with vortex core size (PRB 80, 134524), we propose three new studies examining more deeply the normal state in the vortex core and interactions between vortices. A correlation between scattering inside cores and the viscosity of FFF has not been explicitly determined; this may be investigated by probing the effect of scattering centers created by proton irradiation. Using results of previous irradiation work, one could control the extent of normal state scattering while monitoring effects on FFF. Questions also exist concerning vortex motion in channels with widths approaching that of individual vortices – as determined solely by inter-vortex interactions. Studies have suggested that flux flow through constrictions could imitate “jamming” in the collective motion of grains: Under certain conditions, it is possible for grains to form a barrier, blocking flow. More than just qualitatively comparing flux flow and granular flow to find evidence of jamming, we propose a new experiment for quantitatively modeling flux jamming by realizing the flux flow equivalent of granular jamming in a “hopper”. In the same way, we also propose a FFF equivalent of another granular-flow phenomenon, “non-Newtonian” fluids, where rapid shear causes jamming.

1 Funded by NSF-RUI grant, DMR-0907038.

3:06PM J35.00004 Vortex core size due to the quasiparticle interference effect in cuprate superconductors1, HONG-YI CHEN, National Taiwan Normal University — We investigate the vortex core properties by solving the Bogoliubov-de-Gennes equations for the t-t'-U-V Hamiltonian. The double peaks structure of the local density of states at the vortex core center characterizes the vortex core state. The local density of states maps have been numerically obtained near the slightly underdoping for the energy at the vortex core state. It is found that the field induced spin-density wave would cause the vortex core shrinking as the magnetic increases. We also found that the quasiparticle interference effect would affect the vortex core shrinking that the core size is independent the strength of the applied magnetic field.

1 NSC 101-2112-M-003-005-MY3

3:18PM J35.00005 Field-induced Dirac fermions and Fermi-surface resonance-scattering in the vortex-lattice cores of strongly type-II superconductors, TSOFAR MANIV, VLADIMIR ZHURAVLEV, Technion-Israel Institute of Technology, Haifa 32000, Israel — A remarkable relationship between the formation of Dirac fermions in the vortex lattice of a clean 2D strongly type-II superconductor at high magnetic fields and a peculiar magneto-quantum oscillations effect is revealed. It is shown that at the magnetic fields where the low-lying BdG quasi-particle dispersion has a Dirac cone structure, dHvA oscillations amplitude is sharply modified due to Fermi-surface resonance-scatterings occurring in core regions of the vortex lattice. A Dirac cone is created at each vortex core in the reciprocal vortex lattice at magnetic fields where the effective Zeeman spin-splitting vanishes and the chemical potential is in the middle of a Landau band (M.R.Norman and A.H.MacDonald, Phys.Rev. B54 4239 (1996); Z.Tesanovic and P.Sacramento, Phys.Rev.Lett.80 1521 (1998); T.Maniv, et al., Rev. Mod. Phys.73 867 (2001)). Under these resonance conditions coherent BdG quasi-particle scatterings are singularly enhanced leading to “erratic,” quasi-periodic modulation of the dHvA oscillation amplitude as a function of 1/B (V.Zhuravlev and T.Maniv, Phys.Rev. B85 104528 (2012)). For a spin-triplet superconductor in the presence of commensurate arrays of pinning centers, an “exotic” possibility of field-induced sub-lattices of bound Majorana fermions is discussed.

3:30PM J35.00006 Theory of de Haas van Alphen Oscillations in Superconductors with Pre-formed Pair. YAN HE, PETER SCHERPZEL, KATHRYN LEVIN, University of Chicago — We address recent observations of quantum oscillatory behavior in high temperature superconductors within a preformed pair theory of the pseudogap phase. These non condensed pairs, present in the normal and superconducting phases are shown to be reflective of a slightly distorted vortex lattice phase 1. Importantly they contribute a separate additive (“bosonic”) component to the field dependent thermodynamics in addition to that arising from fermions. In this talk we report our findings that the bosonic component appears to display the same Lifshitz-Kosevich oscillation frequencies as also found in the mixed state of conventional superconductors (associated with gapless fermionic states). We explore the different amplitude weighting factors for the bosonic and fermionic contributions and the effects of varying the pairing symmetry from s to d-wave. For the latter and for many properties, the bosonic component is most strongly associated with the anti-node, while the fermionic contribution comes from the node. Ref.1. Pseudogap Effects in Fermi Gases in the Presence of a Strong Effective Magnetic Field, P. Scherpelz, Dan Wulin, K. Levin and A. K. Rajagopal, ArXiv 1207.4826

3:42PM J35.00007 Quantum oscillations in d-wave superconductors with loop current order, LUYANG WANG, OSKAR VAFEK, National High Magnetic Field Laboratory and Department of Physics, Florida State University — Coexistence of d-wave superconductivity and Fermi pockets in undoped high temperature cuprate superconductors has been suggested by recent quantum oscillation experiments. The origin of Fermi pockets in the superconducting state has been under debate. Here we report numerical results of quantum oscillations of the specific heat in the vortex state of a d-wave superconductor in the presence of loop current order, which gives rise to Fermi pockets coexisting with nodal d-wave superconductivity. First, we calculate the specific heat within a lattice tight-binding model, varying the loop current order and the external magnetic field. Second, we investigate the same problem in the continuum linearized limit, performing Franz-Tesanovic transformation, and find that the Bogoliubov Dirac quasiparticles also couple to a vector-like potential which corresponds to a highly nonuniform magnetic field. The results thus found are consistent with the tight-binding calculation. While the energy spectrum is qualitatively different from Landau levels, we find oscillations of the specific heat that in an intermediate temperature range approximately follow Onsager relation.

3:54PM J35.00008 Oscillations of the Magnetoresistance and the Critical Current in MoGe Thin Films with Hole-arrays in Square Vortex-ice Geometry, MICHAEL LATIMER, GOLIBJON BERDIYOROV, RALU DIVAN, IL WOONG JUNG, **, ZHILI XIAO, ****, FRANCOIS PEETERS, ****, WAI-KWONG KWOK, * Matr. Sci. Div. Argonne National Lab.*, Center for Nanoscale Matr. Argonne National Lab**, Northern Illinois Univ.***, Universiteit Antwerpen**** — Resistivity measurements on MoGe thin films containing hole-arrays in square vortex-ice configuration were carried out to study the formation of a frustrated vortex state. MoGe thin films of 20 nm thick were prepared by sputter-deposition and holes with spacings of 200 nm - 400 nm and diameters from 100 nm to 300 nm were introduced into them using focused-ion-beam milling. We observed unusual matching effects: depending on the hole-hole spacing and the experimental temperature, the pinning enhancement at the half matching field can be stronger than that at the first matching field, as divulged by the deeper dip in the magnetoresistance and the higher peak in the critical current. Computer simulations within the nonlinear time-dependant Ginzburg-Landau theory reveal an origin of vortex jamming in the square vortex-ice state, indicating the first experimental realization of a square vortex-ice.

3 Work supported by the Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357. Nanofabrication done at the Center for Nanoscale Materials, Argonne National Laboratory.
4:06PM J35.00009 Thermal Hall effect in the underdoped cuprate superconductor YBa2Cu3O6.5+δ, PHUAN ONG, MAX HIRSCHBERGER, TIAN LIANG, Princeton University, TOSHIAO LOEW, Max Planck Institute Stuttgart, WEI LI LEE, Princeton University, R. RITZ, Technische Universität München, BERNHARD KEIMER, Max Planck Institute Stuttgart — The thermal Hall conductivity κ_{xy} (Righi-Leduc effect) is tailor-made to probe the transport properties of Bogolyubov quasiparticles (QPs) in a superconductor because neither the phonons nor vortices contribute to the off-diagonal response. We report measurements of κ_{xy} in unwinned crystals of underdoped YBa2Cu3O6.5+δ, extending from 100 K to 15 K in fields H up to 14 T. Several key features will be described. At all temperatures T, the QPs are hole-like. However, there is a small negative contribution that appears just below Tc. Below 30 K, the curve of κ_{xy} vs. H approaches an apparent universal step-like profile that may reflect the behavior of long-lived Dirac excitations confined to orbits around the gap nodes in an intense magnetic field. Measurements to much lower T and higher H (~32 T) are planned.

1Supported by NSF-MRSEC under Grant DMR 0819860

4:18PM J35.00010 Zero field Hall effect in chiral p-wave superconductors near the Kosterlitz-Thouless transition, CHUN KIT CHUNG, Department of Physics, the University of Tokyo, YUSUKE KATO, Department of Basic Science, the University of Tokyo — A theory of vortex dynamics developed by Ambegaokar, Halperin, Nelson, and Siggia is employed to study two-dimensional chiral p-wave superconducting systems. Due to unequal values of drag coefficients of opposite vorticity specific to chiral p-wave cases, we find that a “convective” term, in addition to diffusivity, should enter the dynamical equations governing vortex pair unbinding process. As a consequence, we find a matrix form dielectric function and a new contribution to Hall conductance σ_{xy} automatically follows even in zero magnetic field. We predict both the Hall conductance and power dissipation show a peak across the Kosterlitz-Thouless transition temperature. Their frequency dependence is also discussed. It is found that a set of frequency-dependent length scales, which controls the truncation of renormalization process, depends on both the convective and diffusive motion of vortices.

4:30PM J35.00011 Domain Wall and Rouse Domain Superconductivity in Superconducting/Ferromagnet Hybrid Structures1, S. MOORE, J. FEDOR, Physics Department, Temple University, Philadelphia, PA 19122, V. NOVOSAD, Materials Science Division, Argonne National Laboratory, Argonne, IL 60439, S. CIOLCY, G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA 19104, M. JAVARONE, Physics Department, Temple University, Philadelphia, PA 19122 — We have investigated the effect of inhomogeneous stray fields of a ferromagnet on the nucleation of the superconducting order parameter in superconductor/ferromagnet (S/F) systems magnetically coupled. Low-temperature scanning tunneling microscopy and spectroscopy measurements were performed on a Pb/[Co/Pd] system, which has a nontrivial H–T phase diagram under externally applied magnetic fields. Conductance maps and tunneling spectroscopy of these systems show clear indications of domain wall and reverse domain superconductivity. Close to the temperature (T_c) and in zero applied field, we visualized the emergence of superconductivity in regions above the separation between adjacent magnetic domains on length scales of the order of the coherence length. We also find an increase in T_c for certain values of applied field above magnetic domains of the opposite polarity.

3Supported by Polish NCS grant 2011/01/B/ST3/00462, by the French-Polish Program PICS 2012, by EU grant POIG.01.01.02-00-108/09, and by NSF grants DMR05-20491 and DMR-1053854.

4:42PM J35.00012 Vortex confinement by magnetic domains in superconductor-ferromagnet bilayers1, MARTA Z. CIEPLAK, Z. ADAMUS, Institute of Physics, Polish Acad. Sciences, Warsaw, Poland, M. KONCZYKOWSKI, Ecole Polytechnique, Palaiseau, France, L.Y. ZHU, C.L. CHIEN, Johns Hopkins University, X.M. CHENG, Bryn Mawr College — We use a line of miniature Hall sensors to study the effect of magnetic-domain-induced vortex confinement on the flux dynamics in a superconductor/ferromagnet bilayer. A single tunable bilayer is built of a ferromagnetic Co/Pt multilayer with perpendicular magnetic anisotropy and a superconducting Nb layer, with the insulating layer in between to avoid proximity effect. The magnetic domain patterns of various geometries are reversibly predefined in the Co/Pt multilayer using the appropriate magnetization procedure. The magnetic domain geometry strongly affects vortex dynamics, leading to geometry-dependent trapping of vortices at the sample edge, nonuniform flux penetration, and strongly nonuniform critical current density. With the decreasing temperature the magnetic pinning increases but this increase is substantially weaker than that of the intrinsic pinning. The analysis of the initial flux penetration suggests that vortices may form various vortex structures, including disordered Abrikosov lattice or single and double vortex chains, in which minimal vortex-vortex distance is comparable to the magnetic penetration depth.

3Supported by Polish NCS grant 2011/01/B/ST3/00462, by the French-Polish Program PICS 2012, by EU grant POIG.01.01.02-00-108/09, and by NSF grants DMR05-20491 and DMR-1053854.

4:54PM J35.00013 Magnetic decoration imaging of a superconductor-ferromagnet bilayer, MAXIM MARCHEVSKY, Lawrence Berkeley National Laboratory — Magnetic decoration imaging technique is used to study flux distribution and local vortex order in a superconducting Nb film deposited on a ferromagnetic yttrium-iron garnet substrate. Ambient field-cooled decoration patterns reveal concentration of vortices in the Nb along the labyrinthine magnetic domains of the garnet. Re-magnetization cycles result in a formation of the complex “vortex foam” structure due to a coupled magnetic dynamics of the superconductor-ferromagnet (S/F) bilayer system. We analyze density variations and spatial distribution of vortices in these structures. Flux exit patterns obtained upon removal of an external magnetic field show large-scale inhomogeneity of the vortex flow. Results are compared to the recent theoretical predictions and reported studies of S/F systems by other imaging methods.

5:06PM J35.00014 Vortex coalescence and type-1.5 superconductivity in Sr2RuO4, EGOR BABAEV, University of Massachusetts Amherst and KTH Stockholm, JULIEN GARAUD, University of Massachusetts Amherst, DANIEL AGTERBERG, University of Wisconsin-Milwaukee — Recently vortex coalescence was reported in superconducting Sr2RuO4 by several experimental groups for fields applied along the c-axis. We argue that Sr2RuO4 is a type-1.5 superconductor with long-range attractive, short-range repulsive intervortex interaction. The type-1.5 behavior stems from an interplay of the two orbital degrees of freedom describing this chiral superconductor together with the multiband nature of the superconductivity. These multiple degrees of freedom give rise to multiple coherence lengths, some of which are larger and some smaller than the magnetic field penetration length, resulting in nonmonotonic intervortex forces. The talk is based on Phys. Rev. B 86, 060513(R) (2012)

1supported by Knut and Alice Wallenberg Foundation, Swedish Research Council, NSF Awards No. DMR-0955902 and DMR-0906655 and by (SNIC) Supercomputer Center at Linköping
5:18PM J35.00015 Heirarchical mesophases of vortex matter in layered and multi-component superconductors\textsuperscript{1}, CHRISTOPHER VARNEY, University of Massachusetts, Amherst, KARL SELLIN, Royal Institute of Technology, QINGZE WANG, University of Massachusetts, Amherst / Penn State University, HANS FANGOH, University of Southampton, EGOR BABAEEV, University of Massachusetts, Amherst — Based on several models for Type-1.5 and hybrid Type-1/Type-2 layered superconductors, we examine the zero temperature properties of vortices with Langevin dynamics and Monte Carlo simulations. We demonstrate that inter-vortex forces with multiple length scales can result in unusual mesophases of vortex structures, such as clusters of clusters, concentric rings, clusters in a ring, and stripes in a cluster.

\textsuperscript{1}The authors acknowledge support from NSF Award No. DMR-0955902 and the Supercomputer Center at Linkoping (SNIC).

Tuesday, March 19, 2013 2:30PM - 5:30PM –

Session J36 DCMP: Superconductivity: Properties and Phenomena 344 - Zhigang Wu, Colorado School of Mines

2:30PM J36.00001 Copper Substitution in Iron Telluride: A Phase Diagram , PATRICK VALDIVIA, THOMAS FORRETT, UC Berkeley, COSTEL ROTUNDU, JINSHENG WEN, EDITH BOURRET-COURCHESNE, Lawrence Berkeley Lab, ROBERT BIRGENEAU, UC Berkeley, BIRGENEAU GROUP TEAM — Investigations of superconductivity in the FeCh family (Ch=S,Se,Te) have produced rich physics and notable materials challenges despite the ostensible simplicity of the system. We have studied the effects of copper substitution in iron-telluride. Our interests in this system are two-fold: to compare the properties of copper substitution in iron-telluride with those in the selenium-substituted compounds, and to study if there are additional controllable factors in this system such as the total excess metal content, and the distribution of iron and copper atoms over the two sites. Our initial investigations into this phase diagram involve both diffraction and transport measurements which may be used address these research goals.

2:42PM J36.00002 Kerr effect as evidence of gyrotropic order in the cuprates\textsuperscript{1}, SRINIVAS RAGHU, PAVAN HOSUR, STEVEN KIVELSON, AHARON KAPITULNIK, Stanford University, JOSEPH ORENSTEIN, University of California, Berkeley — The Kerr effect can arise in a time-reversal invariant dissipative medium that is “gyrotropic”, i.e. one that breaks spatial inversion and all mirror symmetries. Examples of such systems include electron analogs of cholesteric liquid crystals, and their descendants, such as systems with chiral charge ordering. We present arguments that the striking Kerr onset, which is not invertible by application of a magnetic field, in the pseudogap phase of a large number of cuprate high temperature superconductors is evidence of chiral charge ordering. We discuss additional experimental consequences of a phase transition to a gyrotropic system.

\textsuperscript{1}DOE Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract DE-AC02-76SF00515

2:54PM J36.00003 Anomalous Hall effect in current-carrying states of matter: topology, commensuration effects, and application to Kerr measurements in the underdoped cuprates\textsuperscript{1}, CATHERINE KALLIN, EDWARD TAYLOR, McMaster University — We calculate the anomalous Hall conductivity for states characterized by patterns of spontaneous currents. Using an exact Ward identity, we find that the DC Hall conductivity is topological provided the current pattern is commensurate and the Fermi surface is fully gapped. For incommensurate patterns, the DC Hall conductivity can be infinite, analogous to the infinite conductivity of a sliding charge density wave. We also discuss the optical Hall conductivity at high frequencies, in connection with Kerr rotation experiments performed on the underdoped cuprates.

\textsuperscript{1}Supported by NSERC, CIFAR, and CRC.

3:06PM J36.00004 ABSTRACT HAS BEEN MOVED TO B29.00015 —

3:18PM J36.00005 Thermodynamic studies of Cu\textsubscript{0.10}TiSe\textsubscript{2} via ac-calorimetry and Hall-probe magnetometry\textsuperscript{1}, ZUZANA PRIBULOVÁ, JOZEF KACMARCIK, PETER SAMUELY, Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Kosice, Slovakia, ZUZANA MEDVECKÁ, VIKTORIA SOLTESZOVÁ, Faculty of Natural Sciences, University of P.J. Safarik, Park Angelinum 9, 040 01 Kosice, Slovakia, PETRA BARANCEKOVA HUSANIKOVA, VLADIMIR CAMBEL, Institute of Electrical Engineering, Slovak Academy of Sciences, Dubravska cesta 9, 84104 Bratislava, Slovakia, GORAN KARAPETROV, Department of Physics, Drexel University, 3141 Chestnut St., Philadelphia, PA 19104, USA — TiSe\textsubscript{2} is a compound with the charge density wave (CDW) transition at 200 K, the CDW state is gradually suppressed when intercalated with copper and for certain amount of Cu superconductivity occurs. We report the studies of the critical fields of an optimally doped sample with a superconducting transition at \( T_c \approx 3.9 \) K. Upper critical field \( H_{c2} \) has been derived from the specific heat measurements while the lower critical field \( H_{c1} \) has been extracted from local magnetization measurements using miniature Hall-probes. The temperature dependence of \( H_{c2} \) and \( H_{c1} \) and its anisotropy will be presented. Moreover, local magnetometry using array of 8 Hall-probes shows that vortices after penetration into the sample move towards the centre resulting into a dome-shape induction profile suggesting relatively low pinning.

\textsuperscript{1}This work was supported by the ERDF EU (European Union European regional development fond) grant, under the contract No. ITMS260220120047.

3:30PM J36.00006 Study of Inhomogeneous Organic Superconductors, CHARLES C. AGOSTA, CHRISTOPHER CONROY, DANIEL ELOWITZ, WILLIAM VON NOPPEN, Clark University — In many anisotropic superconductors, we have found evidence that they are inhomogeneous superconductors, such as those predicted by Fulde and Ferrell and Larkin and Ovchinnikov (FFLO), at the extremes of low temperature and high magnetic field. A FFLO superconductor has an order parameter with nonzero pair momentum that oscillates periodically as a function of distance, unlike traditional superconductors where the order parameter is uniform. During the last several years, our research group at Clark University has made careful and systematic measurements of quasi-2D organic superconductors that suggest an FFLO state can be stabilized in three different organic conductors if a magnetic field is applied precisely parallel to the conducting layers. We will compare our results with theoretical expressions that we have modified from the current literature, with the goal of extracting quantitative results from the phase diagram data such as the Maki parameter and scattering times. We will also describe improvements to our pulsed magnetic field - tunnel diode oscillator penetration depth apparatus.
3:42PM J36.00007 Superconductivity in the misfit compound of (LaSe)$_{1.14}$(NbSe$_2$): STM/S, calorimetric and magnetization studies$^1$ P. SAMUELY, P. SZABO, J. KACMARCIK, Z. PIRIBULOVA, Slovak Academy of Sciences, T. SAMUELY, Safarik University, J.G. RODRIGO, Universidad Autonoma de Madrid, C. MARCENAT, CEA/GrenobleINAC/SPSMS/LATENS, T. KLEIN, Institut Neel, CNRS, L. CARIO, Institut des Matériaux Jean Rouxel — (LaSe)$_{1.14}$(NbSe$_2$) is a low temperature superconductor with $T_c$ around 1.2 K belonging to the family of the lamellar chalcogenides. Electron transfer from the LaSe to the NbSe$_2$ slab results in a natural layered system of the insulating LaSe and (super) conducting NbSe$_2$ sheets. In our previous investigations of the anisotropic transport [P. Szabó et al., Phys. Rev. Lett. 86, 5990 (2001)] indications have been found that this system behaves as a stack of Josephson-coupled superconducting NbSe$_2$ sheets separated by insulating LaSe layers. We test this hypothesis by STM/S measurements at subkelvin temperatures and in magnetic fields. Superconducting energy gap obtained by STM opens at the same temperature and field where the interlayer resistivity starts to increase before drop to zero value. Before any conclusions are made homogeneity of the superconducting parameters is to be tested. STM indicates large areas without any gap but calorimetric measurements have shown the bulk superconductivity and magnetization revealed extremely low pinning. $^1$CFNT MIVEP - Centre of Excellence of Slovak Academy of Sciences, FP7 MNT - ERA.Net II. ESO, EU ERDF grant No. ITMS26220120005, Slovak R&D Agency contract No. APVV-0036-11, VEGA 2/0148/10. Liquid nitrogen has been sponsored by U.S. Steel Kosice, Slovakia

3:54PM J36.00008 Microwave stimulated enhancement of the upper critical field in type-II superconducting films, ANTONIO LARA, AHMAD AWAD, Universidad Autonoma de Madrid, ALEJANDRO SILHANEK, Université de Liege, VICTOR MOSCHALKOV, Katholieke Universiteit Leuven, FARKHAD ALIEV, Universidad Autonoma de Madrid — A few decades ago it was theoretically predicted and experimentally observed that moderate power electromagnetic fields in the GHz range could stimulate superconductivity, increasing the superconducting critical temperature and critical current. Here, on the example of Pb films without / with periodic vortex pinning centers in the form of circular Permalloy dots we investigate experimentally a microwave photovoltaic effect in which the film turns superconducting. A qualitative explanation for the observed difference in the dependence of the upper critical field of the film of up to 0.1% and of the superconducting critical temperature and critical current of up to 10% have been observed at a drive frequency of 6 GHz. A qualitative explanation for the observed difference in the dependence of the upper critical field on the temperature and microwave power, depending on the nearly parallel or perpendicular alignments of the field to the sample, is provided.

4:06PM J36.00009 New Evidences for the observation of the Higgs boson in the Superconductor 2H-NbSe$_2$, MARIE-AUDE MEASSON, BERTRAND CLAIR, YANN GALLAIS, MAXIMILIEN CAZAYOUS, Laboratory Quantum Matter and Penonema- University Paris Diderot-CNRS, PIERRE RODIERE, Institute Neel, CNRS-UJF, LAURENT CARIO, Institut des Materiaux Jean Rouxel (IMN), Universite de Nantes - CNRS, ALAIN SACUTO, Laboratory Quantum Matter and Penonema- University Paris Diderot-CNRS, SQUAP TEAM, SYSTEMES A FORTES CORRÉLATIONS ELECTRONIQUES COLLABORATION, IMN COLLABORATION — We provide here new evidences for the observation of the amplitude mode of the magnetic vortex state, we investigate experimentally the microwave photovoltaic effect in 2H-NbSe$_2$. We report quantitatively comparative electronic Raman measurements on the dichalcogenides 2H-NbSe$_2$, whose superconductivity (SC) coexists with a charge density wave order (CDW), and 2H-NbS$_2$, which exhibits only the SC. A SC pair breaking peak develops below $T_c$ in 2H-NbS$_2$ whose intensity is much smaller than the peak associated with the SC in 2H-NbSe$_2$. Thus, the peak observed in 2H-NbSe$_2$ below $T_c$ certainly doesn't get its intensity only from the superconducting condensate. Moreover, we measure precisely a spectral weight transfer from the amplitude mode of the CDW to the SC peak in 2H-NbSe$_2$, versus decreasing temperature. The total spectral weight for both peaks is constant within ± 3%. This result is consistent with the theory of the observation of a Higgs mode thanks to its coupling with an amplitude developed by Littlewood and Varma. This result complements what was firstly observed by Sooryakumar et Klein under magnetic field.


4:30PM J36.00011 X-ray edge singularity in resonant inelastic x-ray scattering (RIXS), ROBERT MARKIEWICZ, Northeastern University, JOHN REHR, University of Washington, ARUN BANSIL, Northeastern University — We develop a lattice model based on the theory of Mahan, Nozières, and de Dominicis for x-ray absorption to explore the effect of the core hole on the RIXS cross section. The dominant part of the spectrum can be described in terms of the dynamic structure function $S(q, \omega)$ dressed by matrix element effects, but there is also a weak background associated with multi-electron-hole pair excitations. The model reproduces the decomposition of the RIXS spectrum into well- and poorly-screened components. An edge singularity arises at the threshold of both components. Fairly large lattice sizes are required to describe the continuum limit.

4:42PM J36.00012 Using photon to probe spin excitations, CHUNJING JIA, Stanford Institute for Materials and EEnergy Sciences, CHENG-CHIEN CHEN CHEN, Argonne National Lab, BRIAN MORITZ, TOM DEVREUXA, Stanford Institute for Materials and EEnergy Sciences — Elementary spin excitations have attracted considerable attention in the understanding of strongly correlated materials, especially in high temperature superconductors where a full understanding of spin dynamics might reveal important information where the phase emerges in proximity of magnetic order. Photo spectroscopies, such as resonant inelastic x-ray scattering (RIXS) and optical Raman scattering, are powerful tools for the measurement of spin excitations. In this presentation, I will discuss the simulation of various spectroscopies that can reveal spin excitations, using both single- and multi-orbital models. I will show that transition metal in-direct RIXS provides information about two-magnon excitations at low energies in addition to the usual charge transfer excitations; while direct RIXS measures single spin-flip (single magnon) excitations, making it a complementary technique to inelastic neutron scattering. I also will show that Raman scattering can probe two-magnon spin excitations in correlated materials. We track the evolution of these excitations as functions of momentum and doping. These results highlight the nature of spin excitations in correlated materials and are an important step in our understanding of the corresponding experiments in real materials.
4:54PM J36.00013 Investigation of 1/f flux noise in SQUIDs and Superconducting Qubits .
ANTONIO PUGLIELLI, STEVEN SENGELBACH, TAYLOR KLAUS, ROBERT MCDERMOTT, University of Wisconsin-Madison, Department of Physics —
Low-frequency 1/f flux noise is a dominant source of dephasing in the Josephson phase and flux qubits. Recent work has revealed the presence of a high density of unpaired spins at the surfaces of superconducting thin films; it is now believed that these spins are the source of the noise, although the microscopic noise mechanism is not understood. We have recently shown that the dielectric encapsulation of the SQUID loop substantially impacts the noise magnitude and noise exponent. Here we describe experiments on SQUIDs and Josephson phase qubits designed to shed light on the underlying noise mechanism, and we describe efforts to develop Josephson phase qubits with reduced levels of 1/f flux noise and improved dephasing times.

5:06PM J36.00014 Torque magnetization study of superconducting fluctuations in single-layer cuprates: new implications for the phase diagram1 , GUICHUAN YU, R. FRINK, University of Minnesota, D.-D. XIA, X. ZHAO, Jilin University, China, N. BARISIC, CEA-DSM-IRAMIS, France, R.-H. HE, Boston College, N. KANEKO, AIST, Japan, T. SASAGAWA, Tokyo Institute of Technology, Japan, Y. LI, Peking University, China, A. SHEKHTER, Los Alamos National Laboratory, M. GREVEN, University of Minnesota — We have studied the superconducting fluctuations above the transition temperature by angle-dependent torque magnetization in single-layer La2−xSrxCuO4 (LSCO), Bi2(Sr,La)2CuO6+δ (Bi2201), and HgBa2CuO4+δ (Hg1201). The latter is a more ideal compound, with a maximum Tc of 97 K, more than twice the values for LSCO and Bi2201. In all three cases, the diamagnetic signal above Tc vanishes in an unusual exponential fashion, and at a rate that is universal, despite the dramatic differences in Tc [G. Yu et al., arXiv:1210.6942v1]. These observations suggest that anomalies observed at much higher temperatures in both LSCO and Bi2201 are not associated with superconducting fluctuations.

5:18PM J36.00015 Effect of thermal fluctuations in topological p-wave superconductors, BELA BAUER, ROMAN M. LUTCHYN, Station Q, Microsoft Research, MATTHEW B. HASTINGS, Duke University, Department of Physics, MATTHIAS TROYER, Theoretische Physik, ETH Zurich — We study the effect of thermal fluctuations on the topological stability of chiral p-wave superconductors. We consider two models of superconductors: spinless and spinful with a focus on topological properties and Majorana zero-energy modes. We show that proliferation of vortex-antivortex pairs above the Kosterlitz-Thouless temperature $T_{KT}$ drives the transition from a thermal Quantum Hall insulator to a thermal metal/insulator, and dramatically modifies the ground-state degeneracy splitting. Therefore, in order to utilize 2D chiral p-wave superconductors for topological quantum computing, the temperature should be much smaller than $T_{KT}$. Within the spinful chiral p-wave model, we also investigate the interplay between half-quantum vortices carrying Majorana zero-energy modes and full-quantum vortices having trivial topological charge, and discuss topological properties of half-quantum vortices in the background of proliferating full-quantum vortices.

Tuesday, March 19, 2013 7:00PM - 8:00PM —
Session K43 DCMP: DCMP Business Meeting Hilton Baltimore Holiday Ballroom 2 -

7:00PM K43.00001 DCMP BUSINESS MEETING —

Wednesday, March 20, 2013 8:00AM - 11:00AM —
Session M1 DCMP: Invited Session: Tunable, Intense, Coherent THz Emission From a High Temperature Superconductor Ballroom I - Ulrich Welp, Argonne National Laboratory

8:00AM M1.00001 Hot Spot and THz Wave Generation in Bi2Sr2CaCu2O8 Intrinsic Josephson Junction Stacks , REINHOLD KLEINER, University of Tuebingen — Stacks of intrinsic Josephson junctions made of the high temperature superconductor Bi2Sr2CaCu2O8 have been shown to emit coherent radiation at THz frequencies [1]. Emission is observed both in a low bias regime and a high bias regime. While at low bias the temperature of the stack is close to the bath temperature, at high bias a hot spot and a standing wave, formed in the “cold” part of the stack, coexist [2-5]. THz radiation is very stable in this regime, exhibiting a linewidth which is much smaller than expected from a purely cavity-induced synchronization mechanism [6]. We investigate the interaction of hot spots and THz waves using a combination of transport measurement, direct electromagnetic wave detection and low temperature scanning laser microscopy (LTSLM). In this talk recent developments will be presented, with a focus on the mechanism of hot spot formation.


Josephson junction stacks made of high temperature superconductor Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ have been obtained both in a low bias and a high bias regime [1, 2]. While at low bias the temperature distribution in the stack is almost homogeneous, at high bias an over-heated part (hot spot area) and a cold part of the sample coexist [2, 3]. Previous resolution-limited measurements indicated that the linewidth $\Delta f$ of THz emission may be below 1 GHz, showing no difference between two regimes. In this talk, we report on measurements of the linewidth of THz radiation using a Nb/AIN/NbN integrated receiver for detection [4]. While at low bias we found $\Delta f$ to be not smaller than $\sim$500 MHz, at high bias $\Delta f$ turned out to be as narrow as a few MHz. We attribute this to the hot spot acting as a synchronizing element. Also thanks to the variable size of the hot spot and the temperature rise due to the self-heating, the emission frequency can be tuned over a wide range of up to 500 GHz. Last but not least, the emission power was measured to be above 25 $\mu$W. All these properties imply that THz sources made of layered cuprate superconductors can be employed for practical applications.


9:12AM M1.00003 THz Radiation from Mesas of Intrinsic Josephson Junction of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ under Extreme Thermal Inhomogeneity

9:48AM M1.00004 Modelling the coherent THz radiation from Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ mesas of various geometries


10:24AM M1.00005 Intrinsic line shape of electromagnetic radiation from a stack of intrinsic Josephson junctions synchronized by an internal cavity resonance

Work supported by UCAMN Argonne, LLC, under contract No. DE-AC02-06CH11357.

In collaboration with Shi-Zeng Lin (LANL).
8:00AM M2.00001 Unconventional Sequence of Fractional Quantum Hall States in Graphene

BENJAMIN FELDMAN, Harvard University, Department of Physics — Electronic compressibility is a powerful tool for the study of correlated electron phases in two-dimensional electron systems. Using a scanning single-electron transistor, we have measured the local electronic compressibility of suspended graphene in the quantum Hall regime. The local nature of the measurement technique allows us to probe exceptionally clean regions of graphene, revealing delicate many-body effects that are obscured by disorder in global transport studies. In this talk, I will review recent measurements of the fractional quantum Hall effect (FQHE) in graphene. We observe a multitude of FQH states that follow the standard composite fermion sequence between \( \nu = 0 \) and 1, but only occur at even-numerator fractions between \( \nu = 1 \) and 2, suggesting that an underlying symmetry remains. Moreover, we observe a series of phase transitions in the FQH states between \( \nu = 0 \) and 1 that are marked by a decreased energy gap and a narrow region of negative compressibility that cuts across the FQH state. We use a simple model based on crossing composite fermion Landau levels with different internal degrees of freedom to reproduce much of the experimental behavior. Our results provide insight into the interplay between electron-electron interactions and the spin and valley symmetries of graphene.

8:36AM M2.00002 Phase diagram and edge excitations of the \( \nu = 0 \) quantum Hall state in graphene\(^1\).

MAXIM KHARITONOV, Center for Materials Theory, Rutgers University — The interaction-induced broken-symmetry incompressible quantum Hall states in graphene at integer and fractional filling factors have by now been firmly established in transport and compressibility measurements. However, identifying their precise nature (e.g., how the symmetry is broken) still remains a tough challenge: on the experimental side, transport and compressibility probes do not provide direct information about the physical order; on the theoretical side, the presence of additional degrees of freedom to spin, valley and higher internal degrees of freedom in graphene has confounded attempts to formulate a consistent quantum many-body framework for the FQH states in a variety of competing phases in this multicomponent system. As the prime example of this rich behavior, I will present a generic phase diagram for the intriguing \( \nu = 0 \) state, obtained within the framework of quantum Hall “ferromagnetism.” The diagram consists of the canted antiferromagnetic, ferromagnetic, charge-density-wave (charge-layer-polarized), and Kekulé (interlayer-coherent) phases in monolayer (bilayer). I will then discuss the edge excitations of the \( \nu = 0 \) state. Remarkably, the edge excitations are nonuniversal (e.g., can be gapped or gapless) and crucially depend on which phase is realized in the bulk of the system. Besides being of considerable theoretical interest, these unprecedented properties simultaneously allow one to infer about the nature of the phases from the transport experiments. I will present arguments based on this analysis and existing data why the insulating \( \nu = 0 \) state realized in real bilayer (and possibly, monolayer) graphene is likely to be canted antiferromagnetic. Finally, I will mention how this theoretical framework can be generalized to fractional quantum Hall states in graphene, which could shed light on some of the puzzling features of the recent experiments.

\(^1\)This research was supported by the U.S. DOE under contracts No. DE-FG02-99ER45790 and No. DE- AC02-06CH11357.

9:12AM M2.00003 Spin and Valley Quantum Hall Ferromagnetism and Quantum Phase Transitions in Graphene

CORY DEAN, Columbia University — No abstract available.

9:48AM M2.00004 Tunable electron interactions and robust non-Abelian quantum Hall states in graphene and other Dirac materials\(^1\).

DIMITRY ABANIN, Perimeter Institute for Theoretical Physics — Discovery of the fractional quantum Hall effect inspired a concept of quasiparticles with non-Abelian exchange statistics. However, a major limitation for experimental studies of non-Abelian quasiparticles in traditional GaAs-based 2d systems is their lack of tunability: the effective electron interactions in such systems are fixed at values which make non-Abelian states either absent or a very fragile. Therefore it is desirable to find alternative, tunable 2d systems that host robust non-Abelian quantum Hall states. In this talk, we will discuss the phase diagram of fractional quantum Hall states in recently discovered 2d Dirac materials (graphene, bilayer graphene, topological insulators). We will show that the effective interactions in these materials can be naturally tuned in a broad range, in contrast to GaAs. This tunability is achieved by external fields that control the mass gap of Dirac fermions. Alternatively, the effective interactions can be controlled by engineering the dielectric environment of the 2d Dirac electron gas. We will demonstrate that the tunability of interactions in Dirac materials allows one to stabilize non-Abelian states, as well as to drive phase transitions between various correlated phases (quantum Hall states, Fermi-liquid-like states, and states with broken translational symmetry) in a controlled manner. Connecting to experiments, we will argue that a very promising candidate material for tuning interactions and stabilizing non-Abelian states is bilayer graphene, where the gap can be naturally controlled by perpendicular electric field. Our study provides a realistic route towards engineering robust fractional and non-Abelian quantum Hall states in graphene and other Dirac materials.

\(^1\)This work was supported by DOE Grant DE-SC0002140. Discovery of the fractional quantum Hall effect inspired a concept of quasiparticles with non-Abelian exchange statistics. However, a major limitation for experimental studies of non-Abelian quasiparticles

10:24AM M2.00005 Superconducting states in graphene

BRUNO UCHOA, University of Oklahoma — In spite of the remarkable electronic properties of graphene, which include the existence of massless Dirac quasiparticles, the low density of states near the Dirac points seems to conspire against the formation of new many body ground states. In this context, the search for intrinsic superconductivity in graphene has involved either combining graphene with other materials \(^1\), or else exploring ways to modify the electronic density of states at the Fermi level. In this talk, after discussing the classification of symmetry states in the honeycomb lattice and analysing the general thermodynamic properties for Dirac fermion superconductors \(^2\), I will describe a few promising mechanisms to induce superconductivity in graphene. In particular, I will show that in the situation where strain effects lead to a reconstruction of the vacuum into a discrete spectrum of Landau levels due to pseudo magnetic fields, which preserve overall time reversal symmetry, superconductivity is quantum critical at integer filling of the Landau levels, when the system is incompressible. At partial filling, the quenching of the kinetic energy due to the Landau levels leads to a crossover to a non-Fermi liquid regime, where the critical temperature scales linearly with the coupling in the weak coupling limit. I will show that the critical temperature can be orders of magnitude larger than in conventional weak coupling superconductors, and may be triggered by phonons.

\(^1\)B. Uchoa, A. H. Castro Neto, Physical Review Letters 98, 146801 (2007);

Wednesday, March 20, 2013 8:00AM - 11:00AM –
Session M3 DCMP: Invited Session: Novel Quantum Phases in Artificial Lattices and Networks
Ballroom III - Steven Louie, University of California, Berkeley
8:00AM M3.00001 Mott-Hubbard Physics in a Patterned GaAs Heterostructure with Honeycomb Topology

- VITTORIO PELLEGRINI, NEST CNR-NANO and Scuola Normale Superiore, Pisa (Italy) — This talk considers efforts directed towards the design and exploration of novel collective electron states in artificial lattice structures that are realized in semiconductor heterostructures by nanofabrication methods. These studies reveal striking interplays between electron interactions and geometrical constraints (topology). We focus on the honeycomb topology, or “artificial graphene” (AG) [1,2], that supports Dirac fermions. Dirac fermions and the emergence of quantum phases, such as spin liquids and topologically protected states, can be studied by high-demanding inelastic light scattering methods and by electrical transport at low temperatures [3,4]. In particular, we probed the excited spectrum of electrons in the honeycomb lattice in a magnetic field identifying collective modes that emerged from the Coulomb interaction [4], as predicted by the Mott-Hubbard model [5]. These observations allow us to determine the Hubbard gap and suggest the existence of a Coulomb-driven ground state [4]. Studies of electrons confined to artificial lattices should provide key perspectives on strong electron correlation in condensed matter science.

1Work done in collaboration with A. Singh, M. Giberntini, M. Polini, B. Karmakar, M. Katsnelson, S. Yuan, A. Pinczuk, G. Vignale, L.N. Pfeiffer, K.W. West


8:36AM M3.00002 Dirac Fermions in a Nanopatterned Two-Dimensional Electron Gas

- CHEOL-Hwan Park, Department of Physics and Astronomy and Center for Theoretical Physics, Seoul National University — If a lateral periodic potential with triangular (or honeycomb) lattice symmetry is applied to a conventional two-dimensional electron gas (2DEG), the charge carriers behave like massless Dirac fermions [1,2]. A very interesting and useful point of these newly-generated massless mass Dirac fermions is that, unlike the case of graphene, their properties can be tuned through the external periodic potential. In this presentation, I will review the electronic properties of those newly-generated massless Dirac fermions in an artificial 2DEG superlattice system and will discuss how the electronic structure of those massless Dirac fermions changes depending on the external periodic potential [3].

1This work was partly supported by Research Settlement Fund for the new faculty of SNU.

9:12AM M3.00003 Designer Dirac Fermions, Topological Phases, and Gauge Fields in Molecular Graphene

- HARI C. MANOHARAN, Department of Physics, Stanford University / Stanford Institute for Materials and Energy Sciences — The observation of massless Dirac fermions in monolayer graphene has propelled a new area of science and technology seeking to harness charge carriers that behave relativistically within solid-state materials. Using low-temperature scanning tunneling microscopy and spectroscopy, we show the emergence of Dirac fermions in a fully tunable condensed-matter system—molecular graphene—assembled via atomic manipulation of a conventional two-dimensional electron system in a surface state. We embed, image, and tune the symmetries underlying the two-dimensional Dirac equation into these electrons by sculpting the surface potential with manipulated molecules. By distorting the effective electron hopping parameters into a Kekulé pattern, we find that these natively massless Dirac particles can be endowed with a tunable mass engendered by the associated scalar gauge field, in analogy to the Higgs field. With altered symmetry and texturing of the assembled lattices, the Dirac fermions can be dressed with gauge electric or magnetic fields such that the carriers believe they are in real fields and condense into the corresponding ground state, as confirmed by tunneling spectroscopy. Using these techniques we ultimately fabricate a quantum Hall state without breaking time-reversal symmetry, in which electrons quantize in a gauge magnetic field ramped to 60 Tesla with zero applied laboratory field. We show that these and other chiral states now possible to realize have direct analogues in topological insulators, and can be used to guide or confine charge in nontrivial ways [1].


9:48AM M3.00004 Electron-electron interactions in artificial graphene

- ESA RASANEN, Department of Physics, Tampere University of Technology — Recent advances in the creation and modulation of graphene-like systems are introducing a science of “designer Dirac materials.” In its original definition, artificial graphene is a man-made nanostructure that consists of identical potential wells (quantum dots) arranged in an adjustable honeycomb lattice in the two-dimensional electron gas. As our ability to control the quality of artificial graphene samples improves, so grows the need for an accurate theory of its electronic properties, including the effects of electron-electron interactions. Here we determine those effects on the band structure and on the emergence of Dirac points, and discuss future investigations and challenges in this field.

10:24AM M3.00005 Quantum Simulation with Circuit QED

- ANDREW HOUCK, Princeton University — Superconducting circuits and circuit quantum electrodynamics provide an excellent toolbox for non-equilibrium quantum simulation. In circuit QED, the strong interaction of light with two-qubit units can lead to strong quantum-mechanical photon-photon interactions. Recent theoretical proposals have predicted phase transitions in arrays of these cavities, demonstrating that complex matter-like phenomena can emerge with such interacting photons. Due to inevitable photon dissipation and the ease of adding photons through driving, these systems are fundamentally open and a useful tool for studying non-equilibrium physics. I will discuss recent experimental and theoretical progress towards realization of these non-equilibrium quantum simulators. I will focus on a localization-delocalization crossover in a pair of coupled cavities, and discuss preliminary measurements of large cavity arrays. I will discuss a variety of available measurements in these systems, including transport, photon number statistics, and a scanned local quantum probe.

Wednesday, March 20, 2013 8:00AM - 11:00AM

Session M6 DCMP: Graphene: Multilayer and Tunneling

302 - Chun Ning (Jeanie) Lau, University of California, Riverside

8:00AM M6.00001 Quantum Hall Effect in single-, bi- and tri-layer graphene

- ZENG ZHAO, KEVIN MYHRO, DAVID TRAN, HANG ZHANG, JHAO-WUN HUANG, JAIRO VELASCO, YANMENG SHI, FENGLIN WANG, YONGJIN LEE, CHUN NING LAU, University of California, Riverside — Quantum Hall Effect has been extensively studied in single layer, bilayer and trilayer graphene. Our recent studies showed intrinsic gapped state at the charge neutrality point in bilayer and trilayer graphene. Here we describe the fabrication of high-quality single-bilayer and bi-trilayer hybrid graphene devices, and present results from magneto-transport measurements.
Molecules that break the AB symmetry of graphene can produce a band gap in single-layer graphene. Recently atomically flat layers of carbon known as graphene have become the rising star in spintronics as their electrons carry not only the ordinary spin degree of freedom, but they also have a pseudospin degree of freedom tied to the electrons’ orbital motion which could enable new routes for spintronics. Here we focus on bilayer graphene (BLG). Using group theory we have established a complete description of how electrons in BLG interact with electric and magnetic fields. We show that electrons in BLG experience an unusual type of matter-field interactions where magnetic and electric fields are virtually equivalent: every coupling of an electron’s degrees of freedom to a magnetic field is matched by an analogous coupling of the same degrees of freedom to an electric field. This counter-intuitive duality of matter-field interactions allows novel ways to create and manipulate spin and pseudo-spin polarizations via external fields that are not available in other materials. See arXiv:1206.4761.

This work was supported by Marsden Fund contract no. VUW0719, administered by the Royal Society of New Zealand. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357.

8:48AM M6.00005 Coexisting massive and massless Dirac fermions in quasi-freestanding bilayer graphene

KEUN SU KIM, ANDREW L. WALTER, LUCA MORESCCHINI, Lawrence Berkeley National Laboratory, THOMAS SEYLLER, University of Erlangen-Nürnberg, KARSTEN HORN, Fritz-Haber-Institut der Max-Planck-Gesellschaft, ELI ROTENBERG, AARON BOSTWICK, Lawrence Berkeley National Laboratory — The most widely accepted theoretical model to describe charge carriers in bilayer graphene is “massive Dirac fermions”, characterized by a nearly parabolic band pair touching each other at the Dirac energy. This electronic structure of bilayer graphene is widely believed to be unstable towards symmetry breaking either by structural distortions, such as twist and strain, or electronic interactions. In this work, we investigate quasi-freestanding bilayer graphene by angle-resolved photoemission spectroscopy, which shows an unexpected electronic spectrum, consisting of both massive and massless Dirac fermions. The latter has a unique band topology with a chiral pseudospin texture, and its origin will be discussed in terms of symmetry breaking induced by a native imperfection of bilayer graphene.

9:00AM M6.00006 Quasiparticle Energy and Excitonic Effects of Gated Bilayer Graphene

LI YANG, Department of Physics, Washington University in St Louis — By employing the first-principles GW-Bethe-Salpeter equation simulation, we obtain the accurate quasiparticle (QP) band gap and optical absorption spectra of gated bilayer graphene (GBLG). Many-electron effects are shown to be extremely important for understanding these excited-state properties; enhanced electron-electron interactions dramatically enlarge the QP band gap; infrared optical absorption spectra are dictated by bright bound excitons. In particular, these QP band gaps, exciton binding energies, and even the exciton spectra can be tuned in a wide range by the gate field. Our results satisfactorily explain recent experiments. Moreover, our calculation predicts exotic excitonic effects that have not been observed yet, which can be of interest for optoelectronics applications based on GBLG.

9:12AM M6.00007 A theoretical study of symmetry-breaking organic overlayers on single- and bi-layer graphene

JOSUE MORALES-CIFUENTES, T.L. EINSTEIN, Physics & CMTC, Univ. Maryland, College Park — An “overlayer” of molecules that breaks the AB symmetry of graphene can produce (modify) a band gap in single- (bi-) layer graphene. Since the triangular shaped trimesic acid (TMA) molecule forms two familiar symmetry breaking configurations, we are motivated to model TMA physisorption on graphene surfaces in conjunction with experiments by Groce et al. at UMD. Using VASP, with ab initio van der Waals density functionals (vdW-DF), we simulate adsorption of TMA onto a graphene surface in several symmetry-breaking arrangements in order to predict/understand the effect of TMA adsorption on experimental observables.

9:24AM M6.00008 Vortex zero mode and charge of mass skyrmiom in graphene

CHI-KEN LU, IGOR HERBUT, Physics Department, Simon Fraser University, Burnaby, British Columbia, Canada V5A 1S6 — We investigate the skyrmiom formed by the mass order parameters in graphene and bilayer graphene. The skyrmiom out of the three quantum anomalous spin Hall order parameters carries charge of 2e and 4e, respectively, in graphene and BA-stacking bilayer graphene. The origin of the above is related to the counting of vortex zero-mode and the representation of Clifford algebra imposed on the mass order parameters. The doubling of charge in bilayer case is due to the Kramers’ degeneracy implied by the pseudo time-reversal symmetry, which is a result of the quadratic band touching at low-energy.

9:36AM M6.00009 Broken Symmetry Phases in ABC Trilayer Graphene

VLADIMIR CVETKOVIC, OSKAR VAFEK, National High Magnetic Field Laboratory, Florida State University — We study the effects of electron-electron interaction in ABC-stacked trilayer graphene (TLG) within the framework of weak coupling renormalization group (RG). We find that, when the interaction is mainly in the forward scattering channel, the system orders into a gapless phase characterized by breaking of the TLG lattice mirror symmetries. A presence of small but finite back scattering changes the nature of the leading instability and results in gapped phases. The repulsive back scattering favors layered anti-ferromagnetic order, while the attractive back scattering yields the quantum spin Hall phase (gapped in bulk only). By classifying order parameters in TLG according to irreducible representations of the TLG space group, we conclude that any orders that break the rotational symmetry (e.g., the nematic state) in TLG are disfavored compared to the orders that do not break the lattice trifold rotational symmetry. The results are discussed in the context of present experiments on TLG.

Supported by the NSF CAREER award under Grant No. DMR-0955561, NSF Cooperative Agreement No. DMR-0654118, and the State of Florida.
9:48AM M6.00010 Unravelling the intrinsic and robust nature of van Hove singularities in twisted bilayer graphene, FELIX YNDURAIN, IVAN BRIHUEGA, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, PIERRE MALLET, Institut Niéel, CNRS-UJF, BP 166, F-38042 Grenoble, France, HECTOR GONZALEZ-HERRERO, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, GUY TRAMBLY DE LAISSARDIERE, Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise-CNRS, F-95302 Cergy-Pontoise, France, MIGUEL UGEDA, JOSE MARIA GÓMEZ-RODRÍGUEZ, Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain, LAURENCE MAGAUD, JEAN YVES VEUILLEN, Institut Niéel, CNRS-UJF, BP 166, F-38042 Grenoble, France — Extensive scanning microscopy and spectroscopy experiments completed by first principles and parameterized tight binding calculations provide a clear answer to the existence, origin and robustness of van Hove singularities in twisted graphene layers. Our results are conclusive: vHs due to interlayer coupling are present in a broad range of rotation angles. From the variation of the energy separation of the vHs with rotation angle we recover the Fermi velocity of the graphene monolayer as well as the strength of the interlayer interaction. The robustness of the vHs is assessed both by experiments and calculations which test the role of the periodic modulation and absolute value of the interlayer distance. We clarify the origin of the moiré corrugation observed in the STM images.

10:00AM M6.00011 Study on Metal/Metal oxide/Graphene Tunnel Junctions, KE CHEN, YING FENG, RAJA KHALID ZAHIR, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — Metal/metal-oxide/graphene (Metal = Al, Ti, Hf, Zr) tunnel junctions were fabricated by transferring single-layer graphene grown by chemical vapor deposition on Cu onto metal strips by either a wet or dry approach. The metal strips were prepared by dc magnetron sputtering through a shadow mask and were exposed to air for about 10 minutes for native oxides to grow prior to the transfer. Good tunneling properties were observed for all the junctions fabricated by either means of graphene transfer. The zero-bias resistance of these junctions all increases with time to a final value, indicating continuing oxidation of the metals with a self-limited oxidation rate. Some junctions show the final area-normalized zero-bias resistances and self-limited oxidation times for Al, Ti, Hf, Zr are about 0.15, 0.2, 600, 1000 kΩ and 25, 90, 6, 9 hour, respectively. The tunneling spectra were studied at various temperature down to 4.2 K and analyzed by the Brinkman-Dynes-Rowell model to get the height and width of the tunnel barriers, taking into account the electron structure of graphene. The junctions are good candidates for chemical sensing applications.

10:12AM M6.00012 Tunneling Spectroscopy of Graphene using Planar Pb Probes1, YANJING LI, NADYA MASON, University of Illinois at Urbana-Champaign — We show that evaporating lead directly on graphene can create high-quality tunnel probes. By monitoring and comparing the resistances of probes made from Pb, Al and Ti/Au, we have found unique and robust behavior of the Pb probes: the contact resistance between the Pb and graphene first increases and then saturates over a time period of approximately one week. Characterization via transport measurements at low temperature shows that after oxidation a well-formed tunnel barrier is created between the Pb and the graphene. Tunneling spectroscopy using the Pb probes manifests energy-dependent features such as resonances and localization behavior, and can thus be used to probe the microscopic electronics of graphene.

1This work was supported by the NSF DMR-0906521.

10:24AM M6.00013 Mg/MgO/Graphene Tunnel Junctions Made by Dry Transfer of Graphene in Vacuum, YING FENG, KE CHEN, Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — Mg/MgO/Graphene junctions were fabricated by dry transfer of single layer graphene film grown by chemical vapor deposition on Cu Mg strips were deposited onto Si/SiO2 or glass substrates by thermal evaporation through a shadow mask. The tunnel barrier MgO was formed by exposing deposited Mg for about 10 minutes in air prior to the graphene transfer. To prevent degradation of MgO by liquids, a dry transfer technique is used. First a graphene film was transfer onto a free-standing 4µm-thick Cu film using the traditional wet method, then pressed onto a transparent and flexible PDMS stamp followed by etching away the Cu film in FeCl3 solution, and finally stamped onto the Mg strips in vacuum to prevent any gas bubbles that may form between graphene and Mg strips. The dry-transferred graphene has similar properties to traditional wet-transferred graphene, characterized by scanning electron microscopy, atomic force microscopy, Raman spectroscopy, and transport measurements. It has a sheet resistance of 1.6 ∼ 3.4 kΩ/□, charge carrier density of 4.1 ∼ 5.3 × 1012 /cm2 and mobility of 460 ∼ 760 cm2/Vs without doping at room temperature. Mg/MgO/graphene junctions show good tunneling characteristics at temperatures down to 4.2 K. The barrier height and width were obtained by fitting with the Brinkman-Dynes-Rowell trapezoid-shaped barrier model with consideration of graphene electron structure.

10:36AM M6.00014 Intrinsic Dirac Point Energy Level and Band Offset of Graphene/SiO2 interface, KUN XU, Purdue University, National Institute of Standard and Technology, CAIFU ZENG, KANG WANG, University of California, Los Angeles, QIN ZHANG, National Institute of Standard and Technology, PEIDE YE, Purdue University, RUSEN YAN, ALAN SEABAUGH, HUILI XING, University of Notre Dame, JOHN SUEHLE, CURT RICHTER, DAVID GÜNDLACH, NHAN NGUYEN, National Institute of Standard and Technology — Advancing toward the rational design, fabrication, and implementation of graphene(GR)-based electronic and optical devices, the intrinsic barrier height of undoped GR (the Dirac point of GR to the conduction band(CB) edge of an insulator), as well as the intrinsic work function(WF) of GR must be accurately determined. We present an internal photoemission (IPE) investigation of a unique semi-transparent metal/high-k/GR/SiO2/Si structure, and focus our study on the photoemission phenomena at the GR/SiO2 interface. By taking advantage of the optical interference of the SiO2 cavity, the enhanced photoemission from GR was observed. As a result, a complete electronic band alignment at the GR/SiO2/Si interfaces is established. The intrinsic positions of the undoped GR Dirac point with respect to the CB of SiO2, 3.58 eV (Al2O3 TG) and 3.60 eV (HfO2 TG), are obtained. The intrinsic WF of graphene is found to be 4.50 eV. The determination of the WF of GR is of significant importance to the engineering of GR-base devices and the IPE spectroscopy, combined with specific interference cavity structures, would be a valuable measurement technique for other GR-like-D material systems.

10:48AM M6.00015 Point Contacts to Graphene for Corbino Disk Geometry Devices, BIN CHENG, PENG WANG, LEI JING, CHUN NING LAU, MARC BOCKRATH, University of California, Riverside — A Corbino disk geometry raises new possibilities for understanding and manipulating the Dirac fermions of graphene. In this contribution, we present a new type of point contact for Corbino disk geometry devices, which enables the detection of device characteristics under high magnetic fields. The devices are fabricated using focused ion beam techniques and have been tested using low temperature scanning tunneling microscopy. We will discuss the results and their implications for future high-field device applications.


Wednesday, March 20, 2013 8:00AM - 11:00AM – Session M12 DCMP: Topological Insulators: Topological States in Superconductors 314 - Andrew Wray, Lawrence Berkeley National Laboratory
8:00AM M12.00001 Engineering Majorana modes in MBE grown III-V semiconductor heterostructures, PEDRAM ROUSHAN, PETER O’MALLEY, YU CHEN, BROOKS CAMPBELL, Department of Physics, UCSB, BORZOYEH SHOJAEI, JAVAD SHABANI, BRIAN SCHULTZ, CHRIS PALMSTROM, Materials department, UCSC, JOHN MARTINIS, Department of Physics, UCSC. — Several theoretical proposals for realizing Majorana fermions in condensed matter systems have created much excitement and are being intensely followed by experimental groups. A common feature of all these proposals is the large size of the parameter space. We are pursuing a proposal based on coupling a semiconductor nanowire with strong spin-orbit coupling to an s-wave superconductor. Considering only the energy landscape, the size of the induced quasiparticle gap depends on the spin-orbit coupling, Zeeman energy, mobility, coupling between the two materials, and the s-wave superconducting gap. We find that Majorana modes can only be realized through carefully engineered materials. We explore this parameter space and discuss the feasibility of realizing Majorana modes based on measured parameters in our MBE grown semiconductor heterostructures.

8:12AM M12.00002 Tunneling spectroscopy of topological superconducting states – toward detection of Majorana fermions†, WAN KYU PARK, K. COUGHLIN, C. WAN, M. LIU, L. H. GREENE, University of Illinois at Urbana-Champaign, J. SCHNEELOCH, R.D. ZHONG, Z.J. XU, G. GU, Brookhaven National Laboratory. — Topological insulators and superconductors have attracted much research interest recently. These materials are known to possess exotic electronic structures that cannot be adiabatically transformed to topologically trivial ones. The spin-momentum locked (helical) Dirac fermions form surface conduction bands while the bulk is insulating. When they become superconducting, charge-neutral zero-energy modes, the so-called Majorana fermion modes, are predicted to emerge due to the unique quasiparticle properties in such a superconducting state. Aiming at detect them, we investigate two novel superconducting systems using tunneling spectroscopy: i) thin film Nb which is proximity-coupled to the helical Dirac fermions in (Bi, Sb)$_2$Se$_3$; ii) (Sn, In)Te, a potential topological superconductor. Our measurements reveal unusual conductance features in the background and near zero bias. We will report results on their temperature and magnetic field dependences and discuss their implications.

†The work at UIUC is supported by the U.S. DOE under Award No. DE-FG02-07ER46453 and the NSF DMR 12-06706.

8:24AM M12.00003 Transport properties of topological superconductor-Luttinger liquid junctions, ROMAN LUTCHYN, Microsoft Station Q, JACOB SKRABACZ, University of California Santa Barbara. — Devices involving topological superconductor-Luttinger liquid junctions have been fabricated recently [1,2] to detect Majorana zero-energy modes. One of the signatures of Majoranas in such systems is the so-called “zero-bias anomaly” – a quantization of the tunneling conductance at zero temperature. We have developed a framework based on Keldysh formalism to study the corrections to the tunneling conductance due to finite temperature and voltage. Our results are important for understanding the experimental data.


8:36AM M12.00004 Interface currents in topological superconductor-ferromagnet junctions, PHILIP BRYDON, CARSTEN TIMM, Technische Universität Dresden, ANDREAS SCHNYDER, Max-Planck-Institut für Festkörperforschung. — Both fully gapped and nodal pairing states of noncentrosymmetric superconductors (NCS) display non-trivial topological properties, manifested by topologically protected dispersive and flat-band surface states [1,2]. Using a 2D model of an NCS, we show that the surface states typically have strong spin-polarization $s_{\mu} \cdot  \vec{z}(k_y)$, which is odd in the surface-Brillouin-zone momentum $k_y$. Upon placing the NCS in proximity contact with a ferromagnet, the coupling to the exchange field gives a perturbative correction to the energy of these states $\propto s_{\mu}(k_y)$, thus generating an interface charge current $\propto \partial_{k_y} s_{\mu}(k_y)$ in the NCS. This is most clearly realized in a nodal NCS, where the weak dispersion acquired by the singly degenerate zero-energy flat bands leads to a strong enhancement of the interface current at low temperatures. We argue that this effect is a “smoking-gun” signature of the singly degenerate flat bands.


8:48AM M12.00005 Majorana fermions in spin-singlet nodal superconductors with coexisting non-collinear magnetic order, ZIQIANG WANG, Boston College, YUAN-MING LU, University of California, Berkeley. — Realizations of Majorana fermions in solid state materials have attracted great interests recently in connection to topological order and quantum information processing. We propose a novel way to create Majorana fermions in superconductors. We show that an incipient non-collinear magnetic order turns a spin-singlet superconductor with nodes into a topological superconductor with a stable Majorana bound state (MBS) in the vortex core or on the edge. Moreover the topologically-stable point defect of non-collinear magnetic order also hosts a zero-energy MBS. We argue that such an exotic non-Abelian phase can be realized in extended t-J models on the triangular and square lattices. Our proposal suggests a new avenue for the search of Majorana fermions in correlated electron materials where nodal superconductivity and magnetism are two common caricatures.

9:00AM M12.00006 Tuning between s-wave and p-wave superconductors as well as emerging Majorana fermions in extended Hubbard lattices, KUEI SUN, University of Cincinnati, CHING-KAI CHIU, University of Illinois at Urbana-Champaign, JIANSHENG WU, Hong Kong University of Science and Technology. — We study spin-half fermions in one dimensional extended Hubbard lattices in which the superconducting pairing orders are induced by the tuning of nearest-neighbor charge and spin interactions. We derive gap equations for three p-wave (triplet) as well as one s-wave (singlet) pairing orders and obtain a phase diagram characterizing these orders as a function of interaction couplings. We find that the system can evolve between s-wave and p-wave pairing states, with the emergence of Majorana fermions in the p-wave regime, identified as a time-reversal invariant Kitaev Majorana chain. Finally we discuss the effects on the topological non-trivial states when time-reversal or SU(2) symmetry breaks.

9:12AM M12.00007 Robustness of Majorana modes in multiband topological superconductors, SHUSA DENG, Dartmouth College, GERARDO ORTIZ, University of Indiana, Bloomington, LORENZA VIOLA, Dartmouth College. — We investigate the robustness of Majorana modes in a multiband topological superconductor model belonging to symmetry class DIII, against various perturbations. In the three dimensional case, we find that in topological phases where an even number of Kramer pairs of Majorana modes exist on each boundary, these modes may become gapped under a boundary perturbation, despite time-reversal invariance being preserved. Conversely, in two dimensions, the gapless Majorana modes may remain gapless in the presence of certain time-reversal breaking fields or impurities. However, upon changing the strength of an applied longitudinal Zeeman field, a transformation from helical Majorana modes to chiral Majorana modes may be induced, accompanied by a quantum phase transition in the bulk.
9:24AM M12.00008 Majorana end modes in STM Fabricated Atomic Chains on the Surface of a Superconductor: Theory & Experiment, STEVAN NADJ-PERGE, ILYA DROZDOV, JUNGPIL SEO, ANDREI BERNEVIG, ALI YAZDANI, Princeton University — The search for Majorana fermions (MF) in solid state devices has been hampered by the possible absence of disorder which may induce signatures similar to those expected by novel MF boundary states. Therefore it is important to identify clean solid state systems in which MF modes can be easily distinguished from disorder related effects. In this talk, we will present theoretical calculations and preliminary experimental results on chains of magnetic atoms on the surface of an s-wave superconductors. The theoretical efforts show that surprisingly short magnetic chains (20 atoms long or more) support MF under specific conditions depending on spins of the magnetic atoms and their coupling. We will describe these theoretical results along with experiments in which a scanning tunneling microscopy (STM) has been used to assemble chains of magnetic atoms (3d transition metals) on Nb and Pb single crystals. Presence of Majorana boundary modes in these structures can be probed using spatially-resolved STM spectroscopy.

9:36AM M12.00009 Topological defects and subgap excitations in two-band superconductors, KIRILL SAMOKhin, MICHELLE PRZEDBORSKI, Brock University — Phase solitons are topological defects peculiar to two-band superconductors, which are associated with a 2π winding of the relative phase of the two superconducting condensates. The order parameter phase variation in each of the bands leads to the quasiparticle bound states whose energies lie below the bulk gap. We calculate the single soliton energy as well as the interaction energy of two solitons, at arbitrary temperature. Applications to a similar system — one or more domain walls in a chiral p-wave superconductor — are discussed.

9:48AM M12.00010 Symmetry Protected Majorana fermions in topological superconductors, MASATOSHI SATO, Department of Applied Physics, Nagoya University — Recently, there are considerable interests in Majorana fermions in topological superconductors. It has been found that promising schemes to realize Majorana fermions is to break some of symmetries of the system. Indeed, by inducing the spin-orbit interaction and the Zeeman coupling which break inversion and time-reversal symmetries, conventional s-wave superconductors may support Majorana fermions on the boundaries. Moreover, by breaking the spin-rotation symmetry, spin-triplet superconductors may support Majorana fermions. Therefore, one might expect that symmetry is an obstruction to detect Majorana fermions. In this talk, however, we will show that this is not always the case. We show that symmetry may protect Majorana fermions in topological superconductors. As an example, we will show that Majorana Ising character, which gives a detectable signal of Majorana fermion, is stabilized by symmetry of the system. We will also discuss some other roles of symmetry for Majorana fermions in topological crystalline superconductors.

10:00AM M12.00011 Majorana fermions in 3DTI with superconductivity, PEDRO LOPES, Unicamp/UIUC, POUYAN GHAEMI, SHINSEI RYU, UIUC — We study the problem of a strong 3D topological insulator (TI) with intrinsic superconductivity (SC). Particularly we present microscopic calculations using a low energy model of bulk massive Dirac fermions with mean field s-wave SC pairing. Introducing a kink in the mass in one spatial direction we can verify the appearance of localized (around the kink) states which correspond to the TI surface states and, with the further introduction of a vortex in the SC pairing, we are able to bind Majorana zero-modes (MZM’s). The MZM’s are known to be elusive particles in the sense that they are hard to detect. We then introduce a Majorana representation to the system Hamiltonian described above and propose an artificial doubling of this system which gives rise to a O(2) symmetry and allows us to define a conserved charge that can be used to probe for the presence of the MZM’s. This doubled Majorana system then becomes an interesting playground, allowing us to search for masses which mix the different Hilbert spaces and study the behavior of this charge. We finish with a path-integral formulation of the problem through which we can integrate out the fermions and find an effective action for both, the electromagnetic as well as the corresponding to the O(2) conserved charge, gauge fields.

10:12AM M12.00012 Josephson-Majorana cycle in topological single-electron hybrid transistors, NICOLAS DIDIER, Universite de Sherbrooke and McGill University, MARCO GIBERTINI, Scuola Normale Superiore, ALI G. MOGHAD-DAM, University of Duisburg-Essen and IASBS Zanjan, JUERGEN KOENIG, University of Duisburg-Essen, ROSARIO FAZIO, Scuola Normale Superiore — Charge transport through a small topological superconducting island in contact with a normal and a superconducting electrode occurs through a cycle which involves coherent oscillations of Cooper pairs and tunneling in/out the normal electrode through a Majorana bound state, the Josephson-Majorana cycle. We illustrate this mechanism by studying the current-voltage characteristics of a superconductor - topological superconductor - normal metal single-electron transistor. At low bias and temperature the Josephson-Majorana cycle is the dominant mechanism for transport. We discuss a three-terminal configuration that constitutes a direct probe of the non-local character of the Majorana bound states. Non-local cotunneling dominates over the local contributions and the current noise is maximally correlated independently of the length of the wire. Preprint: arXiv:1202.6357

10:24AM M12.00013 Superconducting Klein tunneling and AC Josephson effect in superconductor/topological insulator/superconductor junctions, EWEILINA HANKIEWICZ, GRORY TKACHOV, Wuerzburg University — We consider superconductor(S)/surface state of topological insulator(TI)/superconductor junctions (S) where the S regime describes the surface state of the TI with the proximity with the s-wave superconductor. The novelty of such S/TI/S junctions originates from the electron spin helicity (locking of the momentum and the spin for a surface of TIs) which leads to both the s-wave singlet and the p-wave triplet pairing on the surface underneath the superconductor. Existence of these two superconducting channels lead to interesting features in transport through these junctions. In particular we show that superconducting Klein tunneling and topological Andreev bound state (ABS) (state of hybridized two Majorana fermions) occur for the normal incidence where ABS is protected against backscattering. For transport channels different than for the normal incidence, the scattering from the junction barrier generates an energy gap in the spectrum supporting non-topological ABSs. Due to mixed order parameter, the AC Josephson effect is fractional showing higher odd harmonics. We conclude that favorable conditions for the observation of the topological ABS exist in narrow TI links with a small number of open channels close to one.

13:00AM M12.00014 Josephson currents through topological insulator surfaces, JENS H. BARDARSON, RONI ILAN, UC Berkeley, HEUNG-SUN SIM, KAI, JOEL E. MOORE, UC Berkeley — Motivated by recent experiments carried out on superconductor – 3D topological insulator – superconductor junctions, we study the transport properties of these junctions. Transport is believed to be dominated by the surface states of the topological insulator, and we discuss the effects of the junctions geometry on the Josephson supercurrent in the presence of a magnetic field.
The point is approached. We develop a variational argument which shows that the size of the vortex cores diverges as $1/\sqrt{\lambda}$ that vanishes at the Fermi energy ($E = 0$) is of current interest in connection with impurities in graphene and in unconventional superconductors. The phase diagram of these models has been established previously [1,2]. We study the low-temperature static and dynamical properties of the models using the numerical renormalization-group method, and compare our results against exact and perturbative analytical theories [2], and against calculations performed within the non-crossing approximation. In the vicinity of the quantum critical points separating local-moment and non-Ferrell liquid phases, the static local spin susceptibility is characterized by a set of critical exponents that satisfy the hyperscaling relations expected of an interacting system below its upper critical dimension. The dynamical local susceptibility and the impurity spectral function exhibit forms consistent with frequency-over-temperature scaling, another feature associated with interacting quantum critical points. [1] C. Gonzalez-Buxton and K. Ingersent, Phys. Rev. B 57, 14254 (1998). [2] I. Schneider et al., Phys. Rev. B, 84, 125139 (2011).
dependence of all wave-function renormalization functions is kept. As a consequence, we find non-trivial RG fixed points for all positive integer \( N \).

As a consequence of this phase transition, we use the functional renormalization group to reconsider the problem for \( N \)\, or valence bond solid. We characterize this phase transition by using QMC to study the order parameter, correlation functions, pair density, power spectrum, and addition energies.

1Supported by the U.S. Dept. of Energy (Materials Sciences and Engineering, DE-SC0005237).

9:36AM M19.00009 Construction of local order parameters from non-vanishing mutual information, WING CHI YU, SHI-JIAN GU, Department of Physics, The Chinese University of Hong Kong, HAI-QING LIN, Department of Physics, The Chinese University of Hong Kong; Beijing Computational Science Research Center — In the recent decades, raising attention has been paid in the study of quantum phase transitions (QPTs) from quantum information perspectives. In this talk, we will present a scheme in constructing the local order parameters by investigating the spectra of the reduced density matrices that are used to calculate the mutual information. We will briefly review the relation between non-vanishing mutual information and the presence of long-range correlation in a system. In particular, we will illustrate our scheme using the numerical exact diagonalization result of the one-dimensional Hubbard model.

9:48AM M19.00010 Columnar and superfluid order in an extended Shastry-Sutherland model, KEOLA WIERSCHEM, PINAKI SENGUPTA, Nanyang Technological University — The low temperature magnetic properties of several rare-earth tetraborides have been shown to be well-characterized by an extension of the Shastry-Sutherland model (SSM). This extension includes additional next-nearest-neighbor bonds, and the exchange interaction along all bonds is anisotropic with strictly ferromagnetic transverse exchange. The extended SSM is thus equivalent to a system of hard-core bosons and is free of the quantum Monte Carlo (QMC) sign problem. Using large scale QMC simulations, we study the phase diagram of the extended SSM in a new parameter regime that stabilizes a zero-field columnar antiferromagnetic state. We show how application of an external magnetic field can induce a phase transition to a spin supersolid phase. We compare the overall magnetization process to experimental observations of ErB\(_4\), a rare-earth tetraboride with ground state columnar antiferromagnetic ordering. Finally, we speculate that if the zero-field columnar order present in ErB\(_4\) is driven by similar interactions it may also possess a field-induced supersolid phase.

10:00AM M19.00011 Resummation of divergent fluctuations near to metallic ferromagnetic quantum criticality, CHRIS PEDDER, ANDREW GREEN, London Centre for Nanotechnology & University College, London — Fluctuations near to the metallic ferromagnetic quantum critical point can have profound effects. They lead to new quantum critical scaling at high temperatures, which gives way to reconstruction of the phase diagram at lower temperatures. In the vicinity of the quantum critical point, new spatially modulated magnetic or spin nematic phases appear. These new phases may be revealed by means of non-analytic corrections to Hertz-Millis theory [1], or in the recently-developed quantum order-by-disorder approach [2]. Here we demonstrate a re-summation of all the leading divergences in the latter approach to extend the analysis from the finite-temperature tricritical point down to zero temperature.


1This work was funded by the EPSRC under grant code EP/1004831/1.

10:12AM M19.00012 ABSTRACT WITHDRAWN —

10:24AM M19.00013 Tractable Crossing-symmetric Equations Formalism and Applications in Two Dimensions, KELLY REIDY, KHANDKER QUADER, Kent State University, KEVIN BEDELL, Boston College — The tractable crossing symmetric formalism is developed for the 2D case. We first consider circular Fermi surfaces and then extend this to 2D square lattice systems. Limiting cases, such as small \( q \), vanishing momentum-energy transfer \( q \to 0, \omega \to 0 \), vanishing \( q \) but non-zero \( \omega \) are considered. This is applied to the study of various properties of 2D Fermi systems. Of particular interest is the physics near Pomeranchuk instabilities: in Fermi systems, interactions can cause symmetry-breaking deformations of the Fermi surface, called Pomeranchuk instabilities. In Fermi liquid theory language, this occurs when one of the Landau harmonics \( F_{\alpha}^{\omega} \to -(2\ell +1) \); e.g. \( F_{\ell}^{\omega} \to -1 \) are related to ferromagnetic transition \( \ell \), and density instabilities(s). The corresponding points in parameter space may be viewed as quantum critical points. Using graphical and numerical methods to solve coupled non-linear integral equations that arise in the crossing symmetric equation scheme, we obtain results in the 2D case close to Pomeranchuk instabilities. We compare our 2D results for various response functions and instabilities with the results of recent calculations in the 3D case, which will also be discussed.

10:36AM M19.00014 Strongly-correlated phases in a flatband with incommensurate filling, EVELYN TANG, XIAO-GANG WEN, Perimeter Institute/MIT — We explore strongly-correlated electronic phases in flatband systems (such as on the kagome lattice) with incommensurate filling, in the presence of spin-orbit interactions and ferromagnetism. The competition between Fermi-liquid, charge-density wave and superconducting phases in this system is examined.

Wednesday, March 20, 2013 8:00AM - 11:00AM –
Session M20 DCMP: Focus Session: Metamaterials - Plasmonics

322 - David Smith, Duke University
8:00AM M20.00001 Quantum Plasmonics: Electron transfer processes

Peter Nordlander, Rice University — Plasmon energies can be tuned across the spectrum by simply changing the geometrical shape of a nanostructure. Plasmons can efficiently capture incident light and focus it to nanometer sized hotspots which can enhance electronic and vibrational excitations in nearby structures. Another important but still relatively unexplored property of plasmons is that they can be efficient sources of hot energetic electrons which can transfer into nearby structures and induce a variety of processes. This process is a quantum mechanical effect: the decay of plasmon quanta into electron-hole pairs. We will discuss how plasmon induced hot electrons can be used in various applications: such as to induce chemical reactions in molecules physisorbed on a nanoparticle surface, to inject electrons directly into the conduction band of a nearby substrate, and to induce local doping of a nearby graphene sheet. References [1] J.N. Halas et al., Adv. Mat. 24 (2012) 4842 [2] R. Huchkha et al., JACS 133 (2011) 12247, S. Mukherjee et al. TBP 2012 [3] M.W. Knight et al., Science 332 (2011) 702, Z.Y. Fang et al., NL 12 (2012) 3808 [4] Z.Y. Fang et al., ACS Nano 6 (2012) 10.1021/n304028b

8:12AM M20.00002 Plasmonic electron injection drives ultrafast phase transition by catastrophic phonon collapse I: experiment

Kannatasen Appavoo, Vanderbilt University, Nathaniel F. Brady, University of Alabama-Birmingham, BIN WANG, Vanderbilt University, Minah SEO, Los Alamos National Lab, Joyeeeta Nag, Vanderbilt University, Rohit P. Prasankumar, Los Alamos National Lab, Socrates T. Pantelides, Vanderbilt University, David J. Hilton, University of Alabama-Birmingham, Richard F. Haglund, Vanderbilt University — Phase transitions in quantum materials such as vanadium dioxide (VO$_2$) can provide functionality in nanophotonic devices. Here we report on a novel all-optical mechanism to trigger phase transition (PT) of VO$_2$ faster than its intrinsic single photon period. By optically exciting a spectrally resonant sparse mesh of plasmonic gold nanoparticles, hot electrons created are ballistically injected across the Au/VO$_2$ interface to assist the sub-picosecond PT, lowering the switching threshold by a factor of five. As confirmed by density functional calculations, the injected electrons cause a catastrophic collapse of the 6 THz phonon mode in VO$_2$, essential for triggering its PT (next abstract). This demonstration of plasmon-induced hot-electron-driven PT controlled by this ultrafast technique represents a critical step towards developing hybrid nanomaterials with optimal switching thresholds.

1) (1)DOE-FG02-01ER45916 (2)HDTTRA1-10-1-0047 (3)NSF:ARI-R2 DMR-0963361 and DMR-1207241 (4)McMinn Endowment (6)LANL:DE-AC52-06NA25396 (7)SNL:DE-AC04-94AL85000 (8)GAANN:P200A09001

8:24AM M20.00003 Plasmonic electron injection drives ultrafast phase transition by catastrophic phonon collapse II: theory

Bin Wang, Kannatasen Appavoo, Vanderbilt University, Nathaniel Brady, University of Alabama, Birmingham, Minah Seo, LANL, Joyeeeta Nag, Vanderbilt University, Rohit Prasankumar, LANL, David Hilton, University of Alabama, Birmingham, Richard Haglund, Vanderbilt University, Socrates Pantelides, Vanderbilt University, ORNL — The ultrafast photo-induced phase transition in VO$_2$ is promising for data storage and sensing applications. Our experimental work (the previous talk) shows that in a Au/VO$_2$ hybrid nanostructure, electrons excited in the Au photocathode by an ultrafast laser trigger the insulator-to-metal transition in VO$_2$. Here we report first-principles density-functional calculations showing that the collapse of a 6 THz optical phonon, corresponding to a twisting motion of V atoms, is responsible for the ultrafast phase transition. Above a concentration threshold, we find that injected electrons from Au induce collapse of the VO$_2$ phonon, which stimulates the monoclinic-to-rutile structural phase transition. We also show that hole-doping can induce the same effect. The abrupt change of the critical phonon results from the weakening of the V-V bonds induced by the combined flux of injected electrons and holes. Thus, our results explain the experimental finding of plasmonic-electron-driven ultrafast phase transition and represent a step towards manipulating the photo-induced phase transition by surface modification.

Supported by the Office of Science, US DOE (DE-FG02-01ER45916, DE-AC52-06NA25396, DE-AC04-94AL85000) and DTRA (HDTTRA1-10-1-0047), NSF (ARI-R2 DMR-0963361, DMR-1207241), GAANN Fellowship (P200A090143), McMinn Endowment (STP), and LDRDP.

8:36AM M20.00004 Optical circulation and power flow rotation with nonreciprocal plasmonic structure

Artur Davoyan, Nader Engheta, Department of Electrical and Systems Engineering, University of Pennsylvania — In this work we propose a concept for tailoring the near-zone optical field with the plasmonic nanostructures mixed with MO materials, and demonstrate a novel effect of a subwavelength power flow circulation. We study both analytically and numerically plasmonic nanostructures embedded into magneto-active media, and analyze their resonances and corresponding eigenmode spectra. We show that when the structure is degenerate the magneto-optical activity, when introduced, causes strong interaction between these modes. Such intermodal interaction leads to a formation of a novel set of rotating states and to a frequency splitting between them. We study the plane wave excitation of such nanostructures and reveal a strong power flux circulation around such structures in the presence of magneto-optical activity. We will discuss a possible application of the observed effect and propose a subwavelength optical circulator. In particular, we study numerically a plasmonic nanostructure embedded into the core of the Y-junction formed by single mode optical waveguides. We show that mixing the plasmonic nanostructures with magneto-optical materials it is possible to break significantly the symmetry between the output arms of the junction and almost completely isolate one of them.

This work is supported in part by the US Air Force Office of Scientific Research (AFOSR) grant number FA9500-10-1-0408.

8:48AM M20.00005 Mode matching for optimal plasmonic nonlinear generation

Kevin O’Brien, Haim Suchowski, Jun Suk Rho, Boubacar Kante, XiaoBo Yin, Xiang Zhang, NSF Nano-scale Science and Engineering Center (NSEC), University of California, Berkeley, California — Nanostructures and metamaterials have attracted interest in the nonlinear optics community due to the possibility of engineering their nonlinear responses; however, the underlying physics to describe nonlinear light generation in nanostructures and the design rules to maximize the emission are still under debate. We study the geometry dependence of the second harmonic and third harmonic emission from gold nanostructures, by designing arrays of nanostructures whose geometry varies from bars to split ring resonators. We fix the length (and volume) of the nanostructure on one axis, and change the morphology from a split ring resonator on the other axis. We observed that the optimal second harmonic generation does not occur at the morphology indicated by a nonlinear oscillator model with parameters derived from the far field transmission and is not maximized by a spectral overlap of the plasmonic modes; however, we find a near field overlap integral and mode matching considerations accurately predict the optimal geometry.

9:00AM M20.00006 Theory of plasmon-enhanced metal photoluminescence

Tigran V. Shahbazyan, Jackson State University — Metal photoluminescence (MPL) originates from radiative recombination of photoexcited core holes and conduction band electrons. In metal nanostructures, MPL is enhanced due to surface plasmon local field effect. We identify another essential process in plasmon-assisted MPL excitation of Auger plasmons by core holes - that hinders MPL from small nanostructures. We develop a microscopic theory of plasmon-enhanced MPL that incorporates both plasmonic enhancement and suppression mechanisms and derive enhancement factor for MPL quantum efficiency. Our numerical calculations of MPL from Au nanoparticles are in excellent agreement with experiment.
9:12AM M20.00007 Probing light-matter interactions in plasmonic nanostructures with a single quantum dot

9:24AM M20.00008 Giant circular dichroism of a molecule in a plasmonic nanoparticle dimer

9:36AM M20.00009 Exciton-plasmon coupling in monolayer molybdenum disulfide

9:48AM M20.00010 Optical Properties of Graphene Plasmons in Periodic Gate Structures

10:00AM M20.00011 Optical Properties of Epitaxially Grown Silver Films

10:12AM M20.00012 Hamiltonian Optics Approach for Hybridized Surface Plasmon Polariton in Graded Metal-Dielectric-Metal Waveguide with Periodically Varying Index
were utilized to determine Poisson's Ratio (ν) in the industry. The frequency dispersion and associated light scattering intensities of longitudinal and transverse acoustic standing mode type excitations to characterize the mechanical properties of these highly compact and porous structures. We report on Brillouin light scattering measurements to determine the stability thereby degrading device functionality. Such structural characteristics present limitations with traditional measurement techniques as nanoindentation layers with controlled levels of porosity. However, increased porosity as well as reduced film thicknesses (<100nm) could reduce mechanical and thermal stability thereby degrading device functionality. Such structural characteristics present limitations with traditional measurement techniques as nanoindentation to characterize the mechanical properties of these highly compact and porous structures. We report on Brillouin light scattering measurements to determine the independent elastic constants, and thus the mechanical properties, of dielectric films with thicknesses as low as 25 nm and porosity levels up to 45%, the highest in the industry. The frequency dispersion and associated light scattering intensities of longitudinal and transverse acoustic standing mode type excitations were utilized to determine Poisson’s Ratio (ν) and Young’s Modulus (E). Significant modifications were found in ν and E of these highly porous carbon-doped SiO₂(Si-O-C-H) and amorphous carbon(a-C:H) materials compared to traditional SiO₂ and non-porous low-k materials.

8:00AM M23.00001 Temperature-Dependent Cathodoluminescence of Disordered SiO₂ Layers1, AMBERLY E. JENSEN, JR DENNISON, GREGORY WILSON, JUSTIN DEKANY, USU Materials Physics Group — Optical coatings of disordered thin film SiO₂/SiOₓ dielectric samples on reflective metal substrates exhibited electron-induced luminescence (cathodoluminescence) under electron beam irradiation. These experiments provided measurements of the absolute radiance and emission spectra as functions of incident electron energy, flux and power over a range of sample temperatures (<40 K to >300 K). The overall luminescent intensity increased linearly with increasing power, plateaued, then fell off approximately exponentially. Spectrum data revealed four spectral bands. The structural defects associated with three of the four bands have been identified. Temperature dependence of the peak intensity and central position differs for the lower and higher energy bands. These results are interpreted with a fundamental basis for understanding the dependence of cathodoluminescence on irradiation time and accumulated charge, incident flux and energy, and sample thickness and temperature.

1Work supported by EPSRC

Wednesday, March 20, 2013 8:00AM - 10:48AM – Session M23 DCMP: Optical and Dielectric Properties 325 - Qingteng Zhang, University of Wisconsin

8:12AM M23.00002 Mechanical properties of highly porous low-k dielectric nano-films: A Brillouin light scattering study, J. ZIZKA, S. BAILEY, Department of Physics, The Ohio State University, E. MAYS, D.J. MICHALAK, R. CHEBIAM, S. KING, Intel Corporation, Logic Technology Department, R. SOORYAKUMAR, Department of Physics, The Ohio State University, DEPARTMENT OF PHYSICS, THE OHIO STATE UNIVERSITY COLLABORATION, INTEL CORPORATION, LOGIC TECHNOLOGY DEPARTMENT COLLABORATION — To reduce RC time delays in micro-electronic devices, the semiconductor industry has pursued low dielectric constant (k) hybrid organic-inorganic interconnect layers with controlled levels of porosity. However, increased porosity as well as reduced film thicknesses (< 100nm) could reduce mechanical and thermal stability thereby degrading device functionality. Such structural characteristics present limitations with traditional measurement techniques as nanoindentation to characterize the mechanical properties of these highly compact and porous structures. We report on Brillouin light scattering measurements to determine the independent elastic constants, and thus the mechanical properties, of dielectric films with thicknesses as low as 25 nm and porosity levels up to 45%, the highest in the industry. The frequency dispersion and associated light scattering intensities of longitudinal and transverse acoustic standing mode type excitations were utilized to determine Poisson’s Ratio (ν) and Young’s Modulus (E). Significant modifications were found in ν and E of these highly porous carbon-doped SiO₂(Si-O-C-H) and amorphous carbon(a-C:H) materials compared to traditional SiO₂ and non-porous low-k materials.
8:24AM M23.00003 Power and Charge Deposition and Electron Transport in Disordered SiO2 Layers Under Electron Bombardment1, GREGORY WILSON, JR DENNISON, AMBERLY E. JENSEN, JUSTIN DEKANY, USU Materials Physics Group — Power and charge deposition in multilayer dielectrics from electron bombardment is dependent on the flux and energy-dependent electron penetration depth of the electron beam. Using the Continuous Slow Down Approximation (CSDA), a composite analytical formula has been developed to approximate the electron range which can be related to the dose rate, deposited power and Radiation Induced Conductivity (RIC). Based on the constituent layer geometry and material, the deposited charge can also be inferred. Three separate pulsed electron beam experiments were conducted to measure charge deposition, power dependent cathodoluminescence and RIC. The power and charge deposition experiments measured the net surface potential, electrode currents and electron induced luminescence of disordered SiO2 multilayer dielectrics with a grounded or floating conductive middle layer, using beam energies from 200 eV to 25 keV at <40 K to room temperature. These results showed that the power and charge deposition’s dependence on electron beam flux and incident energy compare favorably with the model predictions. The RIC experiments measured electrode currents using disordered SiO2 layers from <40 K to >320 K with dose rates from 10-5 Gy/s to 10-1 Gy/s. The onset of RIC in the energy-dependant depth of the RIC region provides an explanation for observed retrograde charging.

1This work supported by the NASA Goddard Space Flight Center and an NRC Senior Research Fellowship at AFRL.

8:36AM M23.00004 Structural evolution of nanoporous ultra-low-k dielectrics under voltage stress1, ARCHANRA RAJA, Columbia University, THOMAS SHAW, ALFRED GRILL, IBM Yorktown Heights, ROBERT LAIBOWITZ, TONY HEINZ, Columbia University — High speed interconnects in advanced integrated circuits require ultra-low-k dielectrics. Reduction of the dielectric constant is achieved via incorporation of nanopores in structures containing silicon, carbon, oxygen and hydrogen (SiCOH). We study nanoporous SiCOH films of k=2.5 and thicknesses of 40 - 400 nm. Leakage currents develop in the films under long-term voltage stress, eventually leading to breakdown and chip failure. Previous work* has shown the build-up of trap states as dielectric breakdown progresses. Using FTIR spectroscopy we have tracked the reorganization of the bonds in the SiCOH networks induced by voltage stress. Our results indicate that the cleavage of the Si-C and Si-O bonds contribute toward increase in the density of bulk trapping states as breakdown is approached. AC conductance and capacitance measurements have also been carried out to describe interfacial and bulk traps and mechanisms. Comparison of breakdown properties of films with differing carbon content will also be presented to further delineate the role of carbon. *Atkin, J.M.; Shaw, T.M.; Liniger, E.; Laibowitz, R.B.; Heinz, T.F. Reliability Physics Symposium (IRPS), 2012 IEEE International Symposium.

8:48AM M23.00005 Spectroscopic analysis of erbium doped laser-induced crystals for fiber-laser applications, BRIAN KNORR, ADAM STONE, HIMANSHU JAIN, VOLKMAR DIEROLF, Lehigh University — Laser induced crystallization of glasses is a highly spatially selective process which could be produced to produce crystalline-core optical fibers for fiber-laser applications. Toward this goal, single crystal lines were “written” in Er:LaBGeO glass using a femtosecond pulsed laser. These structures were analyzed using micro-Raman and luminescence spectroscopy in order to determine their viability as waveguiding laser gain media. Two-dimensional scans reveal that the erbium fluorescence is inhomogeneous over the cross-section of the crystal and lacks spatial coordination with the Raman emission, implying a physical ion accumulation in addition to enhancement due to the crystal field. Additionally, erbium fluorescence spectra taken at low temperatures from polycrystals with varying concentrations of erbium were compared to those from the laser-induced crystal lines. Significant differences in the emission energies and intensity ratios of the erbium peaks were observed. These differences may be due to the presence of strain, grain boundaries, or charge resulting from the different crystallization processes used.

9:00AM M23.00006 Luminescence and Local Structure Correlation of Er-doped Glasses and Composites, MATTHEW OTTEN, CARLO SEGRE, JEFF CECIL, MYCHALO CHAVARA, Illinois Institute of Technology, KRIS LIPINSKA, Harry Reid Center for Environmental Studies, University of Nevada Las Vegas, YOSHIMICHI OHKI, Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, Tokyo, Japan, PATRICIA KALITA, Dept. of Physics and Astronomy, University of Nevada Las Vegas — Er-doped (0.05% to 3%) Ga2O3 containing silicate glasses and composites have been prepared by rapid cooling from the melt (glasses), followed by annealing at various temperatures from 800°C to 1100°C. Er3+ luminescence has been measured and will be correlated to the local structural properties of the Er atoms as measured by x-ray absorption spectroscopy (XAS) at the MRCAT (Sector 10) beamline at the Advanced Photon Source. Preliminary analysis of the XAS data indicates that the Er is in an octahedral environment in both the glasses and composites. The glasses show no clustering of Er atoms which would lead to quenched luminescence.

9:12AM M23.00007 Large change in dielectric constant of CaCu3Ti4O12 under violet laser, C. MASINGBOON, Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand, P. THONGBAI, Khon Kaen University, Khon Kaen, 40000, Thailand, P.D.C. KING, University of St. Andrews, St. Andrews, Fife KY16 9SS, United Kingdom, S. MAENSIRI, W. MEEVASANA, Suranaree University of Technology, Nakhon Ratchasima, 30000, Thailand — This work reports the influence of light illumination on the dielectric constant of CaCu3Ti4O12 (CCTO) polycrystals which exhibit giant dielectric constant. When the CCTO samples were exposed to 405-nm laser light, the enhancement in capacitance as high as 22% was observed for the first time, suggesting application of light-sensitive capacitance devices. To understand this change better microscopically, we also performed electronic-structure measurements using photoemission spectroscopy, and measured the electrical conductivity of the CCTO samples under different conditions of light exposure and oxygen partial pressure. All these measurements suggest that this large change is driven by oxygen vacancy induced by the irradiation.

9:24AM M23.00008 Giant dielectric constant in CaCu3Ti4O12-MgB2 composites near the percolation threshold, RUPAM MUKHERJEE, Wayne State University, LUCIA FERNANDEZ, CINN Research Center on Nanomaterials and Nanotechnology, GAVIN LAWES, BORIS NADGORYN, Wayne State University — We have investigated the enhancement of the dielectric constant K in CaCu3Ti4O12 (CCTO)-MgB2 composite near the percolation threshold. To optimize the dielectric properties of pure CCTO we have sintered the samples at various temperatures. We will present the results of the measurements of K in a broad frequency for pure CCTO for the samples sintered at 1100°C and 500°C. Commercially available MgB2 powder was mixed with different weight fractions of CCTO and the pressure of 1GPa was applied to form composite pellets. Near the percolation threshold P_c, CCTO/MgB2 composite system exhibit a dramatic increase of the dielectric constant K by several orders of magnitude, compared to pure CCTO. We will also discuss the magnetic field dependence of the capacitance of CCTO composite powders.

9:36AM M23.00009 Coupling of photonic, plasmonic and electric effects in metal nanostructures, NATALIA NOGINOVA, VINCENT RONTO, Norfolk State University — Strong photonic was observed in thin metal films and nanostructures, with the maximum of the effect at plasmon resonance conditions. To better understand mechanism of the effect and explore the possibility to control it with nanoscale geometry, we studied photoinduced currents in gold films and nanomesh structures in the dependance on the wavelength and period of nanostructure. We showed that nanostructuring of the surface lead to significant (50-fold) increase in the magnitude of the effect. Results are discussed in terms of coupling of optical, plasmonic and electric effects.
9:48AM M23.00010 Plasmons for Coulomb Coupled Spherical Shells, ANTONIOS BALASSIS, Fordham University, ANDRΙUROV, GODFREY GUMBΣ, Hunter College of the CUNY — We report calculations of the collective plasmon excitations for an electron gas confined to the surface of a spherical shell. The energy spectra of the plasmons and particle-hole modes are presented as functions of the radius of the shell as well as the angular momentum quantum number $L$. We compare results for the plasma excitations for a single shell, a pair of concentric shells as well as when two shells have their centers separated by a distance which exceeds the sum of the radii of the two shells. For the single shell and pair of concentric shells, the plasma modes are labelled by the angular momentum quantum number $L$ only. However, for the pair of non-concentric shells, the plasma modes are labelled by both $L$ and $M$, the projection of angular momentum on the $z$ axis. These results have been obtained in the random phase approximation (RPA).

10:00AM M23.00011 High Optical Performance and Practicality of Active Plasmonic devices based on Rhombohedral BiFeO$_3$, PHUONG-KHUONG ONG, HONG-SON CHU, Institute of High Performance Computing, A-STAR, DAVID SINGH, Materials Science and Engineering Division Oak Ridge National Laboratory, JOHN WANG, Department of Materials Science and Engineering National University of Singapore — BiFeO$_3$ is a multiferroic oxide with perovskite type structure, which has been studied extensively for its ferroelectric and magnetic behavior. The magnetoelectric coupling could potentially provide new functionalities. We have studied the electronic and optical properties of Rhombohedral BiFeO$_3$, which we show to be a very promising candidate material to build active nanoplasmonic devices, in particular nanoplasmatic devices. It has a strong switching modulated optical properties and a large optical birefringence $(\Delta n)$ arising from the combination of octahedral tilts, ferroelectricity and G-type antiferromagnetism in BiFeO$_3$. A prototype of a plasmonic resonator with a Rhombohedral BiFeO$_3$ thin film layer is used as an example and shows excellent switch and modulation responses. The proposed approach provides potential opportunities to develop high performance nanoplasmonic devices for optical communication. We find excellent switching and modulation responses. The use of Rhombohedral BiFeO$_3$ provides an effective way to actively control optical performance of plasmonic nanostructures.

1This work was supported by IIPIC, A-STAR under grant A*STAR-ERC 0921540098. Work at ORNL was supported by the Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

10:12AM M23.00012 Taming the flow of light via active magneto-optical impurities, SAMUEL KALISH, HAMIDREZA RAMEZANI, ZIN LIN, TSAMPIKOS KOTTOS, Department of Physics, Wesleyan University, Middletown, CT-06459, USA, VASSILIOS KOVANIS, ILYA VITEBSKIY, Air Force Research Laboratory, Sensors Directorate, Wright Patterson AFB, OH 45433 USA — We demonstrate that the interplay of a magneto-optical layer sandwiched between two judiciously balanced gain and loss layers which are both birefringent in-plane anisotropy, induces unidirectional electromagnetic modes. Embedding one such optically active non-reciprocal unit between a pair of birefringent Bragg reflectors, results in an exceptionally strong asymmetry in light transmission. Remarkably, such asymmetry persists regardless of the incident light polarization. This photonic architecture may be used as the building block for chip-scale non-reciprocal devices such as optical isolators and circulators.

1This research was supported by an AFOSR No. FA 9550-10-1-0433 grant and LIRIR 09RY04COR grant, and by an NSF ECCS-1128571 grant.

10:24AM M23.00013 Gyro-active structures: Unidirectional Reflectionless Isolators and Perfect Absorbers, JUNSIK LEE, Wesleyan University, ZIN LIN, Harvard University, HAMIDREZA RAMEZANI, TSAMPIKOS KOTTOS, Wesleyan University — We propose a novel circuit architecture that consists of gyrotropic elements sandwiched between two judiciously balanced gain and loss constituents. These structures exhibit unique transport characteristics stemming from a generalized parity-time ($PT$)-symmetry. Some of these features include unidirectional reflection-less isolation and perfect absorption as well as asymmetric Anderson localization when disorder is introduced. Realizations as well as applications within the framework of electronic and photonic circuitry are discussed.

1This research was partially supported by the AFOSR and NSF.

10:36AM M23.00014 Local heating of ZnO due to the surface plasmon excitation of Au nanoparticles, OSHADHA RANASINGHA, NETL, Pittsburgh / WVU, Morgantown, CONJUN WANG, NETL, Pittsburgh / URS, Pittsburgh, JAMES P. LEWIS, NETL, Pittsburgh / WVU, Morgantown, CHRISTOPHER MATRANGA, NETL, Pittsburgh — Temperature dependent $E_2$(high) Raman active optical phonon mode was investigated to identify the local heating of ZnO, due to the surface plasmon excitation of the Au nanoparticles. The variation of the linewidth (FWHM) of $E_2$(high) mode for ZnO was investigated from room temperature to 450 °C with 25 °C steps under constant 532 nm laser excitation intensity of $2.0 \times 10^7$ W/m$^2$. Linewidth (FWHM) was increased with the temperature and it was fitted into the theoretical model originally developed by Menendez et al, which contains both cubic and quadratic anharmonicities. After optimizing the cubic and quadratic anharmonic coupling constants, the fit was used to estimate the local temperatures of Au/ZnO, which were irradiated with different laser intensities. The estimated local temperature for Au/ZnO was 613 °C at the laser intensity of 8.1 $\times 10^7$ W/m$^2$. ZnO without Au nanoparticles didn’t show any large temperature variation under the different laser intensities. This is a clear evidence for the heat generation of Au nanoparticles due to the surface plasmon excitation.

1Authors acknowledge use of the WVU Shared Research Facilities.

Wednesday, March 20, 2013 8:00AM - 10:36AM — Session M28 DCMP: Liquid Crystals II 336 - Luz Martinez-Miranda, University of Maryland

8:00AM M28.00001 Stable nematic droplets with handles, JAYALAKSHMI VALLAMKONDU, EKAPOP PAIRAM, Georgia Institute of Technology, VINCENTZ KONING, Instituut-Lorentz Universiteit Leiden, BATES MARTIN, York University, VINCENZO VITELLI, Instituut-Lorentz Universiteit Leiden, ALBERTO FERNANDEZ-NIEVES, Georgia Institute of Technology — We use a simple method to generate nematic liquid crystal droplets with handles. The method relies on the viscous forces exerted by a flowing continuous phase above its yield stress over a liquid crystal which is extruded from an injection needle; the resultant jet is forced to close into a torus, due to the imposed rotation, and is stable against surface tension instabilities, due to the elasticity of the outer phase. We find that the ground state of these nematic liquid crystal toroidal droplets is defect free and exhibits twist, irrespective of the aspect ratio of the torus. By including the splay-splay contribution to the elastic free energy density, we find that this state indeed corresponds to the lowest energy state. For droplets with additional handles, we find there are two surface defects or boojums per additional handle.
8:12AM M28.00002 Nanosecond electrooptics of nematic liquid crystals: induced orientational order and quenching of director fluctuations. Volodymyr Borshch, Sergiu Shiyanovskii, Oleg Lavrentovich, Liquid Crystal Institute and Chemical Physics Interdisciplinary Program, Kent State University, Kent, 44240, OH — We demonstrate a fast (1-100 ns) electrooptic response of a thermotropic nematic liquid crystal in a geometry when a strong electric field (>{10^8 V/m}) does not realign the director and influences only the orientational order and the spectrum of director fluctuations.

8:24AM M28.00003 Impact of Photo-Induced Surface Adsorption of Azo-Dyes on the Liquid Crystal Anchoring Conditions. David Statman, Allegheny College — Using optical techniques, we measured the anchoring conditions of azo-dye doped nematic liquid crystals on rubbed polyimide surfaces. Linearly polarized light induces the formation of a second easy axis on the polymer surface oriented toward the polarization direction of the pump laser beam. This additional easy axis is the result of photo-induced adsorption of the cis isomer of the azo dye. An effective easy axis is the weighted average of the original easy axis and this new easy axis.

8:36AM M28.00004 Surface Nano patterning for aligning Chromonic liquid crystals. Jeong Yeon, Korea Advanced Institute of Science and Technology, Mohan Srinivasarao, Georgia Institute of Technology, Hye Taeg Jung, Korea Advanced Institute of Science and Technology — We present results on planar alignment of several Chromonic Liquid Crystals. We use a high aspect ratio nano pattern of electrically conducting ITO, which was fabricated by employing a new patterning technique that relies on a secondary sputtering phenomenon (SSP). This method is particularly useful in the case of aligning Chromonics which are considerably harder to align in comparison with conventional thermotropics. Berreman’s theory was employed to study the alignment of the Liquid Crystals as a function of the anchoring energy which depend on the dimension of the ITO patterns.

8:48AM M28.00005 Differential Dynamic Microscopy for measuring viscoelastic ratios of Chromonic Liquid Crystals. Karthik Nayani, Jung Ok Park, Mohan Srinivasarao, Georgia Institute of Technology — Differential Dynamic Microscopy (DDM) enables one to access the scattering information from a sample by Fourier analyzing the real space images obtained from a light microscope. Thermal fluctuations of the director about the mean position allows one to study the viscoelastic properties of the nematic. Normally such measurements of the viscoelastic constants require time consuming and sensitive light scattering experiments. DDM enables us to extract the same data just by analyzing a real space movie a few seconds long using a high speed camera. We present results of viscoelastic measurements of Chromonic liquid crystal Sunset yellow using DDM measurements.

9:00AM M28.00006 Phase and Topological Behavior of Lyotropic Chromonic Liquid Crystals in Double Emulsions. ZOEY S. DAVIDSON, JOONWOO JEONG, Department of Physics, University of Pennsylvania, FUQUAN TU, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, MATT LOHR, Department of Physics, University of Pennsylvania, DAeyeon Lee, Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Tom C. Lubensky, A.G. Yodh, Department of Physics, University of Pennsylvania — Lyotropic chromonic liquid crystals, assembled by non-covalent interactions, have fascinating temperature- and concentration-dependent phase behavior. Using water-oil-water double emulsions, we are able control the inner droplet chromonic phase concentration by osmosis through the oil phase. We then study the configurations of the chromonic liquid crystal phases in droplets by varying the oil types, oil soluble surfactants, and inner droplet diameter. We employ polarization microscopy to observe resulting nematic and columnar phases of Sunset Yellow FCF, and we deduce the liquid crystal configuration of both phases within the droplets. Simulations based on Jones matrices confirm droplet appearance, and preliminary observations of chromonic liquid crystal shells in oil-water-oil double emulsions are reported.

9:12AM M28.00007 Homeotropic alignment of the lyotropic chromonic liquid crystal Sunset Yellow FCF using pi-pi stacking chemical interactions. Joowoon Jeong, Ganghee Han, A.T. Charlie Johnson, Tom C. Lubensky, Peter J. Collins, A.G. Yodh, Department of Physics & Astronomy, University of Pennsylvania, Philadelphia, PA 19104, USA — We report on the homeotropic alignment of the lyotropic chromonic liquid crystal, Sunset Yellow FCF (SSY), using pi-pi stacking interactions between the SSY molecules and (1) thin parylene films or (2) a graphene monolayer. The nematic and columnar phases of SSY molecules arise via self-assembly in water into stacks through non-covalent attractions between the SSY molecules. Interestingly, we find that the same non-covalent interactions between SSY molecules and a parylene or graphene alignment layer lead to homeotropic anchoring of these stacks. The nematic phase of SSY is introduced between two glass substrates coated with parylene films or graphene monolayers, and homeotropic alignment of SSY is confirmed by polarized optical microscopy and conoscopic. Additionally, we observe and can explain the stripe domains that occur during cooling of the sample in this cell, and we consider possible novel applications for homeotopically aligned chromonic liquid crystals.

9:24AM M28.00008 Kinetics of Assembly and Dis-assembly of Structures Forming a Chromonic Liquid Crystal at Low Concentrations. Kenneth Nieser, Peter Collins, Department of Physics & Astronomy, Swarthmore College, Swarthmore, PA 19081 — The molecules of the near-IR absorbing dye IR-806 spontaneously assemble in water at very low concentrations, forming a chromonic liquid crystal phase at room temperature when the concentration is above 0.5 wt%. The assembly process proceeds in two steps and results in a complex structure that orientationally orders in a liquid crystal phase. The kinetics of the assembly and dis-assembly of these complex structures can be followed through absorption measurements by rapidly mixing the initial sample with either a small fraction of salt solution (assembly) or a large fraction of water (dis-assembly). The kinetics of dis-assembly is exponential while the kinetics of assembly is non-exponential, both with rate constants depending on the starting and ending conditions, but falling in the 0.1-1.0 s^-1 range. While past equilibrium absorption measurements on IR-806 offer evidence for a threshold concentration for the assembly of these complex structures, the kinetics experiments show with certainty the existence of such a threshold. Similar experiments on Benzopurpurin 4B, another dye that forms a chromonic liquid crystal at low concentrations, reveal kinetics that are slower by two orders of magnitude and a threshold concentration for the assembly of complex structures.

Acknowledgment is made to the donors of the American Chemical Society Petroleum Research Fund for partial support of this research.
9:36AM M28.00009 First energy power expansion for orientationally ordered phases: energy and entropy

SERGIU SHIYANOFSKII, Liquid Crystal Institute, Kent State University—we propose a new approach for description of orientation phase transitions that utilizes the following specific features of the orientational energy $E$ and entropy $S$: (a) $S$ possesses an additional symmetry in comparison with $E$, being invariant under rotation of the molecular frame; and (b) $E$ contributes only to the second order terms because the pair molecular interaction is dominant. The approach is based on minimization of the scaled orientational free energy $\bar{F} = F/T = E/T - S$ instead of $F$ because $\bar{F}$ obeys the standard assumption of the Landau theory that only the second order terms are temperature dependent. We apply the approach to build a model for nematic phases in materials with non-polar parallelepiped-type molecules with symmetry $D_{2h}$. The presented model introduces complex OPs, generalizes the Landau-de Gennes (LdG) theory and predicts the existence of a biaxial nematic phase for the forth order expansion of $F$.

1 This work was supported by DOE grant DE-FG02-06ER 46331

9:48AM M28.00010 Surface topography and rotational symmetry breaking

RAJIRATAN BASU, The US Naval Academy, IAN NEMITZ, Case Western Reserve University, QINGXOANG SONG, ROBERT LEMIEUX, Queen’s University, CHARLES ROESSLBLATT, Case Western Reserve University—The surface electrooptic effect, which is a rotation of the molecular director in the substrate plane proportional to an electric field applied normal to the substrate, requires both a chiral environment and $C_{2h}$ (or lower) rotational symmetry about the field. The two symmetries are created in tandem by manipulating the surface topology, a process that confines their effects. Here we use a pair of rubbed polymer-coated substrates in a twist geometry to obtain our main result, viz., that the strengths of two symmetries, in this case the rub-induced breaking of $C_{2h}$ rotational symmetry and chiral symmetry, can be separated and quantified. Experimentally we observe that the strength of the reduced rotational symmetry arising from the rub-induced scratches, which is proportional to the electrooptic response, scales linearly with the induced topographical rms roughness and increases with increasing rubbing strength of the polymer. Our results also suggest that the azimuthal anchoring strength coefficient is relatively insensitive to the strength of the rubbing.

10:00AM M28.00011 ABSTRACT HAS BEEN MOVED TO Q1.00123

10:12AM M28.00012 Probing Viscoelasticity of Cholesteric Liquid Crystals in a Twisting Cell

JOSEPH ANGELO, ALIREZA MOHEGHI, NICK DIOIO, ANTAL JAKLI, Liquid Crystal Institute—Viscoelastic properties of liquid crystals are typically studied either using Poiseuille flow, which can be produced by a pressure gradient in a capillary tube or Couette flow, which can be generated by a shear between concentric cylinders. We use a different method in which we twist the liquid crystal sandwiched between two cylindrical glass plates, one of which can rotate about its center, the other of which is fixed. When the cell is twisted, there is a force proportional to the twist angle and the twist elastic constant, and inversely proportional to the pitch and sample thickness, normal to the substrates due to the change in pitch in the cholesteric liquid crystal (CLC). Measuring this force on various CLCs with known pitch we could obtain the twist elastic constants. In addition to the equilibrium force, we observed a transient force during the rotation, which is related to the flow of the material, thus allowing us to determine the Leslie viscosity component $\eta_1$, which typically cannot be assessed by other methods. We expect this apparatus to be a useful tool to study the visco-elastic properties of liquid crystals.

1 The authors acknowledge support from NSF grant DMR-0907055.


10:24AM M28.00013 Chiral hierarchal self-assembly in Langmuir monolayers of diacetylenic lipids

1 ELIZABETH MANN, PRITAM MANDAL, PREM BASNET, DOMINIC MALCOLM, Department of Physics, Kent State University, SAHRAOUI CHAIEB, Physical Science and Engineering, KAUST, Thuwal, KSA—A Langmuir monolayer made of chiral lipid molecules forms a hierarchal structure when compressed in the intermediate temperature range below the chain melting temperature. These structures are captured via Brewster angle microscopy. When the liquid monolayer is compressed, an optically anisotropic condensed phase nucleates in the form of long, thin clays. These clays pack closely to form stripes. This appears to be a new mechanism for forming stripes within Langmuir monolayers. In lower temperature range these stripes arrange into spirals within overall circular domains, while near the chain melting transition the stripes arrange into target-structure. We attributed this transition to a change in boundary conditions at the core of the largest-scale circular domains.

1 P. M, P.B.B., D.W.M., and E.K.M. were partially supported by the National Science Foundation under grant number CBET-0730475; S.C. was funded by King Abdullah University of Science and Technology.

2 current: Department of Physics and Astronomy, University of Manitoba

3 current: Biomedical Engineering, University of Rochester

Wednesday, March 20, 2013 8:00AM - 11:00AM –
Session M30 DCMP: Self-Assembly: Janus and other Colloids 338 - Stefano Sacana, New York University

8:00AM M30.00001 Directed Self-Assembly of Colloidal Janus Matchsticks

KUNDAN CHAUDHARY, Harvard University, QIAN CHEN, JAIME JUAREZ, STEVE GRANICK, University of Illinois at Urbana-Champaign, JENNIFER LEWIS, Harvard University—The ability to assemble anisotropic colloidal building blocks into ordered configurations is scientifically and technologically important for developing new classes of soft materials. We are studying the fabrication and electric field driven assembly of end- and side-coated Janus rods. Specifically, we fabricate silica rods (L/D = 2.4) functionalized with hydrophobic gold (Au) patches using a multistep process involving electric field alignment and crystallization, microcontact printing, and selective metallization. In the absence of an applied electric field, the Janus matchsticks (end-coated rods) self-assemble into multi-pods (e.g., bi-, tri- and tetrapods) of varying coordination number and patch angle in aqueous solution. By contrast, both Janus matchsticks and side-coated Janus rods form complex chains in applied AC electric fields of varying magnitude and frequency, whose configurations vary significantly from those formed by pure silica rods.

8:12AM M30.00002 Theory of crystallization and orientational ordering of spherical Janus colloids

HOMIN SHIN, KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign—Amphiphilic Janus particles have two chemically distinct surfaces, one hydrophobic (attractive) and the other hydrophilic (repulsive), resulting in orientationally anisotropic interparticle interactions. In contrast to homogeneous spherical particles, broken rotational symmetry can result in more exotic crystals that possess distinct orientational patterns, and also plastic crystals. We study the rich phase behavior of Janus colloids using a self-consistent phonon theory that includes coupled translational and rotational entropic and enthalpic contributions to the free energy. Ground states are identified based on the compatibility between the patch geometry of particles (e.g., patch coverage, number, shape) and the lattice symmetry. The coupled self-consistent equations for translational and rotational localization parameters are then solved for a given crystal symmetry, thermodynamic state, and patch orientational order, and their stability determined. For two-dimensional diblock AB Janus crystals, we predict the phase sequence of stripes, modulated stripes (zig-zag), and plastic crystals (rotator phases), which depends sensitively on particle chemical composition and pressure. We also study triblock Janus colloids, including the possibility a Kagome lattice.
8:24AM M30.00003 Modeling of tunable structural re-configuration of Janus colloidal particles, DANIEL BELTRAN, RONALD LARSON, Chemical Engineering, University of Michigan, Ann Arbor — Colloidal particles can assemble into a myriad of structures by virtue of the many interaction forces available to them. Variable range attraction and repulsion and the recently explored non-isotropic character, exemplified by Janus particles, are examples of the versatility of colloidal particles as building blocks. A systematic approach to understand the assembly of Janus colloids, as a function of Janus balance and particle concentration is not yet available. In this work we study the phase behavior of Janus particles as a function of the strength of interaction, Janus balance and volume fraction of spherical particles. A secondary goal of this work is the assessment of re-configurability of the structures found. Our results show the range of stability of several structures, including a fluid phase of small clusters, bilayers and worm-like aggregates. We find the bilayer structures are very stable over a range of phase space and provide a good pre-cursor to hexagonally close-packed structures. These findings enable the understanding of the assembly process of Janus building blocks and provide a framework with which to study the kinetics of structure change.

1Work supported by U.S. Army Research Office under Grant Award No. W911NF-10-1-0518

8:36AM M30.00004 Janus Magnetic Rods, Ribbons, and Rings, JING YAN, KUNDAN CHAUDHARY, SUNG CHUL BAE, JENNIFER LEWIS, STEVE GRANICK, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign — Dipolar particles are fundamental building blocks in nature and technology but the roles of anisotropy are seldom explored in their assembly. Here, we fabricate colloidal silica rods coated on one hemicylinder with a thin magnetic layer to satisfy multiple criteria: nearly monodispersed, easily imaged, and magnetic interaction dominant over gravity. We confirm long-predicted features of dipolar assembly and stress the microstructural variety brought about by shape and chemical anisotropy, especially by borrowing knowledge learned from molecules. We describe analogies to liquid crystalline deformations with bend, splay and twist; an analogy to cis/trans isomerism in organic molecules, which in this system can be controllably and reversibly switched; and a field-switching methodology to direct single ribbons into not only single but also multiple rings that can subsequently undergo hierarchical self-assembly. Going beyond earlier investigations of phase behavior, we show that dynamic reconfigurability presents subtle materials issues and possibilities.

8:48AM M30.00005 Study of Aggregation of Janus Ellipsoids, DONOVAN RUTH, Lehigh University, WEI LI, University of California Santa Barbara, SHREeya KHADa, Colgate University, JEFFREY RICKMAN, JAMES GUNTON, Lehigh University — We perform numerical simulations of a quasi-square well potential model of one-patch colloidal particles to investigate the collective structure of a system of Janus ellipsoids. We show that for Janus ellipsoids such that one half is an attractive patch, while the entire ellipsoid has a hardcore repulsion, the system organizes into a distribution of orientationally ordered micelles and vesicles. We analyze the cluster distribution at several temperatures and low densities and show that below certain temperatures the system is populated by stable clusters and depending on temperature and density the system is populated by either vesicles or micelle structures.

9:00AM M30.00006 Amphiphilic Janus cylinders at fluid-fluid interfaces, DAEYEON LEE, BUM JUN PARK, University of Pennsylvania, CHANG-HYUNG CHOI, CHANG-SOO LEE, Chungnam National University — We study the configuration and assembly of amphiphilic Janus cylinders at fluid-fluid interfaces at the single- and two-particle levels using experimental and theoretical approaches. We observe that high aspect ratio Janus cylinders have two configurations – upright and tilted orientation, whereas Janus cylinders with small aspect ratios adopt only the upright orientation. These configurations are confirmed by numerically calculating and minimizing the attachment energy of each Janus cylinder as a function of the orientation angle as well as the vertical displacement with respect to the interface. Unlike homogenous cylinders which show deterministic assembly behaviours at fluid-fluid interfaces, Janus cylinders exhibit a variety of assembly behaviours. We show the origin of such a diversity stems from the attractive capillary interactions between tilted Janus cylinders, which could be explained by the quasi-quadrupolar interface deformation that is caused by the wetting of the fluids on the particle surface. We will also describe our recent results involving the configuration and interactions of asymmetrically hydrophilic cylinders at an air-water interface.

9:12AM M30.00007 Thermodynamically Stable Pickering Emulsions Stabilized by Janus Dumbbells, FUQUAN TU, BUM JUN PARK, DAEYEON LEE, University of Pennsylvania — Janus particles have two sides with different, often opposite, surface properties. Janus dumbbell is one type of Janus particles that consists of two partially fused spherical lobes. It is possible to independently control the geometry and surface wettability of Janus dumbbells. Janus dumbbells can also be produced in a large quantity, making them useful for practical applications such as emulsion stabilization. In this work, we calculate the free energy of emulsion formation using amphiphilic Janus dumbbells as solid surfactants. In contrast to kinetically stable emulsions stabilized by homogeneous particles, emulsion stabilized by Janus dumbbells can be thermodynamically stable. There also exists an optimal radius of droplets that can be stabilized by infinite or limited number of amphiphilic dumbbells in the continuous phase. We demonstrate that the optimal radius of dumbbell-stabilized droplets can be predicted based on the volume of the dispersed phase and the volume fraction of dumbbells in the continuous phase. We believe our calculation will provide guidelines for using Janus dumbbells as colloid surfactants to generate stable emulsions.

9:24AM M30.00008 Analytic Solutions and Numerical Simulation of Self-Assemble Magnetic Colloidal Structures, DAVID PIET, Northwesten University/Argonne National Laboratory, IGOR ARONSON, ALEX SNEZHKO, Argonne National Laboratory, ATHUR STRAUBE, Humboldt University of Berlin — Self-assembled magnetic colloidal structures that lie at a fluid-air interface can have a wide range of behavior, from localized axisymmetric star-like objects to linear, snake-like ones. Modeling these structures requires both the extensive use of the Navier-Stokes Equations from an analytic standpoint as well as the ability to numerically solve and simulate them alongside Newton’s Equations. Analytically, these equations are approximated by an asymptotic expansion with a small viscosity. Using those expressions, simulations are run on GPU’s to utilize their parallel capability. The result is a remarkable, qualitative recapturing of the experimentally observed behavior, namely, the formation of both snakes and stars from a randomized initial condition.

1Work supported by the U.S. DOE, Office of Science, under Contract No. DE-AC02-06CH11357.

9:36AM M30.00009 Dynamic phases in non-equilibrium magnetic colloids at liquid interfaces under in-plane magnetic field driving, ALEXEY SNEZHKO, Argonne National Laboratory, USA, GASPER KOKOT, Josef Stefan Institute, Ljubljana, Slovenia, DAVID PIET, Argonne National Laboratory, IGOR ARONSON, Argonne National Laboratory, USA — Ensembles of interacting colloidal particles subject to an external periodic forcing often develop nontrivial collective behavior. We study emergent phenomena in magnetic colloidal ensembles suspended at a liquid-air interface and driven out of equilibrium by alternating magnetic fields. We use ferromagnetic colloidal micro-particles (so the magnetic moment is fixed in each particle and interactions between colloids is highly anisotropic and directional) suspended over a water-air interface and energized by alternating magnetic fields applied in-plane of the interface. Experiments reveal new types of dynamic self-assembled phases (in particular, “wires,” “rotators”) emerging in such systems in a certain range of excitation parameters. Transition between different self-assembled phases with parameters of external driving magnetic field is observed. Molecular dynamic simulations capture some of the non-equilibrium self-assembled phases in our system.

2The research was supported by the U.S. DOE, Office of Basic Energy Sciences, Division of Materials Science and Engineering, under the Contract No. DE AC02-06CH11357.
Crystalline aggregates of magnetic colloidal particles 1. Joshua E.S. Socolar, Catherine C. Marcoux, Physics Department, Duke University, Durham, NC, Lin Fu, Patrick Charbonneau, Duke Chemistry, Y. E. Yellen, Duke Mechanical Engineering and Materials Science — A colloidal system of magnetic and non-magnetic spheres confined to a 2D monolayer has been found to form a variety of structures, including Kagome, honeycomb, and square lattices, as well as various chain and ring configurations [1]. In these experiments, the layer of beads is immersed in a ferrofluid and placed in an external magnetic field and the different structures are obtained for different values of the relative concentrations of the bead types, the susceptibility of the ferrofluid, and the angle of the field with respect to the assembly plane. We study an approximate model for the potential energy of the system based on self-consistent solutions for the magnetic moments of point dipoles. We find that the model accounts well for the period of the observed phases and the stability of the excitations, possibly stable states for structures with up to ten atoms per unit cell. Further calculations suggest the possibility of creating materials with strong elastic responses to applied magnetic fields.


This work was supported by the NSF’s Research Triangle MRSEC (DMR-1121107).

Using chaotic Faraday waves to create a two-dimensional pseudo-thermal bath for floating particles with tunable interaction potentials, Kyle Welch, Isaac Hasting-Hauss, Raghuveer Parthasarathy, Eric Corwin, Materials Science Institute and Department of Physics, University of Oregon — Whether chaos in actively driven systems can be described by an effective temperature is an unresolved question in the study of nonlinear physics. We use chaotic Faraday waves to create a two-dimensional pseudo-thermal bath to investigate tunable interactions between floating particles. By vertically oscillating a liquid with an acceleration greater than g we excite the Faraday instability and create surface waves. Increasing this acceleration above some critical value causes this instability to become chaotic with fluctuations over a broad range of length scales. Particles placed on the surface are buffeted by random excitations in analogy to Brownian motion. We can change the “temperature” of the pseudo-thermal bath by manipulating the driving frequency and amplitude, a feature of the system we verify using real-time tracking to follow the diffusive movement of a single particle. With an eye toward creating complex self-assembling systems we use this system to measure the tunable interaction potential in two-, three-, and many-particle systems and to probe the effects of particle size, shape, symmetry, and wetting properties.

Twisted results on interior packing and surface energy for filament bundles, Isaac Bruss, Gregory Grason, University of Massachusetts Amherst — Twisted filament bundles are a common structural motif found in both natural and synthetic systems. Examples range from protein assemblies such as collagen and fibrin, to artificial structures such as carbon nanotube ropes and microfabricated materials. They are oftentimes found to self-assemble from fibers via various adhesive interactions, be they depletion, capillary, or other such forces. In these assemblies, twist frustrates the perfect crystalline order of the fibers, requiring the presence of defects in the packing. Through numerical simulations, we discover defect organizations ranging from dislocations and grain boundaries for low twist, to multi-five-fold disclination clusters for high twist. And furthermore, by developing and employing an analytical continuum model, we find that for sufficiently long fibers, twist reduces the surface energy of the assembly. Together, this suggests that the equilibrium lowest energy state of a filament bundle may be twisted regardless of any intrinsic chirality present in the system.

10:36AM 30.0014 Kinetics of Phase Separation in Binary Mixtures, Shaista Ahmad, Department of Chemical Engineering, Pennsylvania State University, University Park, PA - 16802, Subir K. Das, Theoretical Sciences Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Jakkur, Bangalore - 560064, India, Sanjay Puri, School of Physical Sciences, Jawaharlal Nehru University, New Delhi - 110067, India — We present numerical simulation results of the phase separation kinetics in three-dimensional symmetric binary fluid mixtures and binary solid mixtures. In the former system, our extensive molecular dynamics simulation is able to probe an extended period where the domain size grows linearly with time, leading to an unambiguous confirmation of the viscous hydrodynamic regime. On the other hand, for the binary solid mixture, we use Monte Carlo simulation with spin-exchange dynamics to verify the Lifshitz-Slyozov growth law. Despite the differences in the growth mechanisms, the pair correlation functions and structure factors of the two systems overlap, indicating similarity in the morphologies during phase separation.

10:48AM 30.0015 Cooperative Symmetry Breaking from One to Three Dimensions in Multi-Component Double Emulsions, Laura Adams, Physics Department and SEAS Harvard University, Jacy Bird, Mechanical Engineering Department, Boston University, Jiawei Yang, SEAS Harvard University, Thomas Franke, Microfluidic Group, EPI, Universität Augsburg, Universitätstrasse 1, Augsburg, Germany and Harvard University, Vinothan Manoharan, David Weitz, Physics Department and SEAS Harvard University — We follow the evolution of aqueous inner drops confined in a thin sheath of oil in the dimensional crossover from one to three dimensions using a fast camera and microfluidics. Surprisingly, inner drops interact cooperatively to pair with their next nearest neighbor to transform their linear configuration into a three-dimensional composite sphere. The measured time scales of transforming these multi-component double emulsions are investigated as a function of number, size, and composition of inner drops. We model the dynamics to understand and predict how both folding and buckling occur in these complex microfluidic systems.
8:12AM M36.00002 Nonlocal transport in superconducting oxide nanostructures1, JOSHUA VEAEZY, GUANGLEI CHENG, SHICHEMEN LIM, MICHELLE TOMCZYK, PATRICK IRVIN, MENGCHEN HUANG, University of Pittsburgh, CHUNG WUNG BARK, SANGWOO RYU, CHANG-BEOM EOM, University of Wisconsin-Madison, JEREMY LEVY, University of Pittsburgh — We report nonlocal transport signatures in the superconducting state of nanostructures formed at the LaAlO	extsubscript{3}/SrTiO	extsubscript{3} interface using conductive AFM lithography. Nonlocal resistances (nonlocal voltage divided by current) are as large as 200 $\Omega$ when 10 $\mu$m separate the current-carrying segments from the voltage-sensing leads. The nonlocal resistance reverses sign at the local critical current of the superconducting state. Features observed in the nonlocal V-I curves evolve with back gate voltage and magnetic field, and are correlated with the local four-terminal V-I curves. We discuss how nonlocal and local transport effects in LaAlO$_3$/SrTiO$_3$ nanostructures may result from the electronic phase separation and superconducting inhomogeneity reported by others in planar structures.$^1$

$^1$This work is supported by AFOSR (FA9550-10-1-0524) and NSF DMR-0906443


8:24AM M36.00003 Superconductivity in Centimeter Length Indium-Gallium Nanowires1, WEIWEI ZHAO, JESSE BISCHOF, MEENAKSHI SINGH, THOMAS FITZGIBBONS, XIN LIU, CHAOXING LIU, The Pennsylvania State University, LIN WANG, HPsync, Carnegie Institution of Washington, ZHONGHOU CAI, SI CHEN, Advanced Photon Source, Argonne National Laboratory, JOHN HAYES, PIER SAZIO, Optoelectronics Research Centre, University of Southampton, United Kingdom, JOHN BADDING, MOSES CHAN, The Pennsylvania State University — In-doped Ga nanowires 150 nm in diameter and 6mm in length have been formed in silica nanocapillaries. X-ray fluorescence and diffraction measurements performed at the Advanced Photon Source have been used to characterize their chemical composition and crystal structure. Investigation of the low temperature transport properties of these wires reveals a two stage superconducting transition. Magnetoresistance measurements are suggestive of vortex trapping in the wire. The X-ray fluorescence measurements suggest phase separation in the capillaries into Ga nanodroplets and In-Ga eutectic wires. A model to explain the vortex trapping consistent with this observation is being developed.

$^1$This work is supported by the Penn State Materials Research Science and Engineering Center, funded by the National Science Foundation (DMR 0820404). TF and LW are supported by the Energy Frontier Research Center (DE-0001057), DOE.

8:36AM M36.00004 Investigating long-range proximity effect in ferromagnetic Ni and Ni-Fe nanowires1, MEENAKSHI SINGH, JAMES KALLY, WEIWEI ZHAO, MOSES CHAN, Pennsylvania State University — Singlet superconductors and ferromagnets entail incompatible spin orders severely limiting the range of the superconducting proximity effect in a ferromagnet (~1 nm). Contrary to this expectation, a very long-range proximity effect (LRPE, ~ 600 nm) was found in crystalline ferromagnetic nanowires [Wang et al., Nat. Phys. 6, 389 (2010)]. Several mechanisms have been suggested to explain the LRPE, the most intriguing of which is the possibility of triplet superconductivity in the ferromagnet. We have conducted experiments to probe the mechanism of the LRPE. The LRPE persists in granular Ni nanowires, ruling out ballistic transport as a possible mechanism. Surface superconductivity in the oxide layer on the ferromagnetic nanowire is also ruled out based on critical current measurements. On changing the nature of the contacting electrodes, the range of the proximity effect is found to diminish significantly. This indicates that the nature of the interface between the superconductor and the ferromagnet is important as expected for triplet superconductivity. Tunneling measurements probing the superconducting gap in the ferromagnetic nanowire are underway.

$^1$This work is supported by the National Science Foundation (DMR 0820404).

8:48AM M36.00005 Critical current oscillations in superconducting Al strips1, TYLER MORGAN-WALL, BENJAMIN LEITH, NIKOLAUS HARTMAN, ATIKUR RAHMAN, NINA MARKOVIC, Johns Hopkins University — We have studied current-voltage characteristics as a function of temperature and magnetic field in superconducting aluminum strips with varying lengths and cross sections. We find that the critical current oscillates as a function of magnetic field and suggest that the effect depends on the relative energies of vortex configurations in the strips in different transport regimes.

$^1$This work was supported in part by National Science Foundation under DMR-1106167.

9:00AM M36.00006 Ultralow Noise Microwave Amplifier Based on the Superconducting Low-inductance Undulatory Galvanometer, SHAOJIAN ZHU, DAVID HOVER, GUILHEM RIBEILL, ROBERT MCDERMOTT, University of Wisconsin, Madison — We have developed an ultralow noise microwave linear amplifier based on the Superconducting Low-inductance Undulatory Galvanometer (SLUG). The compact SLUG element is straightforward to model at microwave frequencies, allowing separate optimization of the SLUG element and the resonant input matching network. SLUG amplifiers incorporating high-Jc junctions have shown gains of order 15 dB in the frequency range from 3-10 GHz with instantaneous bandwidth up to several hundred MHz. Large-volume normal metal cooling fins have been integrated into the SLUG element to promote thermalization of hot electrons in the resistive shunts at millikelvin temperatures, and the amplifiers have achieved added system noise of one photon in the GHz frequency range. We discuss application of the SLUG amplifier to single shot dispersive readout of the transmon qubit.

9:12AM M36.00007 Flux noise in SQUIDs: Effects of deposited surface films1, S.R. O’KELLEY, S.M. ANTON, J.S. BIRENBACH, JOHN CLARKE, UC Berkeley, G.E. HILTON, H.-M. CHO, K.D. IRVIN, NIST Boulder, C.D. NUGROHO, A.F. DOVE, G.A. OLSON, Z.R. YOSCOVITS, V. ORLYANCHIK, D.J. VAN HARLINGEN, J.N. ECKSTEIN, University of Illinois at Urbana-Champaign — Magnetic flux noise in SQUIDs and superconducting qubits with a spectral density $S_{\Phi}(f)$ scaling as $1/(f^{1/2} Hz)^{\alpha}$ is understood to arise from the random reversal of spins localized at the surface of the superconducting film. We present experimental results showing the effects on $S_{\Phi}(f)$ of Au, SiN$_x$, NbN, and AlO$_3$ films deposited on the upper surface of Nb and NbN dc SQUID loops. For each measurement, we fabricated six identical SQUIDs on a single chip and then copped the surface of either half or all of the SQUID loops. Certain capping layers, such as Au, had no discernible effect on $S_{\Phi}(f)$ with regard to the magnitude, slope $\alpha$, and temperature dependence. On the other hand, some capping layers significantly reduced $S_{\Phi}(1Hz)$—by a factor of about two in the case of SiN$_x$. Furthermore, some layers significantly affected the value of $\alpha$ and the temperature dependence of both $S_{\Phi}(1Hz)$ and $\alpha$. These results further establish the importance of the role of the surface of the SQUID loop on its flux noise. We discuss implications for microscopic models of flux noise in light of these measurements.

$^1$This work was supported by ARO and IARPA
9:24AM M36.00008 Geometry and temperature dependence of low-frequency flux noise in dc SQUIDs. S.M. ANTON, J.S. BIRENBAUM, S.R. O’KELLEY, UC Berkeley, D.S. GOLUBEV, G.C. HILTON, H.-M. CHO, K.D. IRWIN, NIST Boulder, V. BOLKHOVSKY, R.A. BRAJE, G. FITCH, M. NEELEY, R.C. JOHNSON, W.D. OLIVER, MIT Lincoln Laboratory, F.C. WELLSTOOD, Univ of Maryland. JOHN CLARKE, UC Berkeley — Measurements on dc SQUIDs reveal a flux noise spectral density $S_\Phi(f) = A^2 ((f/1Hz)^\alpha$. An analytic model assuming non-interacting spins localized at the surface of the SQUID loop predicts that the mean square noise scales as $R/W$ — the radius and width of the loop, respectively. However, there are no established theories for the scaling of $\alpha$ with geometry or the dependences of $A$ and $\alpha$ on temperature $T$. To test the predicted geometric scaling of this model experimentally, we measured flux noise in ten SQUIDs with systematically varying geometries. We find that, at fixed $T$, $A^2$ scales approximately as $R$. From the measured values of $A$ and $\alpha$, we estimate the mean square flux noise, which does not scale with $R$. As $T$ is lowered, $\alpha$ increases significantly and in such a way that the spectra “pivot” about an approximately fixed frequency. This phenomenon implies that the mean square noise is temperature-dependent, an effect not predicted by the analytic model. We discuss our attempts to reconcile these discrepancies by considering the locking together of spins to form clusters.

3This work was supported by ARO, IARPA, and the US Government.

9:36AM M36.00009 Niobium Nitride Thin Films and Multilayers for Superconducting Radio Frequency Cavities. WILLIAM ROACH, The College of William and Mary, Department of Applied Science, DOUGLAS BERINGER, ZHAOZHU LI, The College of William and Mary, Department of Physics, CESAR CLAVERO, Lawrence Berkeley National Laboratory, ROSA LUKASZEW, The College of William and Mary, Department of Physics — Niobium nitride in thin film form has been considered for a number of applications including multi-layered coatings onto superconducting radio frequency cavities which have been proposed to overcome the fundamental accelerating gradient limit of ~50 MV/m in niobium based accelerators [1]. In order to fulfill the latter application, the selected superconductor’s thermodynamic critical field, $H_C$, must be larger than that of niobium and separated from the Nb surface by an insulating layer in order to shield the Nb cavity from field penetration and thus allow higher field gradients. Thus, for the successful implementation of such multilayered stack it is important to consider not just the materials inherent properties but also how these properties may be affected in thin film geometry and also by the specific deposition techniques used. Here, we show the results of our correlated study of structure and superconducting properties in niobium nitride thin films and discuss the shielding exhibited in NbN/MgO/Nb multilayer samples beyond the lower critical field of Nb for the first time.


9:48AM M36.00010 Induced superconducting FFLO states in patterned island systems and in topological insulators. SMITHA VISHVESHWARA, QINGLEI MENG, TAYLOR HUGHES, NADYA MASON, University of Illinois at Urbana-Champaign — We explore the possibility of inducing an exclusive Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting phase in 2D metal films by means of proximity coupling to patterned superconducting islands. We show that as a function of externally applied magnetic field, such a system not only renders the phase stable for a large region of parameter space but can also be tuned through different spatial ordering wavevectors associated with the FFLO order. We generalize these results to the surface states of 3D topological insulators and metallic surface states with Rashba coupling. We find that these FFLO states can be mapped into BCS states in which a uniform superconductor gap occurs in momentum space and can potentially be accessed in physical systems with relative ease.

10:00AM M36.00011 Evidence for synchronized Andreev reflections in NSN devices. MARTIN P. STEHNO, DALE J. VAN HARLINGEN, University of Illinois at Urbana-Champaign — In mesoscopic NSN devices, in which a short superconducting region separates two metallic electrodes, the Andreev reflection process may delocalize and couple electron- and hole-states on opposite sides of the superconductor. In addition to such nonlocal (or crossed) Andreev reflections, quasiparticles may also tunnel directly between the electrodes. We have studied nonlocal transport and current correlations in Cu/Al/Cu structures. We observe that the current correlations are symmetric in applied bias and show local minima when the applied voltages at the two contacts are equal in magnitude. This behavior matches theoretical predictions for devices with intermediate interface transparency in which the nonlocal exchange of quasiparticles triggers additional synchronized Andreev reflection events at the two interfaces.

1Work supported by the National Science Foundation grant DMR 06-05813

10:12AM M36.00012 Josephson current and density of states in proximity circuits with s+-superconductors. STANISLAV APOSTOLOV, ALEX LEVCHENKO, Michigan State University — We study the emergent proximity effect in mesoscopic circuits which involve conventional superconductor and unconventional pnictide superconductor separated by a diffusive normal or ferromagnetic wire. The focus is placed on revealing signatures of the proposed $s^+-$ state of pnictides from the proximity-induced density of states and Josephson current. We find analytically a universal result for the density of states which exhibits both a Thouless gap at low energies, and peculiar features near the superconducting gap edges at higher energies. The latter may be used to discriminate between $s^+$ and $s^+$ symmetry scenarios in scanning tunneling spectroscopy experiments. We also calculate Josephson current-phase relationships for different junction configurations, which are found to display robust $0-\pi$ transitions for a wide range of parameters.

10:24AM M36.00013 Results of Switching Measurements in MgB$_2$ Josephson Heterojunctions: Search for Multiple Tunneling Channels and Leggett-Mode Signatures. STEVE CARABELLO, JOSEPH LAMBERT, Drexel University, DANIEL CUNNANE, Temple University, WENQING DAI, Penn State University, KE CHEN, Temple University, Qi LI, Penn State University, X. X. XI, Temple University, ROBERTO RAMOS, Indiana Wesleyan University — Josephson tunnel junctions made of multi-gap and single-gap superconducting electrodes provide a useful system for understanding multiple gap superconductivity. Peaks in the differential conductance curve have been used to characterize the energy gaps of such multi-gap materials [e.g. Chen, K. et al., Nat. Commun. 3:619 (2012)]. Superconducting-to-normal switching data can also provide useful insights. While ramping the current from zero to the critical current, the washboard potential is tilted, thereby adjusting the resonant frequency of the potential well, and altering the energy level spacing. By exciting the junction with microwaves, resonant modes may be explored. We report results of conductance and switching experiments on MgB$_2$/Pb and MgB$_2$/Sn junctions, with and without microwaves, in a helium dilution refrigerator with a base temperature 20mK. These results exhibit tunneling modes and resonances not observed in single-gap/single-gap junctions, including a peak in the escape rate that may be consistent with coupling to the Leggett mode.

10:36AM M36.00014 Search for Multiple Tunneling Channels and Leggett-Mode Signatures in MgB$_2$ Josephson Heterojunctions. STEVE CARABELLO, JOSEPH LAMBERT, Drexel University, DANIEL CUNNANE, Temple University, WENQING DAI, Penn State University, KE CHEN, Temple University, Qi LI, Penn State University, X. X. XI, Temple University, ROBERTO RAMOS, Indiana Wesleyan University — Josephson tunnel junctions made of multi-gap and single-gap superconducting electrodes provide a useful system for understanding multiple gap superconductivity. Peaks in the differential conductance curve have been used to characterize the energy gaps of such multi-gap materials [e.g. Chen, K. et al., Nat. Commun. 3:619 (2012)]. Superconducting-to-normal switching data can also provide useful insights. While ramping the current from zero to the critical current, the washboard potential is tilted, thereby adjusting the resonant frequency of the potential well, and altering the energy level spacing. By exciting the junction with microwaves, resonant modes may be explored. We report results of conductance and switching experiments on MgB$_2$/Pb and MgB$_2$/Sn junctions, with and without microwaves, in a helium dilution refrigerator with a base temperature 20mK. These results exhibit tunneling modes and resonances not observed in single-gap/single-gap junctions, including a peak in the escape rate that may be consistent with coupling to the Leggett mode.
10:36AM M36.00014 Evidence for Multi-photon transitions between energy levels in a large Current-Biased Magnesium Diboride Josephson Heterojunction. ROBERTO RAMOS, Indiana Wesleyan University, STEVEN CARABELLO, JOSEPH LAMBERT, Drexel University, DANIEL CUNNANE, Temple University, WENQING DAI, The Penn State University, KE CHEN, Temple University, QI LI, The Penn State University, XIAOXING XI, Temple University — When photons are strongly coupled to a quantum system, multiphoton transitions can be observed between two energy levels when the quantum energy of the exciting radiation, multiplied by an integer, matches the level spacing. This phenomenon can be observed in Josephson junction qubits exposed to weak microwave radiation at very low temperatures. At microwave resonance, the transition probability of a junction from superconducting to normal state is enhanced and these are used to map multiphoton transitions. We report observation of single- and multi-photon transitions between ground and first excited states in current-biased MgB2 thin film junctions by applying RF with frequencies between 0.5 and 3 Ghz. These large (up to 0.2mm x 0.3 mm) junctions consist of an MgB2 electrode insulated by native oxide from a lead (Pb) or tin (Sn) counter-electrode, and have areas at least 600 times bigger than Nb junctions previously shown to exhibit multiphoton transitions. The data is consistent with theoretical models of junctions behaving in the quantum limit and show anharmonicity of the junction potential when biased near the critical current.

10:48AM M36.00015 In-gap States of Josephson Junction with Two-gap Superconductors. JU KIM, LADAN BAHRAINIRAD, University of North Dakota — We investigate the transport property of SIS junctions with two-gap superconductors. The effects of two superconducting condenses on critical current density is estimated by studying the microscopic structure of Josephson current density in a dual-mode tunnel junction with a narrow quasi-classical tunnel barrier. Following the suggestion by Golubov and coworkers [1], we use two Bloch functions to describe the condenses in the two-band superconductors. In this junction, the in-gap states which include the interband interference effect appear at the interfaces due to the discontinuity of the superconducting phase. Also, similar to a Josephson junction [2] involving one-gap and two-gap superconductors, novel broken time-reversal symmetry states are found. We estimate the effects of interband interference and broken time-reversal symmetry on the in-gap bound states and critical Josephson current density.


Wednesday, March 20, 2013 8:00AM - 10:48AM — Session M40 DCMP: Surfaces, Interfaces, and Thin Film Reactions: Kinetics & Dynamics 349
- Brad Conrad, Appalachian State University

8:00AM M40.00001 Effects of Plasmon Excitation on Photocatalytic Activity of Ag/TiO2 and Au/TiO2 nanocomposites1, DINKO CHAKAROV, RAJA SELLAPPAN, Chalmers University of Technology, NISFD TEAM — Model composite photocatalysts consisting of undoped TiO2 films and optically active Ag or Au nanoparticles (NP) were prepared and examined in order to address the role of plasmon excitation in their performance. The particles were either in direct contact or isolated by thin SiO2 layer from TiO2. We found, as measured for the reactions of methanol and ethylene oxidation in two different photoelectrodes, that composites show always enhanced (up to x100) activity compared to pure TiO2. Interfacial charge transfer between TiO2 and NPs plays major role for the enhancement. Plasmonic near-, far-field and thermal effects are present but do not dominate.

1This work has been partly supported by Nordic Energy Research, project 52-NISFD.

8:12AM M40.00002 In-situ coherent x-ray scattering from Ag (001) and Ag (111) surfaces in vacuum and gas-phase environments1, ROBERT KARL, JR., Rochester Institute of Technology, ANDI BARBOUT, Argonne National Laboratory, VLADIMIR KOMANICKY, Safarik University, CHENHUI ZHU, Rochester Institute of Technology, DANIEL HENNESSY, University of Cincinnati Blue Ash, HOYDOO YOU, Argonne National Laboratory, MICHAEL S. PIERCE, Rochester Institute of Technology — We have been able to obtain X-ray photon correlation spectroscopy (XPCS) quality data from the Ag (001) and Ag (111) surfaces at two different locations along the specular scattering rod. We observe dynamic behavior related to temperature and gas-phase composition. We will present the methods of the XPCS analysis routines, as they have been adapted to this specific system, and the preliminary results for the dynamics, such as step edge motion, island growth, and surface phase transitions, of the Ag surface features in these different conditions. These dynamics are also q dependent and vary from slow at low q, to faster dynamics at positions near the Ag (001) anti-Bragg scattering position where the experimental sensitivity is sufficient to detect changes at a monolayer level. This indicates that the dynamics involved are occurring right at the surface and do not involve multiple layers. These results will then be compared to our recent similar measurements on the Au (001) surface [1].


1The work at Safarik University was supported by Slovak grant VEGA 1/0782/12

8:24AM M40.00003 Inhibition of Hydrogen Absorption in Pd by the Formation of a Pd-Ru Surface Alloy1, A.L. CABRERA, P. FERRARI, S. ROJAS, DONOVAN E. DIAZ-DROGUETT, E. RAMOS-MOORE, Pontificia Universidad Catolica de Chile, Departamento de Fisica, LABORATORIO CIENCIA DE MATERIALES TEAM — Hydrogen absorption by palladium has been studied for decades due to the significant importance in a number of applications like production and storage of hydrogen and hydrogen sensors. An increase of the amount of Ru on Pd drastically reduces the absorption properties of the Pd. The fcc crystal structure is preserved but the lattice constant is reduced slightly. In order to understand this phenomenon, we used three samples: a Pd foil, a Pd-Ru(4%) alloy foil, and a Pd foil with a Pd-Ru surface alloy. The surface alloy was made evaporating 8 nm of Ru using an e-beam evaporation technique on top of Pd, followed with a heating the sample up to 700 °C in a high vacuum system. We studied the changes in absorption properties of these samples using Thermal Program Desorption (TPD), resistance changes and grazing incidence X-ray Diffraction (GID).

1Funds from VRI-Puente 10/2012
8:36AM M40.00004 Pd/Ru surface alloys – Creating a “noble” surface from reactive elements. XIANGSHI YIN, MUSTAFA M. ÖZER, HANNO H. WEITERING, The University of Tennessee, Knoxville, TN & Oak Ridge National Laboratory, Oak Ridge, TN. We have studied the growth and reactivity of ruthenium thin films on palladium (111) substrates. To obtain smooth and well-ordered films, the surfaces were annealed to 600 °C. The surface structure, morphology, and chemical composition were investigated with LEED, STM, and AES. The experiments showed that annealed Ru film surfaces contain large concentrations of Pd. The reactivity of this alloy surface towards oxygen was then studied in oxygen gas adsorption experiments at room temperature, and compared to the oxidative properties of bulk Ru and bulk Pd. The surface alloy of the film turns out to be quite inert to oxygen adsorption at room temperature. STM experiments of oxygen adsorption at 112 K reveal that oxygen does adsorb at low temperature but it readily desorbs above 200 K. This surprise finding of a “noble” Pd/Ru surface alloy provides an interesting contrast to the surfaces of bulk ruthenium and palladium, which oxidize easily at room temperature. Research supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division

8:48AM M40.00005 Solid-State Diffusion Mixing in Cu Core/Ni Shell Nanoparticles. KARL UNRUH, BRIAN KELLY, JOHN KLODINICKI, University of Delaware, GERALD POIRIER, Princeton University — Cu core/Ni shell nanoparticles have been prepared in a polyol process using ethylene glycol as the solvent. The reaction of Cu and Ni acetate as the metal sources. The more positive reduction potential of Cu(II) relative to Ni(II) lead to the formation of Cu core/Ni shell nanoparticles. The structural evolution of these core/shell nanoparticle couples was studied by high temperature x-ray diffraction measurements. Between room temperature and 350 °C, the evolution in the diffraction pattern was only due to lattice expansion. At higher temperatures, the elemental Cu and Ni diffraction peaks began to merge until, at a temperature of 600 °C only a single set of diffraction peaks remained, indicating the formation of a single homogeneous Cu-Ni alloy. These diffraction patterns have been decomposed into a set of 11 individual subpeaks corresponding to 9 intermediate Cu-Ni compositions in addition to subpeaks corresponding to pure Cu and Ni. The angular positions of each subpeak were fixed to the values appropriate for their composition and the best fit peak areas determined. These data were then used to reconstruct the radial composition profiles of the diffusion couples as a function of the reaction temperature and time.

9:00AM M40.00006 Investigation of Fe/CuO Interface by X-ray Photoelectron Spectroscopy2. A. CHOURASIA, R.L. MILLER, H. DONG, J.L. EDMONDSON, Texas A&M University-Commerce — The Fe/CuO interfaces have been investigated by x-ray photoelectron spectroscopy. Thin films of iron were deposited on copper oxide substrates at room temperature. The spectral data show considerable reactivity at the interfaces. The spectral data have been compared with those of the oxidized iron and confirms the formation of the iron oxide at the interface. The interface is found to consist of a mixture of iron oxide and elemental copper. Presence of unreacted iron near the interface has been observed for thickness equal to or greater than 0.9 nm of the iron overlay. The interface was also prepared by depositing 2.0 nm of iron on the copper oxide substrate under two different conditions. In one, the substrate temperature was kept constant during the deposition of the iron overlay. In the other, post deposition annealing of the sample was performed. The iron overlay was observed to be completely oxidized at the sample temperatures of 450 °C and the oxidation is independent of the processing conditions. The amount of elemental iron and iron oxide in the samples has been estimated by modeling the spectrum using the spectra of elemental iron and pure iron oxide. The investigation provides a new method of preparing sub-nano-oxide films of iron.

9:12AM M40.00007 Coherent X-ray Scattering Experiments of Pt (001) Surface Dynamics near Roughening Transition. HOYDOO YOU, Argonne National Laboratory, MICHAEL PIERCE, Rochester Institute of Technology, ANDI BARBOUR, VLADIMIR KOMANICKY, DANIEL HENNESSY, Argonne National Laboratory — We will present the results of a series of coherent x-ray scattering experiments from Pt (001) in high vacuum. The resulting speckled diffraction patterns are analyzed with x-ray photon correlation spectroscopy. We find that the hexagonally reconstructed Pt (001) surface exhibits orientational dynamics below 1640 K and a critical behavior as T increases to $T_R = 1834$ K, near the roughening transition as proposed by Abernathy, et al. [Phys. Rev. Lett. 69, 941 (1992)]. The inverse autocorrelation time constant $\tau^{-1}$ of the surface diverges as $T$ approaches $T_R$. The average integrated intensity remains constant below $T_R$ but drops suddenly over a narrow temperature range, indicating abrupt lifting of the hexagonal reconstruction with the roughening transition. This behavior is compared to that of Au (001), for which $\tau^{-1}$ approaches a finite value as the reconstruction lifts gradually over a wide temperature range.

9:24AM M40.00008 A DFT Study of the Interaction of Monometallic Pd$_n$/Pt$_n$ (n=1, 9) Clusters with γ-Al$_2$O$_3$(100) Surfaces. NALIN FERNANDO, New Mexico State University, Las Cruces, TYNE JOHNS, University of New Mexico, Albuquerque, YUE CHI, CHANG KIM, General Motors Global R&D, Warren, MI, ABHAYA D. DADY, University of New Mexico, Albuquerque, BORIS KLECHER, New Mexico State University, Las Cruces, COLLABORATION, UNIVERSITY OF NEW MEXICO, ALBUQUERQUE COLLABORATION, GENERAL MOTORS GLOBAL R&D, WARREN, MI COLLABORATION — The reduction of carbon monoxide and hydrocarbon emissions in advanced low temperature combustion engines has become more difficult for the advanced combustion systems in transportation sector. Exploration of effect of interface formation on the electronic properties of the existing platinum group metals may provide insight for the new material development that rivals platinum. In order to address the effects of the interface on the electronic properties of small Pd$_n$ and Pt$_n$ clusters (n=1–9) with γ-Al$_2$O$_3$(100) support we have performed density-functional-theory (DFT) computations. The preliminary results suggest that the most favorable Pd$_n$ binding geometry is characterized by four Pd atoms binding to both Al and O surface atoms. The average Pd-O bond length across the interface is ~2.2 Å, corroborating the formation of bonds. The preliminary analysis of the electronic density of states shows that the main electronic modifications occur at the Fermi energy, leading to an overall metallic behavior. We will discuss cluster size effects on the character of bonding across the interface, its stability, and electronic structure.

9:36AM M40.00009 Dynamics of tungsten and cobalt carbonyls on silica surfaces. KALIAPPAN MUTHUKUMAR, ROSER VALENTI, HARALD O. JESCHKE, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Metal carbonyl species adsorbed on a substrate are the starting point for the electron beam induced deposition of metallic nanostructures. We employ full-dimensional atomistic simulations to investigate the dynamics of tungsten hexacarbonyl and pentacarbonyl as well as cobalt octacarbonyl precursor molecules on fully and partially hydroxylated silica substrates. We find that physisorbed carbonyls are quite mobile on a silica surface saturated with hydroxy groups, moving around half an Angstrom per picosecond. In contrast, chemisorbed ions like W(CO)$^-$ or Co(CO)$_3$$^-$$^-$ are more stable at room temperature. We determine the vibrational spectra which can provide signatures for experimentally distinguishing the form in which precursors cover a substrate.

9:48AM M40.00010 Effects of biaxial strain on diffusivity of low index tungsten surfaces. ZHENGZHENG CHEN, NASR GHONIEM, Mechanical & Aerospace Engineering Department, University of California Los Angeles — Detailed knowledge of diffusion behaviors is necessary toward fully understanding of damage of tungsten serving as reactor pressure vessels. Using first-principles calculations, we observed different diffusion scenarios on W(001) and W(110) surfaces with external biaxial strains. Hopping is the major diffusion mechanism on the W(110) surface under all kinds of loadings in the present work. On the other hand, the main mechanism on W(001) surface transfers between the atom hopping and the formation and movement of surface crowdings depending on biaxial strains. Our results also indicate high mobile and strong anisotropy of surface crowdings on both surfaces. The microscopic explanation is presented by analyzing the charge density. We have built up the diagram of diffusion on the W(001) surface. This diagram presents that not only the diffusion mechanism, but also the diffusion direction can be modulated by patterns of biaxial strains. These results are important to the future dynamical modeling and simulations. We have further performed kinetic Monte Carlo simulations and observed (1) the modulation of diffusion of single adatom on W(001) surface by strains and (2) the aggregation of multiple adatoms on W(110) surface.
10:00AM M40.00011 Determination of shift in electrodic reaction rates due to the presence of stress1, SWARNAVO SARKAR, Cornell University, USA, WILKINS AQUINO, Duke University, USA — An extension of Butler-Volmer formulation is proposed to determine the stress-induced changes in electrodic reaction rates. Gibbs-Duhem equation is used to determine the stress-dependent chemical potential and the corresponding change in the reaction rate. The scope of possible amplification or reduction in the reaction rates due to tensile and compressive stress fields is explored numerically. Though quantitative experimental validation remains to be pursued, behavioral agreement of the extended Butler-Volmer model with some observations made in the field of corrosive dissolution is established. Our numerical results also indicate that in addition to altering the speed of a reaction, a stress field can modify the shape of an anodic dissolution front. The effect of stress-generated surface patterns is also considered. It is well-established that a stress field can create surface patterns due to surface wrinkling or surface diffusion. We determine the possible significance of such patterns on the reaction rate, and identify the factors that may enhance their contribution to electrodic reaction rates.

1Supported by NSF AWARD #CAREER - 0643618.

10:12AM M40.00012 The model that takes the Marangoni effect into account for drying process of polymer solution coated on a flat substrate, HIROYUKI KAGAMI, Department of Preschool Education, Nagoya College — We have proposed and modified a model of drying process of polymer solution coated on a flat substrate for flat polymer film fabrication supposing resist coating process in photolithography process. And we have clarified dependence of distribution of polymer molecules on a flat substrate on various parameters based on analysis of many numerical simulations of the model. Then we applied the model to thickness control of a thin film after drying through thermal management. Above model consists of two elements. One is vaporization at the gas-liquid interface. The other is the diffusion inside the liquid film on a substrate. The diffusion is divided into two kinds of diffusion, that is, diffusion of solvent with solutes due to gradient of the number density of particles per space and diffusion of diffusion of concentration of solution. Because it is assumed that coated solution film on a flat substrate is very thin and therefore both Rayleigh number and Marangoni number are small enough, it is thought that Bénard convection or Marangoni convection does not occur and therefore it is sufficient to consider only above-mentioned two kinds of diffusion inside the liquid film. However it is thought that there is some sort of Marangoni effect regardless Marangoni convection does not occur. Therefore, in this study we add the Marangoni effect to the existing model. Then we evaluate effects of the Marangoni effect in the drying process through numerical simulation of the modified model.

10:24AM M40.00013 Mesoscopic Aligned and Cu-Coordinated Surface Linear Polymerization at Low Temperature1, QING LI, Oak Ridge National Lab, JONATHAN R. OWENS, Rensselaer Polytechnic Institute, CHENGBO HAN, North Carolina State University, MIGUEL FUENTES-CABRERA, BOBBY G. SUMPTER, Oak Ridge National Lab, WENCHANG LU, JERRY BERNHOLC, North Carolina State University, PETRO MAKSYMOVYCH, Oak Ridge National Lab, VINCENT MEUNIER, Rensselaer Polytechnic Institute, MINGHUA PAN, Oak Ridge National Lab — The on-surface synthesis of covalent organic aggregates and networks has received considerable attention. However, most of the polymerization reactions require high temperatures to overcome the activation barrier. We demonstrate a surface-coordinated linear polymerization, which occurred at 100 K and forms long chain that are well-organized into a “circuit-board” pattern on Cu(100) surface. This highly strained 1D conjugated polymer alters greatly the electronic structure compared to unperturbed polymer and it was investigated by electronic and vibrational spectroscopies, as well as ab initio calculations. More importantly, the processes of polymerization and depolymerization can be controlled locally at the nanoscale by a using a charged metal tip. This work thus demonstrates the feasibility of accessing and controlling chain-growth polymerization at low temperature that may lead to the bottom-up construction of sophisticated architectures for molecular nano-devices.

1Research was conducted at the Center for Nanophase Materials Sciences and sponsored by the Division of Scientific User Facilities, US DOE

10:36AM M40.00014 Surface reactivity/stability and hydration of calcium silicate phases, ENGIN DURGUN, Massachusetts Institute of Tecnology and UNAM-Institute of Materials Science and Nanotechnology, Bilkent University, CAN ATACA, HAMLIN M. JENNINGS, JEFFREY C. GROSSMAN, Massachusetts Institute of Technology — Recent studies on synthetic calcium silicate structures revealed important mechanisms to tune the reactivity of various cement phases. Interaction of water with dicalcium silicate (C2S-belite) and tricalcium silicate (C3S-alite), dominant phases in Portland Cement, are the most important and anticipated reactions. In this work, using first-principles calculations, a fundamental understanding of how water pressure affects the reactivity of C3S and C2S phases is provided. In order to understand the hydration of different phases, as a first step the surface energetics of all lower index orientations are calculated and the stability/reactivity of the surfaces are determined. Taking into account the most and least energetic surfaces of the C3S phase, detailed analyses are carried out in order to understand the induction period in hydration. Surface transformation from highly reactive C3S to low reactive C2S revealed that upon increasing the water pressure, the surface with C2S character becomes energetically more favorable. Reduction of the surface energy is more intense in the case of proton exchange of surface Ca atoms. Our calculations suggest that these processes are the most probable mechanisms underlying the rapid decrease in reactivity in alite hydration.


11:15AM N1.00001 Entanglement and entanglement storage in dipolar coupled diamond defects, JOERG WRACHTRUP, University of Stuttgart — The generation of robust entangled states is one of the key steps in quantum science. Although diamond defects are highly versatile quantum bits mutual entanglement has not been demonstrated so far. The talk will describe the engineering of strongly coupled defect centers as well as their characteristic features. Entanglement generation as well as different means of tomography will be outlined. Correlated photon emission form coupled defect center pairs is analyzed. Robust storage of electron spin entanglement into nuclear spins resulting in entanglement storage lifetime of ms is demonstrated and roads towards efficient generation of strongly coupled defect arrays will be discussed.
1:15AM N1.00002 Mobile quantum sensing with spins in optically trapped nanodiamonds

DAVID D. AWSCHALOM
Center for Spintronics and Quantum Computation, University of California, Santa Barbara, California 93106 — The nitrogen-vacancy (NV) center in diamond has emerged as a powerful, optically addressable, spin-based probe of electromagnetic fields and temperature. For nanoscale sensing applications, the NV center’s atom-like nature enables the close-range interactions necessary for both high spatial resolution and the detection of fields generated by proximal nuclei, electrons, or molecules. Using a custom-designed optical tweezer apparatus, we demonstrate three-dimensional position control of nanodiamonds in solution with simultaneous optical measurement of electron spin resonance (ESR). Despite the motion and random orientation of NV centers suspended in the optical trap, we observe distinct peaks in the ESR spectra from the ground-state spin transitions. Accounting for the random dynamics of the trapped nanodiamonds, we model the ESR spectra observed in an applied magnetic field and estimate the dc magnetic sensitivity based on the ESR line shapes to be ~5 × 10^7 T/√T. We utilize the optically trapped nanodiamonds to characterize the magnetic field generated by current-carrying wires and ferromagnetic structures in microfluidic circuits. These measurements provide a pathway to spin-based sensing in fluidic environments and biophysical systems that are inaccessible to existing scanning probe techniques, such as the interiors of living cells.


In collaboration with Viva R. Horowitz, Benjamín J. Alemán, Paolo Andrich, David J. Christle, and Andrew N. Cleland.

12:27PM N1.00003 Quantum optical networks with diamond nanophotonics

NATHALIE DE LEON
Harvard University Department of Physics — Scalable quantum optical networks require identical single photons from multiple quantum bits and high collection efficiency of these single photons. Nitrogen vacancy (NV) centers in diamond are a promising candidate for quantum information processing because they have quantum mechanical degrees of freedom that can be addressed optically and, as solid-state structures, can potentially be easily integrated into nanophotonic networks. In particular, they have a zero-phonon line (ZPL), which acts as an atom-like cycling transition that can be used for coherent optical manipulation. However, the ZPL only accounts for 3-5% of the total emission, and it is difficult to generate a high density of NV centers with stable ZPL. I will present progress toward gaining both spectral and spatial control over NV emission by coupling NV centers to nanophotonic devices. In particular, we have fabricated high quality factor (Q), small mode volume (V) photonic crystal cavities directly out of diamond, and have deterministically placed them around stable NV centers to enhance the spontaneous emission at the cavity resonance by a factor of 50-100. This emission is guided efficiently into a single optical mode, enabling integration with other photonic elements, as well as networks of cavities, each with their own optically addressable qubit. These nanophotonic elements in diamond will provide a building block for a variety of applications in quantum information processing, such as entanglement of distant NV centers and single photon transistors.

1:03PM N1.00004 Single-shot readout of multiple nuclear spin qubits in diamond under ambient conditions

VINCENT JACQUES, Laboratoire de Photonique Quantique et Moléculaire, Ecole Normale Supérieure de Cachan and CNRS UMR 8537, 94235 Cachan, France — Nuclear spins are attractive candidates for solid-state quantum information storage and processing owing to their extremely long coherence time. However, since this appealing property results from a high level of isolation from the environment, it remains a challenging task to polarize, manipulate and readout with high fidelity individual nuclear spins. A promising approach to overcome this limitation consists in utilizing an ancillary single electronic spin to detect and control remote nuclear spins coupled by hyperfine interaction. In this talk, I will show how the electronic spin of a single Nitrogen-Vacancy (NV) defect in diamond can be used as a robust platform to observe the real-time evolution of surrounding single nuclear spins under ambient conditions. Using a diamond sample with a natural abundance of 13C isotopes, we first demonstrate high fidelity initialization and single-shot readout of an individual 13C nuclear spin. By including the intrinsic 14N nuclear spin of the NV defect in the quantum register, we then report the simultaneous observation of quantum jumps linked to both nuclear spin species, providing an efficient initialization of the two qubits. These results open up new avenues for diamond-based quantum information processing (QIP) including active feedback in quantum error correction protocols and tests of quantum correlations with solid-state single spins at room temperature.

1:39PM N1.00005 Quantum entanglement between diamond spin qubits separated by 3 meters

RONALD HANSON, Kavli Institute of Nanoscience, Delft University of Technology — Entanglement of spatially separated objects is one of the most intriguing phenomena that can occur in physics. This can lead “spooky action at a distance” where measurement of one object instantaneously affects the state of the other object. Besides being of fundamental interest, entanglement is also a valuable resource in quantum information technology enabling secure quantum communication networks and distributed quantum computing. Here we present our most recent results towards the realization of scalable quantum networks with solid-state qubits. We have entangled two spin qubits in diamond, each associated with a nitrogen vacancy center in diamond [1]. The two diamonds reside in separate setups three meters apart from each other. With no direct interaction between the two spins to mediate the entanglement, we make use of a scheme based on quantum measurements: we perform a joint measurement on photons emitted by the NV centers that are entangled with the electron spins. The detection of the photons projects the spins into an entangled state. We verify the generated entanglement by single-shot readout of the spin qubits in different bases and correlating the results. These results open the door to a range of exciting opportunities. For instance, the remote entanglement can be extended to nuclear spins near the NV center. Our recent experiments demonstrate robust methods for initializing, controlling and entangling nuclear spins by using the electron spin as an ancilla [2,3]. Entanglement of remote quantum registers will enable deterministic quantum teleportation, distributed quantum computing tasks and the implementation of an elementary quantum repeater.


Ballroom II - Zhi-Xun Shen, Stanford University
11:15AM N2.00001 Pairing mechanism and gap symmetry in Fe-based superconductors with only electron or only hole pockets, ANDREY CHUBUKOV, University of Wisconsin — The pairing in moderately doped Fe-pnictides and Fe-chalcogenides is generally understood as being due to magnetically enhanced interaction between hole and electron pockets. Recently, however, superconductivity has been observed in AFe$_2$S$_2$ (A = K, Rb, Cs), which contain only electron pockets, and in KFe$_2$As$_2$, which contains only hole pockets. In the talk, I review different (and sometimes conflicting) scenarios for the pairing in these systems and propose my own. I argue that the pairing condensate in systems with only electron pockets necessary contains not only a conventional intra-pocket component, but also inter-pocket component, made of two fermions belonging to different electron pockets. I analyze the interplay between intra-pocket and inter-pocket pairing depending on the ellipticity of electron pockets and the strength of their hybridization and show that with increasing hybridization the system undergoes a transition from a d-wave state to an $s^\pm$ state, in which the gap changes sign between hybridized pockets. This $s^\pm$ state has the full gap and at the same time supports spin resonance, in agreement with the data. Near the boundary between d and $s^\pm$ states the system develops s+i-d state which breaks time-reversal symmetry. For systems with only hole pockets, I argue for $s^\pm$ state in which the gap changes sign between hole pockets. I show that this state is qualitatively different from $s^\pm$ state when both hole and electron pockets are present. I further show that the transition from one s-wave state to the other involves highly unusual s+i state which again breaks time reversal symmetry.

11:51AM N2.00002 Atomic-scale Visualization of Electronic Nematicity and Cooper Pairing in Iron-based Superconductors. MILAN P. ALLAN, Cornell University, ETH Zürich — The mechanism of high-temperature superconductivity in the relatively novel iron-based high-$T_c$ superconductors is unresolved, both in terms of how the phases evolve with doping, and in terms of the actual Cooper pairing process. To explore these issues, we used spectroscopic-imaging scanning tunneling microscopy to study the electronic structure of CaFe$_2$As$_2$ in the antiferromagnetic-orthorhombic 'parent' state from which the superconductivity emerges. We discovered and visualized the now widely studied electronic 'nematicity' of this phase, whose suppression is associated with the emergence of superconductivity (Science 327, 181, 2010). As subsequent transport experiments discovered a related anisotropic conductance which increases with dopant concentration, the interplay between the electronic structure surrounding each dopant atom, quasiparticle scattering therefrom, and the transport nematicity has become a pivotal focus of research. We find that substituting Co for Fe atoms in underdoped Ca(Fe$_{1-x}$Co$_x$)$_2$As$_2$ generates a dense population of identical and strongly anisotropic impurity states that are distributed randomly but aligned with the antiferromagnetic a-axis. We also demonstrate, by imaging their surrounding interference patterns, that these impurity states scatter quasiparticles and thus influence transport in a highly anisotropic manner (M.P. Allan et al., 2013). Next, we studied the momentum dependence of the energy gaps of iron-based superconductivity, now focusing on LiFeAs. If strong electron-electron interactions mediate the Cooper pairing, then momentum-space anisotropic superconducting energy gaps $\Delta_i(k)$ were predicted by multiple techniques to appear on the different electronic bands i. We introduced intraband Bogoliubov quasiparticle scattering interference (QPI) techniques for the determination of anisotropic energy gaps to test these hypotheses and discovered the anisotropy, magnitude, and relative orientations of the energy gaps on multiple bands (Science 336, 563 (2012)). Finally, the electron-electron interactions generating Cooper pairing are often conjectured to involve bosonic spin fluctuations generated by interband scattering of electrons. We explore the STM signatures of both the interband scattering and the electron-boson coupling self-energy in LiFeAs, and detect the signatures of the electron-boson coupling (M.P. Allan et al., in preparation).

12:27PM N2.00003 Spin dynamics in electron and hole-doped iron pnictide superconductors. PENGCHENG DAI, University of Tennessee — No abstract available.

1:03PM N2.00004 ARPES studies of the superconducting gap symmetry of Fe-based superconductors, PIERRE RICHARD, Institute of Physics, Chinese Academy of Sciences — The superconducting gap is the fundamental parameter that characterizes the superconducting state, and its symmetry is a direct consequence of the mechanism responsible for Cooper pairing. Here I discuss about angle-resolved photoemission spectroscopy measurements of the superconducting gap in the Fe-based high-temperature superconductors. I show that the superconducting gap is Fermi surface dependent and nodless with small anisotropy, or more precisely, a function of momentum. I show that while this observation is inconsistent with weak coupling approaches for superconductivity in these materials, it is well supported by strong coupling models and global superconducting gaps. I also stress the importance of scattering and the lifetime of quasiparticles in evaluating the superconducting gap by angle-resolved photoemission spectroscopy and other experimental techniques.

1:39PM N2.00005 Effects of disordered substitutions and vacancies in Fe based superconductors from first principles 1, TOM BERLIJN, University of Florida — Most Fe pnictide and selendire superconductors are created by chemical substitution which inevitably introduces disorder. The relationship between nominal chemical valence, doping, and quasiparticle spectral weight appears to be quite complex. Using a recently developed Wannier function based first principles method for disordered systems [1], we compute the configuration-averaged spectral function $\langle A(k,\omega) \rangle$ of Fe based superconductors containing disordered substitutions and vacancies. In the transition metal doped Ba(Fe$_{1-x}$M$_x$)$_2$As$_2$ with M=Co/Zn we find[2] a loss of coherent carrier spectral weight. For the case of disordered Fe and K vacancies in K$_n$Fe$_x$Se$_2$ we find a disorder induced effective doping to give rise to enlarged electron pockets without adding electrons to the system. For the case of Ru substitutions in Ba(Fe$_{1-x}$Ru$_x$)$_2$As$_2$ we find[4] a cancelation between on- and off-site disorder to give rise to a surprising protection of the Fermi surface.


1Work supported by DOE CMCSN
11:15AM N10.00001 High-speed transport and magneto-mechanical resonant sensing of superparamagnetic microbeads using magnetic domain walls

ELIZABETH RAPOPORT, Massachusetts Institute of Technology — Surface-functionalized superparamagnetic (SPM) microbeads are of great interest in biomedical research and diagnostic device engineering for tagging, manipulating, and detecting chemical and biological species in a fluid environment [1-5]. Recent work has shown that magnetic domain walls (DWs) can be used to shuttle individual SPM microbeads and magnetically tagged entities across the surface of a chip [1-5]. This talk will describe the dynamics of SPM microbead transport by nanotrack-guided DWs, and show how these coupled dynamics can be exploited for on-chip digital biosensing applications. Using curvilinear magnetic nanotracks, we demonstrate rapid transport of SPM microbeads at speeds approaching 1000 \mu m/s [3], and present a mechanism for selective transport at a junction that allows for the design of complex bead routing networks. We further demonstrate that a SPM bead trapped by a DW exhibits a distinct magneto-mechanical resonance that depends on its hydrodynamic characteristics in the host fluid [4, 5], and that this resonance can be used for robust size-based discrimination of commercial microbead populations. By embedding a spin-valve sensor within a DW transport conduit, we show that the resonance can be detected electrically and on-the-fly [5]. Thus, we demonstrate a complete set of essential bead handling functions, including capture, transport, identification, and release, required for an integrated lab-on-a-chip platform.


In collaboration with Daniel Montana, David Bono, and Geoffrey S.D. Beach, Massachusetts Institute of Technology. This work is supported by the MIT CMSE under NSF-DMR-0819762 and by the MIT Deshpande Center.

11:51AM N10.00002 Binary Colloidal Superlattices Assembled by Magnetic Fields

YELLEN, Duke University — Colloidal particle superlattices represent a fascinating class of complex materials which in many cases have corollary structures at the atomic scale. These complex systems thus not only help elucidate the principles of materials assembly in nature, but further provide design criteria for fabrication of novel materials at the macroscopic scale. Methods for assembling colloidal particle superlattices include controlled drying, ionic interactions, and dipolar interactions. However, a general pathway for producing a wider variety of colloidal crystals remains a fundamental challenge. Here we demonstrate a versatile colloidal assembly system in which the design rules can be tuned to yield over 20 different pre-organized lattice structures, including Kagome, honeycomb, square, as well as a variety of chain and ring configurations. We tune the crystal type by controlling the relative concentrations and interaction strengths between spherical superparamagnetic and diamagnetic particles. An external magnetic field causes like particles to repel and unlike particles to attract. The combination of our experimental observations with potential energy calculations of various lattice structures suggest that the lowest energy lattice configuration is determined by two parameters, namely the dipole moment and relative concentration of each particle type.

1 Triangle MRSEC DMR-1121107, NSF 51150110161

12:27PM N10.00003 Magnetic microstructures for regulating Brownian motion

SOORYAKUMAR, The Ohio State University — Nature has proven that it is possible to engineer complex nanoscale machines in the presence of thermal fluctuations. These biological complexes, which harness random thermal energy to provide functionality, yield a framework to develop related artificial, i.e., nonbiological, phenomena and devices. A major challenge to achieving positional control of fluid-borne submicron sized objects is regulating their Brownian fluctuations. In this talk a magnetic-field-based trap that regulates the thermal fluctuations of superparamagnetic beads in suspension will be presented. Local domain-wall fields originating from patterned magnetic wires, whose strength and profile are tuned by weak external fields, enable bead trajectories within the trap to be managed and easily varied between strong confinements and delocalized spatial excursions. Moreover, the frequency spectrum of the trapped bead responds to fields as a power-law function with a tunable, non-integer exponent. When extended to a cluster of particles, the trapping landscape preferentially stabilizes them into formations of 5-fold symmetry, while their Brownian fluctuations result in frequent transitions between different cluster configurations. The quantitative understanding of the Brownian dynamics together with the ability to tune the extent of the fluctuations enables the wire-based platform to serve as a model system to investigate the competition between random and deterministic forces.

1 Funding from the U.S. Army Research Office under contract W911NF-10-1-0353 is acknowledged.

1:03PM N10.00004 Smart Magnetic Materials for Controlling Cell Fate

VITOL, Materials Science Division, Argonne National Laboratory — Toxicity of cancer chemotherapy, often resulting in failure of even healthy organs, represents one of the most vivid and still unavoidable problems of traditional medical approaches to treating a disease. The lack of specificity remains a fundamental obstacle in performing targeted treatment which should ideally affect only the particular cells in a human body. Nanotechnology has recently enabled the possibility to create materials comparable in sizes with cells and subcellular structures opening the opportunities for affecting intracellular processes on the level unattainable by macroscopic techniques. [1-2] Magnetic nanomaterials are especially promising for applications in life sciences due to their bi-functional behavior. On the one hand side, they are inherently stimulus-responsive and their properties can be controlled and modulated remotely. On the other hand, these materials themselves can be used for applying controlled stimulus to a cell thus changing its function and even inducing cell death [3]. For biological applications, such multifaceted functionality opens the unique opportunity to modulate cell behavior by interfacing it with magnetic material. Historically, chemically synthesized superparamagnetic iron oxide particles have been widely studied for biological applications such as magnetic separation, targeting, MRI contrast enhancement and magnetically induced heating [14]. At the same time, there is a growing interest to magnetic materials created by physical fabrication methods which allow for realization of very complex structures in terms of geometry and composition [5]. In this talk, both types of materials will be discussed. Thus, thermo-responsive magnetic micelles were used as nanocontainers for magnetically guided drug delivery and release triggered by heating in the RF frequency a.c. magnetic field. The microfabricated biofunctionalized microparticles targeted to the cancer cells were employed for mechanical stimulation of cell membrane due to oscillation of the disks in the low frequency (10-20 Hz) a.c. magnetic field, resulting in redistribution of free intracellular calcium and subsequent triggering of apoptosis - programmed cell suicide [3,5]. The details of mechanisms by which the cells respond to the stimulus applied by magnetic particles will be discussed.


1 The work at Argonne, including use of the Center for Nanoscale Materials was supported by the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

1 Funding from the U.S. Army Research Office under contract W911NF-10-1-0353 is acknowledged.
atomic resolution Z-contrast images obtained in an aberration-corrected scanning transmission electron microscope, we show that CuInS$_2$ nanocrystals have a hexagonal lattice structure that is different from the bulk chalcopyrite phase. The structure of these nanocrystals has been previously identified as the wurtzite structure in which the copper and indium atoms randomly occupy the cation sites.

This work was supported in part by DOE grant DE-FG02-07ER15842

11:27AM N22.00002 Vibrational and thermodynamic properties of transition-metal nanoclusters$^1$. VALERI G. GRIGORYAN, MICHAEL SPRINGBORG, Physical and Theoretical Chemistry, University of Saarland, Germany — The knowledge of the vibrational spectrum of a cluster, which is the fingerprint of its structure, is necessary for the development of thermodynamics of clusters (melting, heat capacity, solid-solid structural transitions) and for the understanding of experimental vibrational spectra. In summary, the full vibrational spectrum of Ni$_x$ and Cu$_x$ nanoclusters with $N$ from 2 to 150 atoms has been determined using the analytical expression of the embedded-atom method (EAM) for the force-constant tensor for the first time. In the determination of the spectra we have employed the global-minimum structures obtained in our previous unbiased EAM studies (see e.g. Physical Review B, 2004, 2006). Furthermore, using those spectra and the superposition approximation, the thermodynamic properties of the clusters have been calculated quantum mechanically, including their heat capacity and solid-solid transition temperatures for several structural changes in the Ni and Cu clusters. Both the vibrational spectrum and the thermodynamic functions show strong cluster-size effects. We emphasized that our approach is general. It is based on the (common) EAM form of the total energy and applicable to many other many-body potentials.

$^1$This work was supported by the DFG through Project No. Sp439/23-1

11:39AM N22.00003 Material Improvements of ZnCdSe/ZnCdMgSe Heterostructures for Quantum Cascade Laser Applications with Incorporation of Growth Interruptions During MBE Growth. THOR GARCIA, The Graduate Center of CUNY, New York, NY 10016, JOEL DE JESUS, The Graduate Center of CUNY, New York, NY 10016, ARVIND RAVIKUMAR, Princeton University, Princeton, NJ 08544, SONGWOUNG HONG, The City College of New York, New York, NY 10031, CLAIRE GMACHL, Princeton University, Princeton, NJ 08544, AIDONG SHEN, The City College of New York, New York, NY 10031, MARIA TAMARGO, The City College of New York, New York, NY 10031 — We report on the growth of ZnCdSe/ZnCdMgSe/InP Quantum Cascade (QC) structures with improved electrical and material properties. Material quality has been previously addressed by limiting the lattice mismatch to within 0.2% of InP. However, the yields of high quality material have remained low and lasing has not been observed. To address the low growth yields we have investigated possible mechanisms for degradation of the material. Growth interruptions during the MBE growth were added to the active core of the QC laser structure. High resolution XRD and PL were used to evaluate the material quality. Fabricated devices with growth interruptions show a dramatic improvement in the electroluminescence spectral properties.

11:51AM N22.00004 New crystal structures in hexagonal CuInS$_2$ nanocrystals. XIAO SHEN, EMIL A. HERNÁNDEZ-PAGAN, Vanderbilt University, WU ZHOU, Vanderbilt University and Oak Ridge National Lab, YEYGENIY S. PUZYREV, Vanderbilt University, JUAN C. IDROBO, Oak Ridge National Lab, JANET E. MACDONALD, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Lab, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Lab — CuInS$_2$ is one of the best candidate materials for solar energy harvesting. Its nanocrystals with a hexagonal lattice structure that is different from the bulk chalcopyrite phase have been synthesized by many groups. The structure of these CuInS$_2$ nanocrystals has been previously identified as the wurtzite structure in which the copper and indium atoms randomly occupy the cation sites. Using first-principles total energy and electronic structure calculations based on density functional theory, UV-vis absorption spectroscopy, X-ray diffraction, and atomic resolution Z-contrast images obtained in an aberration-corrected scanning transmission electron microscope, we show that CuInS$_2$ nanocrystals do not form random wurtzite structure. Instead, the CuInS$_2$ nanocrystals consist of several wurtzite-related crystal structures with ordered cation sublattices, some of which are reported for the first time here. This work is supported by the NSF TN-SCORE (JEM), by NSF (WZ), by ORNL’s Shared Research Equipment User Program (JCI) sponsored by DOE BES, by DOE BES Materials Sciences and Engineering Division (SJP, STP), and used resources of the National Energy Research Scientific Computing Center, supported by the DOE Office of Science under Contract No. DE-AC02-05CH11231.
12:03PM N22.00005 Measuring the Elastic Modulus of the Grain Boundary Component of Nanocrystalline Copper, GUO-JIE GAO, YUNJIA NANG, SHIGENOBU OGATA, Osaka University — In the past twenty years, it has been widely accepted that the Young’s modulus of the grain boundary (GB) part of nanocrystalline metals is about 70% of that of the crystalline core component. However, this belief is an assumption based on numerical studies of specific grain boundary like 225 twist boundary where atoms interact with one another via simplified Lennard-Jones potential at 0K or experimental studies assuming the GB behaves like amorphous alloys. A thorough investigation driven from completely realistic atomic simulation at finite temperature is still lacking. We reexamine this assumption by measuring the Young’s modulus of pure copper (Cu) with grain size ranging from 3 to 25 nm at 300K using molecular dynamics (MD) uniaxial tensile tests. We implement a novel Voronoi protocol to build nanocrystalline structures of fully dense pure Cu with well-controlled grain size distribution and Mishin embedded atom model (EAM) potential. We find the following key results concerning the stiffness for nanocrystalline metals at finite temperature: 1) The GB is more thermally sensitive and therefore elastically much softer than the crystalline interior. 2) The Young’s modulus of the GB is about 20% or less of that of the grain interior.

12:15PM N22.00006 Structural and compositional characterization of “covetics” a new class of materials containing high C concentration, R.A. ISAACS, University of Maryland College Park, A. HERZING, National Institute of Standards and Technology, D.R. FOREST, A.N. MANSOUR, Naval Surface Warfare Center, M.C. LEMIEUX, Chemical Engineering Department, Stanford University, J. SHUGART, Third Millennium LLC, L. SALAMANCA-RIBA, University of Maryland College Park — “Covetics” are a new class of materials formed by the incorporation of high concentrations (> 6wt%) of nanoscale carbon in a metal matrix. The carbon incorporates into the crystal structure of the host metal and remains dispersed after subsequent melting and re-solidification. The carbon is highly stable in these materials despite the absence of a predicted solid solution at such concentrations in the binary phase diagrams. Covetics have been shown to exhibit enhanced electrical, mechanical and thermal properties when compared with non-covetic metals. We have performed energy dispersive X-ray spectroscopy (EDS), X-ray photoelectron spectroscopy (XPS), X-ray absorption spectroscopy (XAS), SEM, TEM, STEM/electron energy loss spectroscopy (EELS), AFM, and Raman spectroscopy to investigate the structure of Al, Cu, and Ag covetics. Both bulk samples and thin films are investigated. Carbon was detected in the form of nanoparticles 5 nm - 200 nm in diameter with an interconnecting carbon matrix. The carbon is detectable by EDS and XPS, but not by analytical methods such as LECO and GDMS. Raman indicates a similar signal to that of CNTs in covetics. A detailed investigation of the morphology of the nanocarbon and the structure of several covetics will be presented.

12:27PM N22.00007 Computational Investigations of a Possible New Class of Materials: A Superatom Ionic Solid, KARL SÖHLMER, VIOLETA NASTO, Drexel University — A “superatom” is a cluster of atoms that shows high stability. High stability can arise from the geometric arrangement of the atoms in the cluster. For example, when atoms are closed packed, clusters containing an integer number of closed shells of atoms, (i.e. 13, 55, 137...) atoms exhibit enhanced stability and are termed “magic clusters.” High stability can also arise from the electronic structure. High symmetry metal clusters that have exactly 8, 20, 40,..., valence electrons show enhanced stability. Superatons can act chemically like a single atom of a different element. We have used electronic structure calculations to test the idea that a new class of materials may be formed by the periodic arrangement of superatom ions, instead of the periodic atomic or polyatomic ions of a conventional ionic solid. A solid is formed based on crystalline packing of anionic (Al@Cu_{13}) and cationic (Ce@C_{60}), nearly spherical superatom species that show exceptional stability. According to radius-ratio rules, these ions will favor a CsCl crystal structure with a body-centered (bcc) type of unit cell. Calculations on this material suggest that it is stable, semiconducting and less dense than common metal oxides, but that the metal anion clusters deform within the material.

12:39PM N22.00008 Electronically Guided Self Assembly within Quantum Corrals, RONGXING CAO, BINGFENG MIAO, ZHANGFENG ZHONG, LIANG SUN, BIAO YOU, WEI ZHANG, WEI BAO, Department of Physics, Nanjing University, SAMUEL BADER, Center for Nanoscale Materials, Argonne National Laboratory, HAIFENG DING, Department of Physics, Nanjing University, LOW DIMENSIONAL MAGNETISM TEAM, CENTER FOR NANOSCALE MATERIALS COLLABORATION — A grand challenge of nanoscience is to master the control of structure and properties in order to go beyond present day functionality. The creation of nanostructures via atom manipulation by means of a scanning probe represents one of the great achievements of the nano era. Here we build on this achievement to self-assemble nanostructures within quantum corrals. We constructed circular and triangular Fe quantum corrals on Ag(111) substrate via STM manipulation and studied the quantum confinement of electronic states and the diffusion of Gd atoms inside the corrals. Statistical results reveal the motion of the Gd atoms forming several individual orbits that are closely related to the local density of states. We experimentally demonstrate that different self-organized Gd atomic structures are formed within 30-nm circular and triangular Fe quantum corrals with a step-by-step guiding process. The findings demonstrate that quantum confinement can be used to engineer atomic structures and atom diffusion. And 30-nm resolution can be reached by means of advanced lithography. Adding quantum engineering to augment it opens new possibilities for local functionality design down to the atomic scale.

1Work at Nanjing is supported by the State Key Program for Basic Research of China (Grant No. 2010CB923401), NSFC (Grants Nos. 10974087, 10834001, and 11023002) and PAPD.

12:51PM N22.00009 Simultaneous hypersonic and optical mirrors in nanometric porous silicon multilayers, JESUS MANZANARES-MARTINEZ, Departamento de Investigacion en Fisica, Universidad de Sonora, Apartado Postal 5-088, Hermosillo, Sonora 83180, Mexico, PAOLA CASTRO-GARAY, DAMIAN MOCTEZUMA-ENRIQUEZ, YOHAN JASID RODRIGUEZ-VIVEROS, Departamento de Fisica, Universidad de Sonora, Blvd. Luis Encinas y Rosales, Hermosillo, Sonora 83180, Mexico. — We study by theoretical simulations the non-perpendicular propagation of electromagnetic and elastic waves in Porous Silicon Multilayers (PSM). Our work is inspired by recent experimental results where the angular variation of light was observed in PSM. [L. C. Parsons and G. T. Andrews, J. Appl. Phys. 111, 123521 (2012)] We proceed in three steps. First, we found the conditions to obtain a simultaneous hypersonic-phononic mirror at normal incidence. Second, we determined the angular variation of the mirrors computing the projected band structure. Finally, we found the conditions to obtain omnidirectional mirror for hypersonic waves. However, we have found that for the optical case the mirror is limited to an angular cone.

1:03PM N22.00010 Dynamic Structural Disorder in Supported Nanoparticles, F.D. VILA, J.J. REHR, Dept. of Physics, U. of Washington, Seattle, WA 98195, S.D. KELLY, S.R. BARE, UOP LLC, Des Plaines, IL 60016 — Supported Pt based nanoclusters are of wide interest in nano-scale physics and have many industrial applications, yet an understanding of their structure is far from complete. Experimental probes such as x-ray absorption spectroscopy (XAS) only yield globally averaged properties, e.g., mean bond distances and mean-square radial disorder (MSRD), which can give a misleading characterization of such complex systems. To obtain a more detailed picture we have carried out finite temperature DFT/MD simulations of Pt and PtSn nanoclusters up to 600 K (operando conditions). These show that the nano-scale structure and charge distribution are inhomogeneous and dynamically fluctuating over several time-scales, ranging from fast (200-400 fs) bond vibrations to slow fluxional bond breaking (>10 ps). In particular the anomalous behavior of the MSRD is not static, but rather due to “dynamic structural disorder” (DSD) driven by stochastic motion of the center of mass over 1-4 ps time-scales. In addition the nanoclusters exhibit a semi-melted, Sn-rich surface. These findings show that, and how an improved XAS interpretation of supported nano-scale structure must take into account DSD and other structural inhomogeneities.

1Supported by NSF Grant PHY-0835543 with computer support from DOE - NERSC.

2F. Vila et al., UW preprint (2012).
A promising method for fabricating regular nanowire arrays with controlled wire separation. The thinnest YSi$_2$ nanowires have been grown epitaxially on the Si(110) surface. In contrast to epitaxial growth on the Si(100) surface, YSi$_2$ nanowires on Si(110) grow in a single orientation and show a clear preference of nucleating at terrace edges, thus providing a promising method for fabricating regular nanowire arrays with controlled wire separation. The thinnest YSi$_2$ nanowires have a cross section of $\sim 0.5 \times 2.8$ nm$^2$ with wire lengths of up to a few hundred nm, while thicker nanowires can grow up to several $\mu$m long. Scanning tunneling microscopy measurements on individual nanowires indicate that the nanowires have metallic properties while the surface between the nanowires has a band gap of $\sim 1$ eV. These nanowires thus represent an ideal platform for studies of quasi one-dimensional electrical transport. Such studies are currently underway in our laboratory.

Epitaxial growth of YSi$_2$ nanowires on the Si(110) surface

Absence of Dirac electrons in silicene on Ag (111) Surfaces

Engineering of the static interface dipole in metal/organic nanohybrid materials

Self-organized growth of single crystalline copper nanobead strings by electrodeposition

The Orientation Control of Iodine Molecules inside nano-scale channels

Formation of heterogeneous toroidal-spiral particles – by drop sedimentation and interaction

This work was supported by NSF CBET Grant CBET-1039531.
11:27AM N30.00002 ReaxFF Reactive Force Field Study of Oriented Attachment of TiO$_2$ Nanocrystals in Vacuum and Humid Environments, MURALIKRISHNA RAJU, Dept of Physics, The Pennsylvania State University, KRISTEN FICHTHORN, Dept of Chemical Engineering, Dept of Physics, The Pennsylvania State University, ADRI VAN DUIN, Dept of Mechanical and Nuclear Engineering, The Pennsylvania State University — We use a ReaxFF reactive force field to study the aggregation of various titanium dioxide (anatase) nanocrystals in vacuum and humid environments. The nanocrystals are in the 2-6nm size range, with shapes dictated by the Wulf construction. In vacuum, the nanocrystals tend to merge along their direction of approach, resulting in a polycrystalline structure. By contrast, in the presence of water vapor, the nanocrystals tend to reorient themselves and aggregate via the oriented attachment mechanism to form a single or twinned crystal. We find that adsorbed water molecules and hydroxyl groups play multiple roles in the aggregation process. Specifically, adsorbed water molecules and hydroxyl groups prevent their immediate aggregation. These adsorbed species create a hydrogen bonding network, which aligns the nanocrystals in registry. Upon the eventual elimination of these species, the nanocrystals fuse into a single-crystal or twinned aggregate. We observe this aggregation mechanism for anatase(101), anatase(112), and anatase(001) surfaces, as is also seen experimentally. This indicates the important role that solvent plays in nanocrystal aggregation and how solvent can be a powerful tool for directing and controlling nanocrystal growth.

11:39AM N30.00003 Improving reaction rates by confinement within biocompatible polymers, CECILE MALARDIR-T JUGROOT, XIA LI, MICHAEL N. GROVES, Department of Chemistry and Chemical Engineering, Royal Military College of Canada, MANISH JUGROOT, Department of Mechanical and Aerospace Engineering, Royal Military College of Canada — The most efficient catalytic systems have been developed and optimized by living systems. Indeed, in vivo enzyme-catalyzed reactions are several orders of magnitude more efficient than platinum based catalyzed reactions. However, the rate of reaction and equilibrium interactions are considerably reduced when the biological systems are studied in vitro. This phenomenon is largely attributed to the effect of confinement or macromolecular crowding present in the cell. This paper will present the comprehensive characterization of amphoteric amphiphilic template and hydrophobic cores inducing 1D and 2D confinement on hydrophobic reactants diffusing within the templates. The paper will show that effect of confinement allows reactions to occur without external factors essential for these reactions to occur in the bulk. The products synthesized in a very controlled environment within amphiphilic polymeric nanotubes and nanosheets are monodispersed at the nanoscale (~2nm). The effect of confinement opens new possibilities for environmentally friendly synthesis of novel nanoscale materials.

11:51AM N30.00004 Unraveling the Mechanism of Nanotube Formation by Chiral Self-Assembly of Amphiphiles, DGANIT DANINO, Technion - Israel Institute of Technology and the Russell Berrie Nanotechnology Institute — The self-assembly of nanotubes from amphiphiles and peptides is still poorly understood. Here, we present the first complete path to nanotubes by chiral self-assembly studied with C$_{12}$-β$_2$, a tailored molecule designed to have unique hybrid architecture. Using direct-imaging cryo-transmission electron microscopy (cryo-TEM) we show the time-evolution from micelles to closed nanotubes, passing through several types of 1-dimensional (1-D) intermediates such as elongated fibrils, twisted ribbons, and coiled helical ribbons. Scattering and diffusion techniques confirm that the fundamental unit is a monolayer lamellae with the hydrophobic tails in the gel state and beta-sheet arrangement. The lamellae are held together by a combination of hydrophobic interactions, and 2 sets of hydrogen bonding networks. Our data exclusively indicate that twisted ribbons are the precursors for coiled ribbons, and we show this transition is directly linked to the ribbon width. Furthermore, quantitative analysis shows that neither the “growing width” model nor the “closing pitch” model accurately describe the process of nanotube formation, and both ribbon width and pitch grow with maturation, maintaining a linear growth in their ratio. We also show that chirality is a key requirement for nanotube formation. References: [1] Ziserman L et al., J Am Chem Soc 133(8), 2511-2517 (2011) [2] Ziserman L et al., Phys Rev Lett 106, 238105 (2011)

12:03PM N30.00005 Programmable Mesoscopic Architecture using Directionally-Functionalized Nanoparticles, JONATHAN HALVERSON, ALEXEI TKACHENKO, Brookhaven National Laboratory — Nanoparticles that have been isotropically-functionalized with complementary DNA strands have been shown to self-assemble into a variety of crystalline morphologies. To produce a nanoparticle assembly with a finite size and arbitrary shape, the NPs must be endowed with directional interactions. Directionally-functionalized nanoparticles (dfNPs) can be constructed by grafting ssDNA at specific locations on the particles, and proof-of-principle experiments have successfully demonstrated the self-assembly of such particles. Using these building blocks we have previously demonstrated with numerical simulations that a variety of target mesosopic structures, each with a programmed local morphology and complex overall shape, can be self-assembled in near perfect yield. Here we present a model to describe the kinetics of assembly of a structure composed of dfNPs. The capability to produce these structures can be utilized in a variety of applications where bottom-up construction of 3D nano-objects with well-defined composition and architecture is required (e.g., nanoplastomics, nanomedicine, metamaterials).

1Research carried out in whole at the Center for Functional Nanomaterials, Brookhaven National Laboratory, which is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, under Contract No. DE-AC02-98CH10886.

12:15PM N30.00006 Biomimetic DNA emulsions: specific, thermo-reversible and adjustable binding from a liquid-like DNA layer, LEA-LAETITIA PONTANI, LANG FENG, Department of Physics, New York University, REMI DREYFUS, Complex Assemblies of Soft Matter, Centre National de la Recherche Scientifique-Rhôdia-University of Pennsylvania, NADRIAN SEEMAN, Department of Chemistry, New York University, PAUL CHAIKIN, JASNA BRUJIC, Department of Physics, New York University — We develop micron-sized emulsions coated with specific DNA sequences and complementary sticky ends. The emulsions are stabilized with phospholipids on which the DNA strands are grafted through biotin-streptavidin interactions, which allows the DNA to diffuse freely on the surface. We produce two complementary emulsions: one is functionalized with sticky ends and dyed with red streptavidin, the other displays the complementary sticky ends and green streptavidin. Mixing those emulsions reveals specific adhesion between them due to the short-range S-S’ hybridization. As expected this interaction is thermo-reversible: the red-green adhesive droplets dissociate upon heating and reassemble after cooling. Here the fluid phospholipid layer also leads to diffusive adhesion patches, which allows the droplets to rearrange to nanotubes through this novel mechanism. In this way we break the strong interaction between two droplets and build a theoretical framework that captures the observed trends through parameter studies such as the size of the droplets, the DNA surface density, the various DNA constructs or the temperature. This colloidal-scale, specific, thermo-reversible biomimetic emulsion offers a new versatile and powerful tool for the development of complex self-assembled materials.

12:27PM N30.00007 Hybridization dynamics to DNA guided crystallization, TING LI, Northwestern University, RASTKO SKNEPNK, Syracuse University, MONICA OLVERA DE LA CRUZ, Northwestern University, NORTHWESTERN UNIVERSITY TEAM — DNA nanostructure design inspires an elegant protocol to design versatile nanoparticle assemblies. Although great achievements in DNA programmed periodic structures have been obtained, it took over a decade to realize even the basic crystal structures like FCC and BCC in an experiment. We use molecular dynamics simulations to discuss the dynamic aspects of the assembly mechanism and identify ingredients that are key to successfully assemble nanoparticle superlattices through DNA hybridizations. The scale-accurate coarse-grained model [1,2] faithfully captures the relevant dynamics of the DNA hybridization, and is able to recover the in situ formation of all to date experimentally reported binary superlattices (BCC, CsCl, AuBi2, Cr$_3$Si and Cs6C60 lattices). We used a multi-scale simulation approach to study the assembly mechanism in systems with up to $10^9$ degrees of freedom and found that the assembly process is enthalpy-driven. Finally, we investigated the optimal strength of DNA linkers, hybridization dynamics, and percentage of hybridizations for different binary systems. Based on these results, we suggest a protocol for future nanomaterial designs with versatile DNA interactions. [1] Knorowski, C., et al. P.R.L. 2011,106,215501; [2] Li, T.I.N.G., et al. Nano Letters 2012,12,2509.

This work is funded by the AFORS MURI FA9550-11-1-0275 and the NSF NEEF FA9550-10-1- 0167.
et al. The system is equivalent to f-star polymer systems, and consists of bcc, also with rotator, orientational glass or cubatic orientational order as well as sc. We also study self-assembly for spherical nanoparticles [1,2] without fitting parameters, to the case of nanocubes. We show that the phase diagram consists of bcc and sc lattices, to self-assemble into an array of superlattices. In this talk, we extend our previous model [1], which successfully predicted equilibrium phases and dynamics of self-assembled systems.

CHRISTOPHER KNOROWSKI, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA, ALEX TRAVESSET, Iowa State University Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA, 478, 225-228(2011) DOI: 10.1039/c2sm26832a

This work is funded by DOE through the Ames Lab under Contract DE-AC02-07CH11358. Most simulations are performed on the Exalted GPU cluster, which is funded by a grant from Iowa State University and Nvidia Corp.

1:27PM N30.00012 Colloidal Clusters via Short, Specific, and Isotropic DNA Interactions
JESSE W. COLLINS, Harvard SEAS, VINOTHAN N. MANOHARAN, Harvard SEAS and Physics — DNA is increasingly being used as a tool for guiding the self-assembly of particle-based systems. The transient bridging of grafted, complementary DNA strands induces specific, attractive interactions that can direct nanoparticles or colloids to form clusters, ordered crystal lattices, or other interesting structures. In most cases, the DNA-induced binding strength is a monotonic and near exponential function of temperature, resulting in a single, narrow temperature window for equilibrium assembly that may frustrate efforts to make multicomponent or hierarchical structures. Here, we present and quantitatively demonstrate a new approach to controlling the temperature dependence of DNA-induced colloidal interactions using toehold exchange hybridization, a concept borrowed from dynamic DNA nanotechnology. These competitive hybridization pathways allow additional control over the thermodynamics of bridge formation and provide a simple way to engineer novel temperature dependences that need not be exponential or monotonic. This additional functionality will be useful in the rational design of new multicomponent, hierarchical, or reconfigurable self-assembling systems.

1:39PM N30.00013 Phases and Dynamics of Self-Assembled DNA Programmed Nanocubes1
CHRISTOPHER KNOROWSKI, Department of Physics and Astronomy and Ames Laboratory, Iowa State University, Ames, IA, ALEX TRAVESSET, Iowa State University Department of Physics and Astronomy and Ames Lab DOE — Systems of Nanoparticles grafted with complementary DNA strands have been shown to self-assemble into an array of superlattices. In this talk, we extend our previous model [1], which successfully predicted equilibrium phases and dynamics of assembly for spherical Nanoparticles [1,2] without fitting parameters, to the case of nanocubes. We show that the phase diagram consists of bcc and sc lattices, depending on DNA length. The bcc lattices are either rotator and orientational glass or cubatic. For temperatures above the DNA melting temperature, the system is equivalent to f-star polymer systems, and consists of bcc, also with rotator, orientational glass or cubatic orientational order as well as sc. We also study self-assembly for spherical nanoparticles [1,2] without fitting parameters, to the case of nanocubes. We show that the phase diagram consists of bcc and sc lattices, to self-assemble into an array of superlattices. In this talk, we extend our previous model [1], which successfully predicted equilibrium phases and dynamics of self-assembled systems.

1:51PM N30.00014 Assembly of tetrahedral gold nanoclusters from binary colloidal mixtures1
NICHOLAS B. SCHADE, Harvard University, DAZHI “PETER” SUN, Brookhaven National Laboratory, MIRANDA C. HOLMES-CERFON, ELIZABETH R. CHEN, EMILY W. GEHRELS, JONATHAN A. FAN, Harvard University, OLEG GANG, Brookhaven National Laboratory, VINOTHAN N. MANOHARAN, Harvard University — We experimentally investigate the structures that form when colloidal gold nanospheres cluster around smaller spheres. We use nanoparticles coated with complementary DNA sequences to assemble the clusters, and we observe them under electron microscopy. Previous experiments using polystyrene microspheres indicate that a 90% yield of tetrahedral clusters is possible near a critical diameter ratio; random sphere packing serves as a useful model for understanding this phenomenon. Here we examine how this approach can be scaled down by an order of magnitude in size, using gold building blocks. We study how this method can be used to assemble tetrahedral plasmonic resonators in order to create a bulk, isotropic, optical metamaterial.

1This work is funded by DOE through the Ames Lab under Contract DE-AC02-07CH11358. Most simulations are performed on the Exalted GPU cluster, which is funded by a grant from Iowa State University and Nvidia Corp.
**2:03PM N30.00015 Field-directed assembly of colloidal ellipsoids**

PETER J. BELTRAMO, ERIC M. FURST, University of Delaware — Self-assembly of colloidal building blocks into ordered structures has become a rapidly evolving area of research due to the novel properties (thermal transport, photonic, electromagnetic) imparted by periodicity. Assembly of anisotropic particles presents numerous challenges, namely kinetic arrest at high particle volume fractions due to glasy dynamics. This prevents the realization of theoretically predicted close-packed phases. In this work, we use AC electric fields to align dilute polystyrene ellipsoidal particles in suspension and a drying front to concentrate the particles into orientationally ordered thin films. Results using several aspect ratio particles are presented. The dilute electrokinetic properties which enable this field-directed assembly are characterized by dielectric spectroscopy and electrophoretic mobility measurements. Light scattering is used to evaluate the frequency and field strength dependence of particle alignment. Finally, the nanomechanical and phononic properties of the films are evaluated by Brillouin light scattering.

1Funding from the U.S. Department of Energy (Basic Energy Sciences Grant DE-FG02-09ER46026) is gratefully acknowledged.

2M. Grzelczak et al. ACS Nano, 4, 3591 (2010)


**Wednesday, March 20, 2013 11:15AM - 2:15PM**

**Session N36 DCMP: Superconductivity: Mesoscopic Techniques and Applications**

**11:15AM N36.00001 Cantilever micro-susceptometry of mesoscopic Bi2212 samples**

HRYHORIY POLSHYN, RAFFI BUDAKIAN, University of Illinois at Urbana-Champaign, GENDA GU, Brookhaven National Laboratory — Fluidic quantization provides a direct means to study phase coherence. In cuprate superconductors, there have been observations which suggest that phase coherent superconducting fluctuations may persist at temperatures significantly above Tc. The focus of this work is to study the vortex states in mesoscopic cuprate superconducting samples to directly probe phase coherence over a wide range of temperatures. We present cantilever torque susceptometry measurements of micron and sub-micron size Bi2212 rings and disks. The high sensitivity of this technique allowed observation of transitions between different fluxoid states of a single ring, and the discrete vortex states of micron size disks. The dependence of magnetic susceptibility on diameter and wall thickness of the ring was investigated. Measurements were made at different values of the in-plane magnetic field, and over a wide range of temperatures.

1This work was supported by the Center for Emergent Superconductivity, an Energy Frontier Research Center funded by the US DOE, Office of Science.

**11:27AM N36.00002 Measuring superconducting delta-doped strontium titanate bilayers using the scanning SQUID technique**

HILARY NOAD, KATJA C. NOWACK, HISASHI INOUE, CHRISTOPHER BELL, YASUYUKI HIKITA, HAROLD Y. HWANG1, KATHRYN A. MOLER2, Stanford Institute for Materials and Energy Science, Stanford University, SLAC National Accelerator Laboratory, Menlo Park, CA 94025, USA — Delta-doped strontium titanate is a highly tunable system well-suited for studying two-dimensional superconductivity. Bilayer structures, in particular, offer the possibility of modifying interlayer coupling between sheets of superconducting electrons. We can locally probe superconductivity and magnetism as a function of temperature using scanning SQUID susceptometry. We will discuss prospects for using the scanning SQUID technique to measure unusual effects, such as multi-component superconductivity, that may arise in delta-doped strontium titanate bilayers.

1Second affiliation: Department of Applied Physics, Stanford University, Stanford, CA 94305

2Second affiliation: Department of Applied Physics, Stanford University, Stanford, CA 94305

**11:39AM N36.00003 Fabrication of La2−xSrxCuO4 Superconductor Nanodevices**

NICHOLAS LITOMBE, Harvard University, ANTHONY BOLLINGER, IVAN BOZOVIC, Brookhaven National Laboratory, JENNY HOFFMAN, Harvard University — In order to investigate dimension-limited superconductivity in cuprates, we explore methods of nanopatterning La2−xSrxCuO4 (LSCO). We use high resolution e-beam and photo-lithographic fabrication techniques, coupled with appropriate chemical and physical pattern transfer techniques. In particular, we focus on quasi-1D LSCO nanowire devices where we study random telegraph noise (RTN) signals from possible nematic domain fluctuation dynamics.

1This research was supported by the New York Community Trust–George Merck Fund

**11:51AM N36.00004 Development of a Nb-AlxOy-Nb trilayer process at the University of Washington**

ANDREW WAGNER, University of Washington, AXION DARK MATTER EXPERIMENT COLLABORATION — We present progress made at the Washington Micro-Fabrication Facility toward the production of SQUID amplifiers from a Nb – AlxOy – Nb trilayer process. Details of a simplified trilayer process are presented and the capability to fabricate 3 micrometer Josephson Junctions from the process with controllable critical current densities is demonstrated. We discuss how these results can be applied to the production of SQUID, SLUG or Josephson Parametric amplifiers operating in the microwave band for the Axion Dark Matter eXperiment (ADMX) located at the University of Washington.

1University of Washington MicroFabrication Facility and CENPA

**12:03PM N36.00005 Superconducting spin switch with infinite magnetoresistance**

BIN LI, Francis Bitter Magnet Lab, MIT, NIKLAS ROSCHEWSKY, FBML, MIT and Georg-August-Universitaet, Gottingen, MARKUS MUNZENBERG, Georg-August-Universitaet, Gottingen, MARIUS EICH, FBML, MIT, MARGUERITE EPSTEIN-MARTIN, FBML, MIT and Spencer School, New York, JAGADEESH S. MOODERA, FBML and Physics Department, MIT — Nearly five decades ago de Gennes theoretically predicted that below the superconducting transition temperature Tc the resistance in a FI/S/FI (FI-ferromagnetic insulator; S-superconductor) trilayer structure depends on the magnetization direction of the two FI layers [de Gennes, Phys. Lett. 123, 10 (1966)]. This prediction is experimentally demonstrated here. We present magneto-transport properties in a EuS/Al/EuS structure, showing an infinite magnetoresistance by tuning the internal exchange field at the FI/S interface. The superconducting order parameter was suppressed when the magnetic moment of the two EuS layers aligned in parallel whereas it was least affected when the two EuS layers have their magnetizations in antiparallel alignment: one could tune between the superconducting and normal states by the FI magnetization configuration. Importantly either of these two states could be maintained in zero applied fields, thus creating a nonvolatile two-level memory state. It was also shown that this is entirely an interface proximity effect and could be destroyed by introducing just a monolayer of Al2O3 barrier in between the interfaces. Furthermore the observed resistance switching field correlated with the surface anisotropy of the EuS layers.

1This work was supported by NSF DMR-1207469 and DOE DE-SC0001088.
12:15PM N36.00006 Thin semi-rigid coaxial cables for cryogenics applications. AKIHIRO KUSHINO, Asahikawa National College of Technology, SOICHI KASAI, COAX CO., LTD. — We have developed cryogenic coaxial cables for low temperature signal readout from sensitive devices, such as transition edge sensors, superconducting tunnel junctions, and kinetic inductance detectors. In order to reduce heat penetration into cryogenic stages, low thermal conductivity metals were chosen for both conductor and outer electrical conductors. Various types of coaxial cables, employing stainless-steel, cupro-nickel, brass, beryllium-copper, phosphor-bronze, niobium, and niobium-titanium, were manufactured using drawing dies. Thermal and electrical properties were investigated between 1 and 8 K. Coaxial cables made of copper alloys showed thermal conductance roughly consistent with literature, meanwhile Nb coaxial cable must be affected by the drawing process and thermal conductance was lowered. Attenuation of superconducting Nb and NbTi coaxial cables were observed to adequately small up to above 10 GHz compared to those of normal conducting coaxial cables, which are subject to the Wiedemann-Franz law. We also measured normal conducting coaxial cables with silver-plated center conductors to improve high frequency performance.

12:27PM N36.00007 Novel structural transformation in the ultrathin films of cuprates and its influence on electronic and magnetic properties. D. SAMAL, University of Twente, TAN HAIYAN, University of Antwerp, H. MOLEGRAAF, B. KUIPER, University of Twente, W. SIEMONS, Oak Ridge National Lab, SARA BALS, JO VERBEECK, GUSTAAF VAN TENDELOO, University of Antwerp, Y. TAKAMURA, University of California, Davis, ELKE ARENHOLZ, CATHERINE JENKINS, Advanced Light Source. G. RIJNDERS, GERT J AN KOSTER, University of Twente — We report on the evidence found for structural transformation in ultrathin films of two cuprate systems viz. SrCuO$_2$(SCO) and CuO. In case of SCO ultrathin films, we show a transformation from the bulk planar to chain-like structure, below a critical thickness, due to associated electrostatic instability. Results based on X-ray diffraction, X-ray photoelectron diffraction and scanning transmission electron microscopy reveal an elongation of the unit cell by ∼0.5Å along the c-axis and the presence of oxygen in the Sr plane for chain-like structure. Polarized X-ray absorption spectroscopy reveals a preferential occupation of Cu $d_{x^2-y^2}$ orbital in case of the chain like structure unlike to the planar one. For the case of ultrathin CuO films, we find strain induced structural transformation from monolonic to tetragonal phase, akin to other 3d transition metal monoxides and reveals relatively higher Neel temperature. Our findings point to a unique structural stabilization process for ultrathin cuprate layers and provide new insight for the experimental realization of novel hybrids to look for enhanced superconducting properties. References: Zhong et al, PRB 85, 124411(R) (2012); Siemons et al, AI PRB 79,195122 (2009)

12:39PM N36.00008 Dynamical I-V Characteristics of SNS Junctions. KEVIN SPAHR, JONATHAN GRAVELINE, CHRISTIAN LUPIEN, Université de Sherbrooke, MARCO APRILI, Université Paris-Sud, BERTRAND REULET, Université de Sherbrooke — We probe the dynamics of a Superconductor /Normal Metal/ Superconductor junction (SNS: Nb / Al above its critical temperature / Nb) by measuring its voltage / current characteristics while applying an ac current of frequency in the range 1-200 MHz. We observe a dynamical phase transition as a function of the frequency and amplitude of the ac current. At low frequency there is a continuous change in the dynamical behavior of the junction, replaced an abrupt change and hysteresis at high frequency. The crossover frequency between the two regimes has a strong temperature dependence similar to that of the electron-phonon interaction rate.

12:51PM N36.00009 Spectroscopy of Andreev Bound States: revealing the hidden side of the Josephson effect. ÇAĞLAR GIRIT, LANDRY BRETHEAU, HUGUES POTHIER, DANIEL ESTEVE, CRISTIAN URBINA, Groupe quantonome CEA Saclay — The Josephson effect describes how phase coherence is established between two weakly coupled superconductors. Microscopically, the Josephson current is carried by Cooper pairs, occupying Andreev Bound States, localized at the weak link. Andreev Bound States, which come in particle-hole symmetric pairs, constitute a spin-like degree of freedom. In our experiment, we detect the transition to the excited Andreev bound state in a superconducting atomic contact using a Josephson junction as a broadband (5-90 GHz) spectrometer. Not only do we clearly resolve the Andreev transition, but we also identify spectroscopic lines arising from anticrossings with a Josephson plasma mode of the environment. Our results demonstrate the accessibility of a pseudospin degree of freedom in the Josephson effect.

1:03PM N36.00010 X-ray Structural Studies of Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ Exfoliated Nanocrystals. ANDREEA LUPASCU, Department of Physics, University of Toronto, RENFEI FENG, Canadian Light Source. LUKE J. SANDILANDS, ZIXIN NIE, VIKTORIYA BAYDINA, Department of Physics, University of Toronto, GENDA GU, Condensed Matter Physics & Materials Science Department, Brookhaven National Laboratory, SHIMPEI ONO, Central Research Institute of Electric Power Industry, YOICHI ANDO, Institute of Scientific and Industrial Research, Osaka University, KENNETH S. BURCH, YOUNG-JUNE KIM, Department of Physics, University of Toronto — Structural studies of nanocrystals produced via mechanical exfoliation are not only essential for examining structure quality or structural changes at reduced-dimensionality, but also for understanding the role of substrates in the exfoliation process. Highly focused, tunable synchrotron X-ray beams enable the use of non-destructive characterization tools to study exfoliated samples on a variety of substrates. We demonstrate that structural and spectroscopic information can be obtained on nanocrystals as thin as 6 nm, by using a combination of micro X-ray fluorescence ($\mu$ XRF), micro X-ray absorption near-edge spectroscopy ($\mu$ XANES), and X-ray microdiffraction ($\mu$ XRD) techniques. $\mu$ XRF is used to locate the sample of desired thickness, $\mu$ XANES and $\mu$ XRD are used to obtain electronic and structural information, respectively. We report a substantial substrate effect for Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ nanocrystals exfoliated on Si/SiO$_2$ and mica substrates. The “4.7 b” structural modulation, characteristic of bulk crystals, vanishes below a thickness of 60 nm on mica, and is drastically suppressed below 60 nm for the Si/SiO$_2$ substrate.

1:15PM N36.00011 Mechanical detection of single-quantum-level fluxoid relaxation in an Nb micro-ring. JAE-HYUK CHOI, HEON-HWA CHOI, YUN-WON KIM, Division of Physical Metrology, Korea Research Institute of Standards and Science, Daejeon, Korea, SOON-GUL LEE, Department of Display and Semiconductor Physics, Korea University, Jochiwon, Chungnam, Korea, MAHN-SOO CHOI, Department of Physics, Korea University, Seoul, Republic of Korea — We developed a highly sensitive static force magnetometry, originally proposed for sub-pico-newton force standard, which enabled the observation of single fluxoids selectively and their dynamics in a superconducting micro-ring. For an Nb micro-ring with inner diameter of 4.0 µm and outer diameter of 8.0 µm, we observed a preferential occupation of Cu $d_{x^2-y^2}$ orbital in case of the chain like structure unlike to the planar one. For the case of ultrathin CuO films, we find strain induced structural transformation from monolonic to tetragonal phase, akin to other 3d transition metal monoxides and reveals relatively higher Neel temperature. Our findings point to a unique structural stabilization process for ultrathin cuprate layers and provide new insight for the experimental realization of novel hybrids to look for enhanced superconducting properties. References: Zhong et al, PRB 85, 124411(R) (2012); Siemons et al, AI PRB 79,195122 (2009)

1:27PM N36.00012 Studying phonon and quasiparticle heating effects on SINIS Coolers. THOMAS AREF, HUNG NGUYEN, JUHA MUHONEN, JUKKA PEKOLA, O.V. Lounasmaa Laboratory, Aalto University — A Normal-Insulating-Superconductor (NIS) tunnel junction can function as an electronic cooler. This is typically done in the SINIS configuration where the normal metal island is the object being cooled. By applying proper biasing, the bandgap in the superconductor can be used as an energy filter, allowing hot electrons to escape from the normal island and cold electrons to enter the island from the superconductor. This narrows the Fermi distribution of the electrons on the island, effectively lowering their temperature. By coupling this electronic refrigeration to phonons, the phononic temperature can be reduced as well. These SINIS coolers have potential for replacing other cryogen based refrigeration techniques at low temperatures. One primary aim is to produce an efficient, solid-state, cooling platform that cools small devices and their electronic components.

References: Zhong et al, PRB 85, 124411(R) (2012); Siemons et al, AI PRB 79,195122 (2009)
Coupling carbon nanotube mechanics to a superconducting circuit.

HELENE BOUCHIAT, Laboratoire de Physique des Solides, F-91405 Orsay, FRA — Most properties of a non superconducting (N) metal connected to two contacts can be seen as resulting from the phase dependent Andreev states (AS) in N. Density of states in N is then drastically modified from displacements of the nanotube. Incorporating this SQUID into superconducting resonators and qubits should enable the detection and manipulation of nanotube mechanical quantum states at the single-phonon level.

Spin-precession-assisted tunneling in hybrid superconducting point contacts.

CECILIA HOLMQVIST, WOLFGANG BELZIG, University of Konstanz, MIKAEL FOGELSTROM, Chalmers University of Technology — The charge and spin transport properties of a quantum point contact coupled to a nanomagnet depends strongly on the dynamics of the nanomagnet's spin. We analyze the current-voltage characteristics of a junction coupled to a spin whose dynamics is modeled as Larmor precession brought about by an external magnetic field. The interaction between the spin dynamics and the Josephson effect leads to a rich subgap structure due to spin-precession-assisted multiple Andreev reflections. Additionally, the spin current displays Shapiro-like resonances due to the interplay between the ac Josephson current and the Larmor precession.

Probing the Dynamics of Andreev States in Coherent Normal/Superconducting ring: Evidence for a noisy supercurrent.

BASTIEN DASSONNEVILLE, Laboratoire de Physique des Solides, F-91405 Orsay, FRA, FRANCESCA CHIodzi, Institut d'Electronique Fondamentale, F-91405 Orsay, FRA, SOPHIE GUERON, MEYDI FERRIER, HELENE BOUCHIAT, Laboratoire de Physique des Solides, F-91405 Orsay, FRA — Most properties of a non superconducting (N) metal connected to two superconductors (an SNS junction) can be seen as resulting from the phase dependent Andreev states (AS) in N. Density of states in N is then drastically changed with the emergence of a small energy gap, the minigap. Whereas AS equilibrium properties are well understood, AS dynamics is a more complex issue.

We perform experiments on a phase (φ) biased NS ring coupled to a superconducting resonator. The modification of the resonances (f from 200 MHz up to 14 GHz) yields the complex phase dependent susceptibility ∂′′ χ = χ′′ + iχ′ which is proportional to the current flow through the ring. A more striking finding [2] is the existence of a dissipative χ′ related to the supercurrent flowing through the ring. Moreover, as f increases we show that the main dissipation mechanism changes from population relaxation to microwave-induced transitions across the minigap.

References:

Wednesday, March 20, 2013 2:30PM - 5:30PM –
Session R1 DCMP GMAG: Invited Session: Controlling Magnetism Without Magnetic Fields
Ballroom I - Ramamoorhey Ramesh, University of California at Berkeley

Electric Field Control of Magnetization Using Multiferroic BFO.

SAYEEL SALAHUDDIN, University of California, Berkeley — No abstract available.

Controlling Magnetism by light.

THEO RASING, Radboud University Nijmegen — From the discovery of sub-picosecond demagnetization over a decade ago to the recent demonstration of magnetization reversal by a single 40 femtosecond laser pulse, the manipulation of spins by ultra short laser pulses has become a fundamentally challenging topic with a potentially high impact for future spintronics, data storage and manipulation and quantum computation. In addition, when the time-scale of the perturbation approaches the characteristic time of the exchange interaction (~ 10-100 fs), the magnetization dynamics enters a novel, highly non-equilibrium, regime, which was recently demonstrated by both fs optical and X-ray experiments. Theoretically, this field is still in its infancy, using phenomenological descriptions of the nonequilibrium dynamics between electrons, spins and phonons via 2- or 3-temperature models and atomistic spin simulations. A proper description should include the time dependence of the exchange interaction and nucleation phenomena on the nanometer length scale. Such developments need to be supported by experimental investigations of magnetism at its fundamental time and length scales, i.e. with fs time and nanometer spatial resolution. Such studies require the excitation and probing of the spin and angular momentum contributions to the magnetic order at timescales of 10fs and below, a challenge that could be met by the future fs X-ray FEL’s but in some cases also with purely optical techniques.

Recent references:

This work is supported by the Netherlands Organization for Scientific Research (NWO) and the FP7 programme of the EU.
range of approximately 90 degrees at room temperature in these hybrids. On the other hand, I will show that the spin mechanics scheme also is operational at anisotropy and thus induces a magnetization reorientation. This allows for a voltage-controlled, fully reversible magnetization orientation manipulation within a range of approximately 90 degrees at room temperature in these hybrids. On the other hand, I will show that the spin mechanics scheme also is operational at GHz frequencies. In the corresponding experiments, we use surface acoustic waves (SAWs) propagating in Ni/LiNbO₃ hybrid devices for the all-elastic excitation and detection of ferromagnetic resonance (FMR). Our SAW magneto-transmission data are consistently described by a modified Landau-Lifshitz-Gilbert approach [2], in which the magnetization precession is not driven by a conventional, external microwave magnetic field, but rather by a purely virtual, internal tickle field stemming from radio-frequency magneto-elastic interactions. This causes a distinct magnetic field orientation dependence of elastically driven FMR, observed in both simulations and experiment. Last but not least, I will address perspectives for spin mechanics experiments, e.g., the study of magnon-phonon coupling, or acoustic spin pumping [3] in normal metal/ferromagnet hybrid structures.


4:18PM R1.00004 Control of Magnetic Properties Across Metal to Insulator Transitions¹. JOSE DE LA VENTA, University of California San Diego — Controlling the magnetic properties of ferromagnetic (FM) thin films without magnetic fields is an on-going challenge in condensed matter physics with multiple technological implications. External stimuli and proximity effects are the most used methods to control the magnetic properties. An interesting possibility arises when ferromagnets are in proximity to materials that undergo a metal-insulator (MIT) and structural phase transition (SPT). The stress associated with the structural changes produces a magnetoelastic anisotropy in proximity coupled ferromagnetic films that allows controlling the magnetic properties without magnetic fields. Canonical examples of materials that undergo MIT and SPT are the vanadium oxides (VO₂ and V₂O₅). VO₂ undergoes a metal/rutile to an insulator/monoclinic phase transition at 340 K. In V₂O₅ the transition at 160 K is from a metallic/rhombohedral to an insulating/ monoclinic phase. We have investigated the magnetic properties of different combinations of ferromagnetic (Ni, Co and Fe) and vanadium oxide thin films. The (0.32%) volume expansion in VO₂ or the (1.4%) volume decrease in V₂O₅ across the MIT produces an interfacial stress in the FM overlayer. We show that the coercivities and magnetizations of the ferromagnetic films grown on vanadium oxides are strongly affected by the phase transition. The changes in coercivity can be as large as 168% and occur in a very narrow temperature interval. These effects can be controlled by the thickness and deposition conditions of the different ferromagnetic films. For VO₂/Ni bilayers the large change in the coercivity occurring above room temperature opens the possibilities for technological applications.


4:54PM R1.00005 Controlling Magnetism with electric fields, LEONID ROKHINSON, Purdue University — No abstract available.

Wednesday, March 20, 2013 2:30PM - 5:30PM –
Session R2 DCMP: Invited Session: New Developments in Organic Spintronics Ballroom II - Markus Wohlgemann, University of Iowa

2:30PM R2.00001 Electrically detected magnetic resonance in organic light emitting diodes¹, CHRISTOPH BOEHME, Department of Physics and Astronomy, University of Utah, Salt Lake City, 84112 UT, USA — Due to the built-in weak spin-orbit coupling of carbon based materials, electronic transitions in organic semiconductors are subjected to strong spin-selection rules that are responsible for a number of interesting electron spin- and even nuclear spin-dependent electrical and optical properties of these materials, including device efficiencies of organic light emitting diodes and solar cells or magnetoresistive and magneto-optic effects. In recent years, we have studied how these effects work and how they can be utilized for organic semiconductor device improvement and new device applications. Our focus has been in particular on the effects of spin on π-conjugated polymer based bipolar injection devices (more commonly known as organic light emitting diodes, OLEDs). In OLEDs, spin-interactions between recombining charge carriers do not only control electroluminescence rates but also the magnetoresistance. We have shown that spin-coherence can be observed through current measurements [1] and that these effects can be utilized for a coherent, pulsed electrically detected magnetic resonance spectroscopy (pEDMR) which enables us to encode the qualitative nature of spin-dependent mechanisms (the polaron pair mechanism [2,3] and the triplet polaron recombination [4]) and the their dynamical nature (spin-relaxation, electronic relaxation, hopping times [5]). The insights gained from these studies have led to the invention of a robust absolute magnetic field sensor based on organic thin film materials with absolute sensitivities of <50nT/Hz²/² [6].


¹Acknowledgment is made to the DOE (#DESC0000909) and NSF through a MRSEC Project (#1121252) and a CAREER Project (#0953225).
3:06PM R2.00002 Direct measurements of spin propagation in organic spin valves by low-energy muon spin rotation

3:42PM R2.00003 Percolative Theory of Organic Magnetoresistance and Fringe-Field Magnetoresistance

4:18PM R2.00004 Spin-polarized organic light emitting diode based on a novel bipolar spin-valve

4:54PM R2.00005 Spin-orbit coupling in organic spintronics

Wednesday, March 20, 2013 2:30PM - 5:30PM – Session R3 GSNP DCMP: Invited Session: Nonequilibrium Relaxation and Aging in Materials Ballroom III - Uew Tauber, Virginia Polytechnic Institute and State University
2:30PM R3.00001 Nonequilibrium behavior in strongly correlated electron systems¹, DRAGANA POPOVIĆ, National High Magnetic Field Laboratory, Florida State University — There is growing evidence that nonequilibrium behavior may underlie many complex phenomena exhibited by strongly correlated electronic materials with disorder. A two-dimensional electron system (2DES) in Si metal-oxide-semiconductor field-effect transistors has emerged as an excellent model system for studying glassy or nonequilibrium charge dynamics near the metal-insulator transition (MIT). In particular, studies of both conductance relaxations and noise on disordered samples, using several different experimental protocols, have established that the 2DES in Si exhibits all the main manifestations of glassiness: slow, correlated dynamics, non-exponential relaxations, diverging equilibration time (as temperature \( T \to 0 \)), aging and memory. The results provide strong evidence that many such universal features are robust manifestations of glassiness, regardless of the dimensionality of the system. In addition, the experiments show that the 2D MIT is closely related to the melting of this Coulomb glass. The observations are consistent with predictions of the theoretical models that describe the MIT as a Mott transition with disorder. Some effects that are unique to Coulomb glasses have also been revealed, which should have important implications for theoretical modeling of the glassy dynamics in a 2DES and other strongly correlated materials.

¹Supported by NSF DMR-0905843 and NHMFL via NSF DMR-0654118.

3:06PM R3.00002 Universally slow, ARIEL AMIR, Harvard University — Glassy systems are very common in nature, from disordered electronic and magnetic systems to window glasses and crumpled paper. Among their key properties are slow relaxations to equilibrium without a typical timescale, and dependence of relaxation on the system’s age. After reviewing some of these physical systems, I will describe our approach to the problem, and show how it leads to a novel class of aging. The slow relaxations result from a broad distribution of “relaxation eigenmodes,” which relates to a particular class of random matrices. I will discuss recent results on the structure and localization properties of these modes, and their implications.

3:42PM R3.00003 Dynamical symmetries in ageing phenomena, MALTE HENKEL, Institut Jean Lamour, Universite de Lorraine Nancy — Systems undergoing physical ageing can be characterised by (i) undergoing slow relaxation (ii) absence of time-translation-invariance and (iii) dynamical scaling. Specific examples are obtained by quenching many-body systems from a high-temperature initial state to below their critical temperature. Here, we shall consider consequences of an assumed extension of dynamical scaling to a larger group of local scale-transformations. Explicit scaling forms of two-time responses and correlators are obtained. These will be compared with simulational data in simple magnets, as well as in many-body systems without an equilibrium stationary state, such as critical directed percolation or domain-growth in the Kardar-Parisi-Zhang universality class.


4:18PM R3.00004 Probing equilibrium by nonequilibrium dynamics: Aging in Co/Cr superlattices¹, CHRISTIAN BINEK, University of Nebraska-Lincoln — Magnetic aging phenomena are investigated in a structurally ordered Co/Cr superlattice through measurements of magnetization relaxation, magnetic susceptibility, and hysteresis at various temperatures above and below the onset of collective magnetic order. We take advantage of the fact that controlled growth of magnetic multilayer thin films via molecular beam epitaxy allows tailoring the intra and inter-layer exchange interaction and thus enables tuning of magnetic properties including the spin-fluctuation spectra. Tailored nanoscale periodicity in Co/Cr multilayers creates mesoscopic spatial magnetic correlations with slow relaxation dynamics when quenching the system into a nonequilibrium state. Magnetization relaxation in weakly correlated spin-systems depends on the microscopic spin-flip time of about 10 ns and is therefore a fast process. The spin correlations in our Co/Cr superlattice bring the magnetization dynamics to experimentally better accessible time scales of seconds or hours. In contrast to spin-glasses, where slow dynamics due to disorder and frustration is a well-known phenomenon, we tune and increase relaxation times in ordered structures. This is achieved by increasing spin-spin correlation between mesoscopically correlated regions rather than individual atomic spins, a concept with some similarity to block spin renormalization. Magnetization transients are measured after exposing the Co/Cr heterostructure to a magnetic field set for various waiting times. Scaling analysis reveals an asymptotic power-law behavior in accordance with a full aging scenario. The temperature dependence of the relaxation exponent shows pronounced anomalies at the equilibrium phase transitions of the antiferromagnetic superstructure and the ferromagnetic to paramagnetic transition of the Co layers. The latter leaves only weak fingerprints in the equilibrium magnetic behavior but gives rise to a prominent change in nonequilibrium properties. Our findings suggest that scaling analysis of nonequilibrium data can serve as a probe for weak equilibrium phase transitions.

¹Financial support by NRI, and NSF through EPSCoR, and MRSEC 0820521 is greatly acknowledged.

4:54PM R3.00005 Aging processes in disordered materials: High-\( T_c \) superconductors and ferromagnets¹, MICHEL PLEIMLING, Virginia Tech — Physical aging is generically encountered in systems far from equilibrium that evolve with slow dynamics. Well known examples can be found in structural glasses, spin glasses, magnetic systems, and colloids. Recent years have seen major breakthroughs in our understanding of aging processes in non-disordered systems. Progress in understanding aging in disordered systems has been much slower though. In this talk I discuss non-equilibrium relaxation in two different types of disordered systems: coarsening ferromagnets with disorder, characterized by a crossover from an initial power-law like growth of domains to a slower logarithmic growth regime, and interacting vortex lines in disordered type-II superconductors, where the interplay of vortex-vortex interaction and pinning results in a very rich non-equilibrium behavior.

¹This work is supported by the US Department of Energy through grant DE-FG02-09ER46613.

Wednesday, March 20, 2013 2:30PM - 5:30PM –
Session R4 DCMP: Topological insulators: Nanostructures and Possible Applications: Transport phenomena • Ballroom IV • Vidya Madhavan, Boston College

2:30PM R4.00001 ABSTRACT WITHDRAWN –
2:42PM R4.00002 Thermoelectric power factor of topological insulator Bi$_2$Sb$_2$Te$_3$... TE CHIH HSUING, TING YUAN CHEN, LI ZHAO, YI HSIN LIN, YANG YUAN CHEN, Institute of Physics, Academia Sinica, Taipei, Taiwan — Topological insulator (TI) is a new quantum material. The surface states of TIs are protected by time-reversal symmetry which allows charge carrier to propagate on the edge of surface conducting channel without scattering. Bi$_2$Sb$_2$Te$_3$... is a well-known TI [1] and thermoelectric material because of its promising thermoelectric performances at room temperature. The conversion efficiency of thermoelectric material is characterized by the dimensionless figure of merit ZT. Decades of effort were devoted to ZT optimization either through composition alteration or nanostructure fabrication. In this study, the temperature dependence of resistance of bulk (exfoliated specimen with 140 μm thickness) shows semiconductor behavior (0.04 Ω cm at 300 K) without saturating regime in lower temperatures. In contrast, its nanoflake counterpart (100-500 nm) [2] shows a transition from semiconductor to metallic behavior near 100 – 150 K with decreasing temperature and saturation at 10 K. Surface contribution to the total conductance of exfoliated specimens was acquired through Hall effect measurements in the magnetic field ranging from -9 to 9 Tesla. Surface contribution of BSTS samples increases from 3% to 70% as thickness decreases from 140 to 7 μm. In this work, we report a systematic study of thermoelectric power factor for various thicknesses of BSTS specimens to examine the thermoelectric power factor of their surfaces.


2:54PM R4.00003 Spin-dependent Peltier effect in 3D topological insulators... PARIJAT SENGUPTA, TILLMANN KUBIS, MICHAEL POVOLOTSKYI, GERHARD KLIMECK, Purdue University — The Peltier effect represents the heat carrying capacity of a certain material when current passes through it. When two materials with different Peltier coefficients are placed together, the Peltier effect causes heat to flow either towards or away from the interface between them. This work utilizes the spin-polarized property of 3D topological insulator (TI) surface states to describe the transport of heat through the spin-up and spin-down channels. It has been observed that the spin channels are able to carry heat independently of each other. Spin currents can therefore be employed to supply or extract heat from an interface between materials with spin-dependent Peltier coefficients. The device is composed of a thin film of Bi2Se3 sandwiched between two layers of Bi2Te3. The thin film of Bi2Se3 serves both as a normal and topological insulator. It is a normal insulator when its surfaces overlap to produce a finite band-gap. Using an external gate, Bi2Se3 film can be again tuned in to a TI. Sufficiently thick Bi2Te3 always retain TI behavior. Spin-dependent Peltier coefficients are obtained and the spin Nernst effect in TIs is shown by controlling the temperature gradient to convert charge current to spin current.

3:06PM R4.00004 Surface-to-surface scattering in three-dimensional (3D) topological insulator (TI) thin films... GEN YIN, DARSHANA WICKRAMARATNE, ROGER LAKE, Department of Electrical Engineering, University of California, Riverside — When the thickness of a 3D TI material is reduced below approximately 6nm, hybridization of the opposite surfaces states can result in inter-surface tunneling. Due to the rotational symmetry of the thin film, the k-s locking relation on opposite surfaces also has opposite chirality. Thus, in this inter-surface scattering mechanism, back-scattering is allowed without the flip of the spin. This effect breaks the protection of TI surface states against back-scattering. To investigate the influence of the inter-surface scattering mechanism, we study different near-elastic scattering mechanisms in the surface state transport using Boltzmann transport equations within the relaxation time approximation. The effect of screened Coulomb impurities, low-energy acoustic phonons and surface magnetic impurities on the TI surface states will be discussed. The response of the inter-surface scattering of TI states to various external stimuli such as a Rashba-like splitting and the orientation of the impurity magnetic moments will also be presented. Using simulation results, we propose possible experimental methods to modulate the back-surface protection of TI surface states in thin film TI materials.

3:18PM R4.00005 Realization of Negative Capacitance with Topological Insulator Based MOS Capacitor... HUI YUAN, GMU, KAI ZHANG, ODU, HAO ZHU, HAITAO LI, DIMITRIS IOANNOU, GMU, HELMUT BAUMGART, ODU, CURT RICHTER, NIST, QI LIANG LI, GMU, ECE, GEORGE MASON UNIVERSITY TEAM, SEMICONDUCTOR AND DIMENSIONAL METROLOGY DIVISION OF NIST TEAM, ECE, OLD DOMINION UNIVERSITY TEAM — Negative capacitance is one of way to achieve steep subthreshold slope exceeding its thermal limit in metal-oxide-semiconductor field effect transistor (MOSFET). The common materials under study for negative capacitance are ferroelectric thin films. However, the integration of regular ferroelectric materials (e.g., PZT) into semiconductor based devices is usually difficult due to the high temperature required for crystallization and precise control of oxygen percentage in ferroelectric materials. In this work, we found that negative capacitance can be achieved by introducing a topological insulator interlayer into a conventional MOS capacitor. Three-dimensional topological insulators inherently contain a insulator/semiconductor bulk and a gapless conducting surface. When an electric field is added to topological insulator interlayer, imbalanced charge carriers (electrons and holes) would be generated and then accumulate on either surface of the film, resulting in a temporary residual polarization. As a result, a ferroelectric-like hysteresis and negative capacitance are achieved. We believe this approach will be very attractive to achieve steep subthreshold using negative capacitance.

1Supported by NSF Career grant 0846649.

3:30PM R4.00006 Transport measurements of the topological surface states in Bi$_2$Te$_3$ nanoribbon field effect devices... LUIS A. JAUREGUI, Purdue University, MICHAEL T. PETTES, LI SHI, University of Texas at Austin, LEONID P. ROKHINSON, YONG P. CHEN, Purdue University — We have grown nanoribbons (NRs) of Bi$_2$Te$_3$, a prototype topological insulator, by CVD and characterized them by TEM, Raman Spectroscopy and EDS. We fabricate backfield gate effect devices where the chemical potential is tuned and ambipolar field effect has been observed. The as-grown NRs are n-type and the 4-terminal resistance (R4p) versus temperature (T) shows a metallic behavior. Applying a sufficiently negative Vg, the R4p vs T displays an insulating behavior that saturates in a plateau at T < 100K, suggesting a metallic surface conduction dominant at low temperatures. Aharonov-Bohm (AB) oscillations of surface conducting carriers are observed in the magneto-resistance (MR) with a magnetic (B) field parallel to the NR axis. We have also measured the Shubnikov de Haas (SdH) oscillations with the B-field perpendicular to the NR axis at different carrier densities (n). The extrapolated Landau level crossing at 1/B = 0 is ~0.5 and the extracted cyclotron mass from the T-dependence of the SdH oscillations is proportional to 1/√n, providing direct evidence of the Dirac fermion nature of the topological surface state. Gate-tunable weak anti-localization is observed and the extracted number of decoupled coherent conduction channels is 2 at the charge neutrality point.

3:42PM R4.00007 Majorana qubit rotations in microwave cavities... CHRISTOPH BRUDER, ANDREAS NENNENKAMP, THOMAS L. SCHMIDT, Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — Majorana bound states have been proposed as building blocks for qubits on which certain operations can be performed in a topologically protected way using braiding. However, the set of these protected operations is not sufficient to realize universal quantum computing. We show that the electric field in a microwave cavity can induce Rabi oscillations between adjacent Majorana bound states. These oscillations can be used to implement an additional single-qubit gate. Supplemented with one braiding operation, this gate allows to perform arbitrary single-qubit operations.
3:54PM R4.00008 Electrical transport studies of Topological Insulator Bi$_2$Te$_3$ Nanotubes . RENZHONG DU, WEIWEI ZHAO, Department of Physics, Penn State Univ., JIAN WANG, ICQM, PKU, YUEWEI YIN, SINING DONG, XIAOGUANG LI, Department of Physics, USTC, CHAOXING LIU, MOSES CHAN, QI LI, Department of Physics, Penn State Univ. — We have studied electrical transport properties of candidate topological insulator Bismuth Telluride (Bi$_2$Te$_3$) nanotubes. Bi$_2$Te$_3$ nanotube samples were synthesized by solution phase method, with the outer diameters in the range of 70±5 nm and inner diameter 50±5 nm and the length of 3 to 10 um. Platinum contact leads were fabricated on the nanotubes by focusing ion beam assisted deposition. Electrical transport measurements were conducted at low temperatures and high magnetic fields (up to 9T). The nanotubes showed good insulating behavior in comparison with the thin films which are often metallic. Resistance oscillation as a function of magnetic field was observed when the magnetic field is applied parallel to the nanotubes. The periods range from 6000 Oe to 8350 Oe, which correspond to the diameter of 80 to 100 nm according to Aharonov-Bohm oscillation formula. This is close but slightly larger than the outer diameter of the nanotubes. The amplitude of the oscillations decays rapidly as field increases, possibly due to scattering. When the magnetic field was applied perpendicular to the nanotube, no resistance oscillation was observed. The possible origins of the oscillation effect will be discussed.

4:06PM R4.00009 Surface state transport in MBE-grown topological insulator (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ thin films and field effect transistors . JIFA TIAN, Department of Physics, Purdue University, CIUZI CHANG, Department of Physics, Tsinghua University, HELIN CAO, Department of Physics, Purdue University, JIUNING HU, Electrical Engineering, Purdue University, TAI-LUNG WU, Department of Physics, Purdue University, KE HE, XUCUN MA, IOP, CAS, QIKUN XUE, Department of Physics, Tsinghua University, YONG CHENG, Department of Physics, Purdue University — Topological insulators feature spin-helical, Dirac fermion surface states, promising potential applications in both nanoelectronics and spintronics. However, experimental identification of a clear transport signal of the surface state conduction is still challenging. Here, we report a systematical study of the gate tunable magneto-transport in MBE grown (Bi$_{1-x}$Sb$_x$)$_2$Te$_3$ (x=0.96) thin film on SrTiO$_3$ substrate. We observed an ambipolar field effect and a sign change in the Hall resistance as the gate voltage ($V_g$) crosses the Dirac point ($V_D$). Temperature ($T$) dependence of the resistance at different $V_g$ shows a transition from a metallic to an insulating bulk with 100% surface conduction at low $T$. Weak antilocalization measurements indicate a $\pi$ Berry phase near $V_D$. We also performed spin valve measurements and observed a resistance asymmetry (which reverses with reversing current direction) between the positive and negative in-plane magnetic fields, demonstrating the predicted locking between spin and momentum for the surface state. We also studied the thermal-electric transport, demonstrating a sign change of the thermoelectric power across the $V_D$ as the carrier type switches from electron to hole.

4:18PM R4.00010 ABSTRACT WITHDRAWN —

4:30PM R4.00011 Detection of Majorana Fermions in circuit QED . JEROME BOURASSA, CLEMENS MUELLER, ALEXANDRE BLAIS, Universite de Sherbrooke — Superconducting quantum circuits, such as the flux and the transmon qubits, have been proposed to measure and control the quantum state of topological qubits based on pairs of Majorana fermions [1-4]. This is possible by making the superconducting qubit transition frequencies sensitive to the fermionic parity representing the topological qubit state. In this talk, we propose to measure the fermionic parity using a flux qubit integrated in a microwave resonator. In this proposal, the flux qubit always remains in its ground state and is used as a passive circuit element which modifies the resonance frequency of the resonator depending on the charge state of a nearby pair of Majorana fermions. Since it is always in its ground state, the requirements on the qubit coherence properties and fabrication parameters are less stringent than in other proposals.


4:42PM R4.00012 Antimony arsenide: Chemical ordering and order-disorder transition in SbAs . DANIEL SHOEMAKER, Argonne National Laboratory, THOMAS CHASAPIS, Northwestern University, DAT DO, Michigan State University, MELANIE FRANCISCO, DUCK YOUNG CHUNG, Argonne National Laboratory, S. D. MAHANTI, Michigan State University, ANNA LLOBET, Lujan Neutron Scattering Center, LANL, KATZIRIKAUSKIEN KEKI, ICQM, CAS, A. ALI, Argonne National Laboratory — The A7 structure of the Group V elements can display chemical ordering of Sb and As, which were previously thought to mix randomly. Our structural characterization of the compound SbAs is performed by single-crystal and high-resolution synchrotron x-ray diffraction, and neutron x-ray pair distribution function analysis. All least-squares refinements indicate ordering of Sb and As, resulting in a GeTe-type structure without inversion symmetry. This lowering of symmetry does not result in any new Bragg reflections, so high-quality scattering data are required. High-temperature diffraction studies reveal an ordering transition around 550 K. Transport and infrared reflectivity measurements, along with first-principles calculations, find that SbAs has a direct band separation larger than that of Sb or As. Because even subtle substitutions in the semimetals, notably Bi$_{1-x}$Sb$_x$, can open semiconducting energy gaps, a further investigation of the interplay between chemical ordering and electronic structure on the A7 lattice is warranted.

4:54PM R4.00013 Probing Topological Superconductors with Elastic Strain Fields . DAVID SCHMELTZER, City College of the City University of New York, AVADH SAXENA, Los Alamos National Lab — We introduce a model for superconductivity in a topological insulator. The response of this system is probed by applying an external stress. We find that the strain field introduces connections in the superconductor and the response of the superconductor is given by the chiral anomaly which is proportional to the disclination density (for s-wave) or dislocations density (for the p-wave) superconductor. This result modifies the sound wave equations. In particular, we find that the core of the disclinations contains the normal matter in a superconductor. The presence of the long-range field induced by the topological response modifies the elastic properties of the solid which can be probed experimentally. The effect of rotating magnetic fields is also considered. Due to the Larmor theorem it is shown that the rotations replace the magnetic field by an effective magnetic field.

5:06PM R4.00014 High resolution spin- and angle-resolved photoelectron spectroscopy for 3D spin vectorial analysis . TAIUCHI OKUDA, KOJI MIYAMOTO, Hiroshima Synchrotron Radiation Center, Hiroshima University, AKIO KIMURA, Graduate School of Science, Hiroshima University, HIROFUMI NAMATAME, Hiroshima Synchrotron Radiation Center, Hiroshima University, MASAHIRO TAKAGI, University of Tsukuba, SHOICHI KODA, RIKO OUTI KANATZIDIS, Argonne National Laboratory — Topological superconductors make use of spin-polarized quasiparticles from the surface states of a topological insulator. Harnessing these states for applications requires detailed knowledge of the spin structure of the surface states. Here, we present a high resolution spin- and angle-resolved photoelectron spectroscopy (SARPES) instrument that we have developed to measure this two-dimensional spin structure. By combining a high brilliance synchrotron source and a novel, high-speed analyzer, we demonstrate that our system can be used to make high resolution (ΔE < 10 meV, Δθ ~ 0.2 °) compatible with the SARPES measurements. By placing two VLEED spin detectors orthogonally we have realized the polarization measurement of all spin components (x, y and z) with the high resolution. Some examples of the three-dimensional spin observation will be presented. [1] M. Hoesch et al., J. Electron Spectrosc. Relat. Phenom. 124, 263 (2002). [2] T. Okuda et al., Rev. Sci. Instrum. 81, 095101 (2010). [3] S. Souma et al., Rev. Sci. Instrum. 82, 103302 (2011).

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study the absorption mechanisms in graphene by selecting between conventional photovoltaic effects and photo-thermoelectric effects. Experiments suggest phonon scattering is suppressed and is predicted to lead to increased carrier lifetimes and enhanced photo-response. Using electrostatic gating, we are able to necessary to fabricate electrostatically controlled p-n junctions due to the longer optical length scales. Moreover, at these low energies (1 – 300 K) in the frequency range 0.3 – 3 THz. On top of a Drude-like response, we see a strong and narrow peak in \( \sigma(\omega) \) at \(~2.7\) THz. We analyze the overall Drude-like response using a disorder-dependent (unitary scattering) model, then attribute the peak at 2.7 THz to an enhanced density of states at that energy, that is caused by the presence of van Hove singularities arising from a commensurate twisting of the two graphene layers.

In the graphene physics, there are growing interests toward bilayer and trilayer graphene, whose electronic structures are distinct from that of monolayer graphene. It is then interesting to ask how the variety of low-lying electronic structures will affect optical responses, i.e., optical longitudinal and optical Hall conductivities, where the former describes the absorption while the latter the Faraday and Kerr rotations. Thus we study the optical conductivities in bilayer and trilayer graphene systems. We shall show for bilayer graphene that the Lifshitz transition associated with the trigonal warping greatly affects the resonance structures in Faraday rotation not only on low-energy scale where Dirac cones emerges but also in the higher-energy range with parabolic bands as a sequence of satellite resonances. For trilayer graphene, on the other hand, we shall show that the optical conductivities are dominated by the difference in the stacking order. In ABA trilayer, the resonance spectrum is a superposition of effective monolayer and bilayer contributions with band gaps, while ABC trilayer exhibits a distinct spectrum peculiar to the cubic-dispersed bands. In the latter, the trigonal warping effect becomes strong with a larger Lifshitz transition energy (~10 meV).

3:06PM R5.00004 Graphene’s Dynamic Conductivity in THz Regime, SUFEI SHI, UC Berkeley and Lawrence Berkeley National Laboratory, TSUNG-TA TANG, BO ZENG, LONG JU, UC Berkeley, FENG WANG, UC Berkeley and Lawrence Berkeley National Laboratory — Graphene, a single layer of carbon atoms arranged in honeycomb structure, has linear dispersion relation. The conductivity of graphene in the THz regime is highly tunable due to its gapless dispersion relation, which makes graphene a promising candidate for THz application. Using optical excitation as the pump, we probe graphene with a THz beam and study the THz conductivity in the time domain. This study sheds light on the carrier relaxation in graphene after intense optical excitation and provides information for designing future graphene-based opto-electronic device.

3:18PM R5.00005 Mid-Infrared Graphene Photoresponse, ALLEN HSU, Massachusetts Institute of Technology, PATRICK HERRING, Harvard University, YONG CHEOL SHIN, Massachusetts Institute of Technology, KI KANG KIM, Dongguk University, JING KONG, Massachusetts Institute of Technology — Graphene is a two-dimensional (2D) material that has attracted great interest for electronic devices since its discovery in 2004. Due to its zero band gap band structure, it has a broad-band optical absorption ranging from the far-infrared all the way to the visible making it potentially useful for infrared photodetectors. Electrostatically gated p-n junctions have demonstrated photocurrents in the near-IR (\( \lambda = 850\)nm), primarily due to hot carrier mechanisms. In order to study these mechanisms at longer wavelengths (\( \lambda = 10\) \( \mu \)m), high quality chemically vapor grown (CVD) graphene is necessary to fabricate electrostatically controlled p-n junctions due to the longer optical length scales. Moreover, at these low energies (~125 meV), optical phonon scattering is suppressed and is predicted to lead to increased carrier lifetimes and enhanced photo-response. Using electrostatic gating, we are able to study the absorption mechanisms in graphene by selecting between conventional photovoltaic effects and photo-thermoelectric effects. Experiments suggest that the photocurrent signal is enhanced by electrostatic gating near the Dirac peak and reduced disorder in the graphene sample.
3:30PM R5.00006 Ga Nanoparticle/Graphene Platforms: Plasmonic and Charge Transfer Interactions, CONGWEN YI, TONG-HO KIM, ECE, Duke University, YANG YANG, Physics, Duke University, MARIA LOSURDO, Institute of Inorganic Methodologies and of Plasmas, IMIP-CNR, Italy, APRIL S. BROWN, ECE, Duke University — Metal nanoparticle (NP) – graphene multifunctional platforms are of great interest for numerous applications, such as sensing and catalysis, and for fundamental studies on charge transfer and light-matter interactions. To understand platform-plasmon interactions, it is important to articulate the coupling of photon-based excitations, such as the interaction between plasmons in each of the material components, as well as their charge-based interactions dependent upon the energy alignment at the metal/graphene interface. Herein, we use liquid metal Ga nanoparticles, which can be deposited at 300K on graphene, to explore the surface-enhanced Raman spectroscopy modulation induced by the NPs. The localized charge transfer between Ga NPs and graphene are investigated, and enhancement of the Raman modes is correlated with metal coverage the transfer of electrons from Ga to graphene creating local regions of enhanced electron concentration which modify the electron-phonon interaction in graphene.

3:42PM R5.00007 Terahertz and mid-infrared reflectance of epitaxial graphene, CRISTIANE N. SANTOS, BENNOIT HACKENS, IMCN/NAPS, Université catholique de Louvain, Belgium, FRÉDÉRIC JOUCKEN, ROBERT SPORKEN, LMPME, Université de Namur (FUNDP), 5000 Namur, Belgium, JESSICA CAMPOS DELGADO, JEAN-PIERRE RASKIN, ICTM/ELEN, Université catholique de Louvain (UCL), 1348 Louvain-la-Neuve, Belgium, DOMINOS DE SOUSA MEÑESES, PATRICK ECHEGUT, CEMHTI-CNRS, 45071 Orléans cedex 2, France — Epitaxial graphene grown by thermal decomposition on SiC substrate has been widely investigated as a promising material for electronics and optics. Here, we investigate the infrared (IR) optical properties of few-layer (FL) and multilayer (ML) graphene on the C-terminated face of 6H-SiC substrates [1]. Contrary to IR transmission spectroscopy, which is hampered over a large part of the IR range by the SiC restrahlen band and multphonon absorption, IR reflectance gives access to invaluable information from terahertz (THz) to mid-infrared (MIR). Experimental data are well fitted with an explicit model over the entire spectral range using the SiC dielectric function and the graphene optical conductivity, taking into account both intraband and interband transitions. The number of layers extracted from our data in the FL and ML graphene corroborates with the X-ray photoelectron spectroscopy (XPS) measurements. We demonstrate that this consistent and simultaneous analysis leads to precise information on the carrier properties, doping level and the number of layers, even in the case of thick ML (30 layers or more). MIR microscopy was also used to check the sample homogeneity. [1] F. Joucken et al., Phys. Rev. B 83, 161408(R) (2012).

3:54PM R5.00008 Self-Energy and Excitonic Contributions to the Drude Conductivity of Doped Graphene, FELIPE JORNADA, STEVEN LOUIE, UC Berkeley — There has been a growing interest in the far infrared AC conductivity of doped graphene because of possible applications in optoelectronics, but there is still disagreement between recent experiments [1,2] and theories [3] with respect to the Drude weight. In this work we study from an ab-initio GW-BSE perspective the effects of the electron-electron interactions and excitons on the renormalization of the Drude weight. We discuss the role of quasiparticle lifetimes due to electron-electron and electron-phonon interactions, and we determine the AC conductivity in the forbidden region (i.e., for ω ≪ 2E_F). This work was supported by NSF grant No. DMR10-1006184, U.S. DOE under Contract No. DE-AC02-05CH11231 and the U.S. DOD - Office of Naval Research under RTC Grant No. N00014-09-1-1066. Computational resources have been provided by NERSC. [1] J. Horng et al., PRB 83, 165113 (2011). [2] H. Yan et al., ACS Nano 5, 9854 (2011). [3] S. H. Abedinpour et al., PRB 84, 045429 (2011).

4:06PM R5.00009 Tuning optical conductivity of large-scale CVD graphene by strain engineering, GUANGXIN NI, JING WU, ORHAN KAHYA, CHEE TAT TOH, Department of Physics, National University of Singapore, JONG HYUN AHN, School of Mechanical Engineering, Sungkyunkwan University, VITOR M. PEREIRA, BARBAROS ÖZYILMAZ, Department of Physics, National University of Singapore — Strain engineering has been widely recognized as an effective way to tailor the electrical properties of graphene. In the optical domain, the strain effect is also predicted to alter the optical conductivity of graphene, making graphene possible for the atomically thin optical elements. However, a direct experimental observation is still missing. Using the nanopillar structure, here we show that optical conductivity of CVD graphene under nonuniform strain exhibits periodic modulation as a function of polarization. The optical absorption can be further modulated via the application of an external uniaxial strain, which is confirmed by Raman spectroscopy as well as AFM images. Our experimental observations are quantitatively interpreted within the Kubo-Greenwood formalism. The manipulation of the optical properties of graphene demonstrated in this study can be effectively utilized in the novel type of optical devices and strain sensor applications.

4:18PM R5.00010 Tunable magneto-plasmons in graphene: an infrared study, ZHIGUO CHEN, National High Magnetic Field Laboratory, HUGEN YAN, XUESONG LI, WENJUAN ZHU, PHAEDON AVOURIS, FENGNIAN XIA, IBM T. J. Watson Research Center, ZHIQIANG LI, National High Magnetic Field Laboratory — Plasmons, collective oscillations of electrons, in graphene have attracted much attention due to their important roles in understanding the intriguing physics of graphene and potential applications in optoelectronic devices. Using infrared spectroscopy, we investigated the optical response of the plasmons in micrometer-sized graphene disks in high magnetic fields up to 18 T. Our study shows that the plasmon resonance splits into edge and bulk modes in magnetic fields. Due to the band structure of graphene, the splitting exhibits a sensitive doping dependence, which is not observed in the two-dimensional electron gas but is two-dimensional. By tuning the thickness of the graphene films, with the edge plasmons developing increasingly longer lifetimes in high fields. The latter behavior can be understood from the suppression of backscattering at the edges. Our work not only opens an avenue to explore the magneto-plasmon and edge physics in graphene but also supports the great potential of graphene for tunable magneto-optical devices.


4:30PM R5.00011 Long-range plasmon-assisted energy transfer over doped graphene1, KIRILL VELIZHANIN, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, TIGRAN SHAHBAZYAN, Department of Physics, Jackson State University, Jackson, MS 39217, USA — Förster resonance energy transfer (FRET) between spatially separated donor and acceptor fluorophores, such as dye molecules or semiconductors quantum dots, underpins diverse phenomena in physics, chemistry and biology. However, the range of present and potential applications of FRET is limited by its intrinsically short-range nature (∼1/FF). We demonstrate that longitudinal plasmons in doped monolayer graphene can mediate highly efficient long-range (∼1/R) energy transfer between nearby fluorophores, e.g., semiconductor quantum dots. We derive a simple analytical expression for the energy transfer efficiency that incorporates all the essential processes involved. We perform numerical calculations of the transfer efficiency for a pair of PbSe quantum dots near graphene for inter-fluorophore distances of up to 1 μm and find that the plasmon-assisted long-range energy transfer can be enhanced by up to a factor of ∼103 relative to FRET in vacuum.

1Work at LANL was performed under the NNSA of the U.S. DOE at LANL under Contract No. DE-AC52-06NA25396. Work at JSU was supported by the NSF under Grant No. DMR-1206975 and No. HRD-0833178 and under EPSCOR program.

4:42PM R5.00012 Graphene multilayers as hyperbolic metamaterials, ASHLEY DASILVA, ALLAN MACDONALD, University of Texas Austin — Graphene and multilayer graphene systems show promise for numerous electronic and optical applications in part due to the extraordinary tunability of graphene via gate voltage. We discuss the optical properties of electrically decoupled multilayer graphene systems. These can be described by the reflection and transmission coefficients, which we calculate using a transfer matrix approach. This point of view allows an explicit comparison between graphene multilayers and metal/dielectric multilayer metamaterials. In particular, we will compare multilayer graphene systems to hyperbolic metamaterials which have extreme anisotropy in the effective dielectric constant: εx = εy < 0 and εz > 0.
Session R10 GQI DCMP: Invited Session: New Platforms for Non-Abelian Statistics Majoranas and Beyond  309 - Kirill Shtengel, University of California, Riverside

2:30PM R10.00001 Coulomb-assisted braiding of Majorana fermions in a Josephson junction array , CARLO BEENAKKER, Leiden University, Instituut-Lorentz — We show how to exchange (braid) Majorana fermions in a network of superconducting nanowires by control over Coulomb interactions rather than tunneling. Even though Majorana fermions are charge-neutral quasiparticles (equal to their own antiparticle), they can have an effective long-range interaction through the even-odd electron number dependence of the superconducting ground state. The flux through a split Josephson junction controls this interaction via the ratio of Josephson and charging energies, with exponential sensitivity. By switching the interaction on and off in neighboring segments of a Josephson junction array, the non-Abelian braiding statistics can be realized without the need to control tunnel couplings by gate electrodes. This is a solution to the problem how to operate on topological qubits when gate voltages are screened by the superconductor.

3:06PM R10.00002 Zero-bias peaks and splitting in an Al–InAs nanowire topological superconductor as signature of Majorana fermions1 , MOTY HEIBLUM, Weizmann Institute of Science — Majorana fermions are the only fermionic particles that are expected to be their own antiparticles. While elementary particles of the Majorana type were not identified yet, quasi-particles with Majorana like properties, born from interacting electrons in the solid, were predicted to exist. Here, we present thorough experimental studies, backed by numerical simulations, of a system composed of an aluminum superconductor in proximity to an indium arsenide nanowire, with the latter possessing strong spin-orbit coupling and Zeeman splitting. Induced one-dimensional topological superconductor, supporting Majorana fermions at both ends, is expected to form. We concentrate on the characteristics of a distinct zero bias conductance peak (ZBP) and its splitting in energy - both appearing only with a small magnetic field applied along the wire. The ZBP was found to be robustly tied to the Fermi energy over a wide range of system parameters. While not providing a definitive proof of a Majorana state, the presented data and the simulations support its existence.

1Partial support by the European Research Council under the European Community’s Seventh Framework Program (FP7/2007-2013) / ERC Grant agreement # 227716.

3:42PM R10.00003 Exotic non-Abelian anyons from conventional fractional quantum Hall states1 , DAVID CLARKE, Caltech — Non-Abelian anyons are widely sought after for the exotic fundamental physics they harbor as well as for quantum computing applications. There now exist numerous blueprints for stabilizing the simplest type of non-Abelian anyon, defects binding Majorana fermion zero modes, by judiciously interfacing widely available materials. Following this line of attack, we introduce a device fabricated from conventional fractional quantum Hall states and s-wave superconductors. We show that a new type of zero mode is bound at the interface between the quantum Hall state and the superconductor. These zero mode operators have parafermionic rather than fermionic commutation relations, implying a topologically protected ground state degeneracy larger than that of Majoranas. We discuss how these modes might be experimentally identified (and distinguished from Majoranas) using Josephson measurements.

1Supported by NSF Grant DMR-1055522

4:18PM R10.00004 Fractionalizing Majorana Fermions: Non-Abelian Statistics on the Edges of Abelian Quantum Hall States , NETANEL LINDNER, California Institute of Technology — We study the non-Abelian statistics characterizing systems in which the edges of fractional quantum Hall states are gapped by proximity coupling to superconductors and ferromagnets. We show that as more superconductor-ferromagnet interfaces are introduced, the ground state degeneracy grows with a quantum dimension of a square root of an even integer, corresponding to a new family of non-Abelian anyons. Topologically protected braiding of two anyons can be achieved by a sequence of adiabatic manipulations of the system. We show that the unitary transformations resulting from these braiding operations realize a richer set of representations of the braid group than those realized by non-Abelian anyons based on Majorana fermions. We discuss how these modes might be experimentally identified (and distinguished from Majoranas) using Josephson measurements.

4:54PM R10.00005 Genons, twist defects, and projective non-Abelian statistics , MAISSLAM BARKESHLI, Stanford University — An intense focus in the condensed matter community currently is the search for Majorana fermions in solid state systems. Defects which localize Majorana zero modes obey the simplest kind of non-Abelian statistics, and are of interest partially for the goal of achieving topological quantum computing. In this talk, I will present recent advances in our understanding of how to synthesize a much more general class of non-Abelian defects using conventional topological states. After discussing the new theoretical foundations, I will present an experimental proposal using only conventional bilayer fractional quantum Hall states and a simple geometry of top and bottom gates. I will also discuss how these ideas can be used to perform universal topological quantum computing (TQC) using non-abelian states that by themselves are not universal for TQC.
2:42PM R19.00002 Berezinskii-Kosterlitz-Thouless Transition in Heavy Fermion Superlattices

JIAN-HUANG SHE, Los Alamos National Laboratory, ALEXANDER BALATSKY, Los Alamos National Laboratory and Nordita — We propose an explanation of the superconducting transitions discovered in the heavy fermion superlattices by Mizukami et al. (Nature Physics 7, 849 (2011)) in terms of Berezinskii-Kosterlitz-Thouless transition. We observe that the effective mass mismatch between the heavy fermion superconductor and the normal metal regions provides an effective barrier that enables quasi 2D superconductivity in such systems. We show that the resistivity data, both with and without magnetic field, are consistent with BKT transition. Furthermore, we study the influence of a nearby magnetic quantum critical point on the vortex system, and find that the vortex core energy can be significantly reduced due to magnetic fluctuations. Further reduction of the gap with decreasing number of layers is understood as a result of pair breaking effect of Yb ions at the interface. Reference: Jian-Huang She, Alexander V. Balatsky, Phys. Rev. Lett. 109, 077002 (2012).

2:54PM R19.00003 Theory for ESR in the heavy fermion system $\beta$-YbAlB$_4$

ALINE RAMIRES, PIERS COLEMAN, Rutgers University — We propose a theory to explain the unusual temperature dependence of the Electron Spin Resonance (ESR) lines of the critical heavy fermion superconductor $\beta$-YbAlB$_4$. This system shows a conduction electron ESR signal at high temperatures, but at low temperatures its g-factor shifts to the f-electron g-factor and it develops strong anisotropy. With our theory we are able to explain this dichotomy based on the fact that the lower crystal field configuration of the local moments in this system is a pure $\pm (5/2)$. Because of its Ising nature these spins can not be directly probed by ESR, and the f-electron features that appear at low temperatures can be explained by an emergent hybridization model. We can account for the origin of this signal and its main characteristics qualitatively, including g-factor shift and the hyperfine structure with the assumption that the scattering rate is unusually small.

3:06PM R19.00004 Effects of correlated hybridization in the single-impurity Anderson model

WALTER LIBERO, RODRIGO VEIGA, Sociedade Brasileira de Física — The development of new materials often depends on the theoretical foundations which study the microscopic matter, i.e., the way atoms interact and create distinct configurations. Among the interesting materials, those with partially filled d or f orbitals immersed in nonmagnetic metals have been described by the Anderson model, which takes into account Coulomb correlation ($U$) when a local level (energy $E_j$) is doubly occupied, and an electronic hybridization between local levels and conduction band states. In addition, here we include a correlated hybridization model, which depends on the local-level occupation number involved. This term breaks particle-hole symmetry (even when $U + 2E_j = 0$), enhances charge fluctuations on local levels and as a consequence strongly modifies the crossover between the Hamiltonian fixed-points, even supressing one or other. We exemplify these behaviors showing data obtained from the Numerical Renormalization Group (NRG) computation for the impurity temperature-dependent specific heat, entropy and magnetic susceptibility. The interleaving procedure is used to recover the continuum spectrum after the NRG-logarithmic discretization of the conduction band.

3:18PM R19.00005 Friel's sum rules for one- and two-channel Kondo models and unitarity paradox via bosonization-refermionization approach

MAXIM KHARITONOV, NATAN ANDREI, PIERS COLEMAN, Center for Materials Theory, Rutgers University, Piscataway, NJ 08884, USA — We calculate the single-particle Green’s functions and scattering amplitudes of the one-channel and channel-anisotropic two-channel Kondo models at the Toulouse and Emery-Kivelson lines, respectively, where exact solutions via the bosonization-refermionization approach are admitted. We demonstrate that in this approach the Friel's sum rules — the relations between the trapped spin and “flavor” moments and the scattering phase shifts in the Fermi-liquid regime — arise naturally and elucidate on their subtleties. We also recover the “unitarity paradox” [1,2] — the vanishing of the single-particle scattering amplitude at the channel-symmetric point of the two-channel Kondo model — stemming from non-Fermi-liquid behavior. We discuss the implications of these results for the development of composite pairing in heavy fermion systems.

3:30PM R19.00006 Kondo destruction and superconducting correlations in the two-impurity Bose-Fermi Anderson model

LILI DENG, KEVIN INGERSEN, U. of Florida, JEDEDIAH PIXLEY, QIMIAO SI, Rice U. — The Bose-Fermi Kondo and Anderson models are among the simplest models for Kondo destruction, the phenomenon believed to underlie the anomalous physics of certain heavy-fermion materials. From our recent studies on heavy fermions [1], we have frequently observed strongly bias-dependent and asymmetric conductance behaviors. Based on a Fano resonance model in a Kondo lattice [2], we attribute them to energy-dependent quasiparticle scattering off hybridized renormalized electronic states, dubbing it QPS. We will present our QPS results on several heavy-fermion systems and discuss QPS as a novel technique to probe the bulk spectroscopic properties of the electronic structure. For instance, it reveals that the hybridization gap in URu$_2$Si$_2$ opens well above the hidden order transition [1].

3:42PM R19.00007 Quasiparticle scattering spectroscopy (QPS) of Kondo lattice heavy fermions

L.H. GREENE, S.M. NARASIWODEYAR, P. BANERJEE, W.K. PARK, University of Illinois at Urbana-Champaign, E.D. BAUER, P.H. TOBASH, R.E. BAUMBACH, F. RONNING, J.L. SARRAO, J.D. THOMPSON, Los Alamos National Laboratory — Point-contact spectroscopy (PCS) is a powerful technique to study electronic properties via measurements of non-linear current-voltage characteristic across a ballistic junction. It has been frequently adopted to investigate novel and/or unconventional superconductors by detecting the energy-dependent Andreev scattering. PCS of non-superconducting materials has been much rarely reported. From our recent studies on heavy fermions [1], we have frequently observed strongly bias-dependent and asymmetric conductance behaviors. Based on a Fano resonance model in a Kondo lattice [2], we attribute them to energy-dependent quasiparticle scattering off hybridized renormalized electronic states, dubbing it QPS. We will present our QPS results on several heavy-fermion systems and discuss QPS as a novel technique to probe the bulk spectroscopic properties of the electronic structure. For instance, it reveals that the hybridization gap in URu$_2$Si$_2$ opens well above the hidden order transition [1].

References:

This work was supported by National Science Foundation grants DMR 0907179 (MK, PC) and DMR 1006684 (NA).

3:30PM R19.00006 Kondo destruction and superconducting correlations in the two-impurity Bose-Fermi Anderson model

LILI DENG, KEVIN INGERSEN, U. of Florida, JEDEDIAH PIXLEY, QIMIAO SI, Rice U. — The Bose-Fermi Kondo and Anderson models are among the simplest models for Kondo destruction, the phenomenon believed to underlie the anomalous physics of certain heavy-fermion materials. From our recent studies on heavy fermions [1], we have frequently observed strongly bias-dependent and asymmetric conductance behaviors. Based on a Fano resonance model in a Kondo lattice [2], we attribute them to energy-dependent quasiparticle scattering off hybridized renormalized electronic states, dubbing it QPS. We will present our QPS results on several heavy-fermion systems and discuss QPS as a novel technique to probe the bulk spectroscopic properties of the electronic structure. For instance, it reveals that the hybridization gap in URu$_2$Si$_2$ opens well above the hidden order transition [1].

References:

This work was supported by National Science Foundation grants DMR 0907179 (MK, PC) and DMR 1006684 (NA).
3:54PM R19.00008 Quantum Phases of the Shastry-Sutherland Kondo Lattice. JEDEDIAH PIXLEY, RONG YU, QIMIAO SI, Rice University — Motivated by the discovery of the geometrically frustrated heavy fermion metal Yb2Pt2Pb[1], which has a quasi two dimensional Shastry-Sutherland lattice structure, we consider the Heisenberg-Kondo lattice model on a two dimensional Shastry-Sutherland geometry. Using a large-N method, we obtain the phase diagram and, in particular, the quantum transitions between a valence bond solid phase and a heavy Fermi liquid phase. Interestingly, we find intermediate states that break the C4 symmetry. We discuss the implications of our results for the experiments on Yb2Pt2Pb and related 221 materials [1], as well as the possible placement of these systems in a proposed global phase diagram for heavy fermion metals [2]. [1] M. S. Kim and M. C. Aronson, arXiv:1202.0220 (2012). [2] Q. Si, Phys. Status Solidi B 247, 476-484 (2010).

4:06PM R19.00009 Kondo hole route to incoherence in the periodic Anderson model. PRAMOD KUMAR, N.S. VIVYADHIRAJA, Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India 560064 — The interplay of disorder and interactions in strongly correlated electronic systems is a subject of perennial interest. In this work, we have investigated the effect of Kondo hole type disorder on the dynamics and transport properties of heavy fermion systems. We employ the periodic Anderson model within the framework of coherent potential approximation and dynamical mean field theory. The crossover from lattice coherent behaviour to an incoherent single-impurity behaviour is reflected in all aspects: a highly frequency (ω)-dependent hybridization becomes almost flat, the coherence peak in resistivity (per impurity) gives way to a Hamann form that saturates at low temperature (T); the Drude peak and the mid-infrared peak in the optical conductivity vanish almost completely. The zero temperature resistivity can be captured in a closed form expression, and we show how the Nordheim’s rule gets strongly modified in these systems. The thermopower exhibits a characteristic peak, which changes sign with increasing disorder, and its location is shown to correspond to the low energy scale of the system (ω⊥). In fact, the thermopower appears to be much more sensitive to disorder variations that the resistivity. A comparison to experiments yields quantitative agreement.

4:18PM R19.00010 Bose-Fermi Kondo model with a local transverse field and its implications for the global phase diagram of heavy fermions. EMILIAN NICA, QIMIAO SI, Rice University, KEVIN INGERSENT, University of Florida — Recent studies of the global phase diagram of quantum critical heavy fermion metals [1] have motivated us to consider the interplay between the quantum fluctuations within the local-moment system and those associated with the Kondo interaction. Towards this goal, we studied a Bose-Fermi Kondo model with local anisotropy in the presence of a local transverse field. Using the numerical renormalization group method for co-existing fermionic and bosonic baths [2], we found that tuning the transverse field gives rise to a continuous phase transition between a local moment phase and a Kondo screened phase. We determine the critical fixed point structure by studying the transitions accessed by varying the transverse field for different initial values of the coupling to the dissipative boson bath. Finally, we discuss the implications of these results for the global phase diagram of the Kondo lattice.

4:30PM R19.00011 Kondo Metal and Ferrimagnetic Insulator on the Triangular Kagome Lattice. YAO-HUA CHEN, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, Texas 77204, USA, HONG-SHUAI TAO, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, DAO-XIN YAO, State Key Laboratory of Opolectronic Materials and Technologies, Sun Yat-sen University, Guangzhou 510275, China, WU-MING LIU, Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing 100190, China — We obtain the rich phase diagrams in the Hubbard model on the triangular kagome lattice as a function of interaction, temperature and asymmetry, by combining the dynamical cluster effective-field theory with the continuous time quantum Monte Carlo method. The phase diagrams show the asymmetry separates the critical points in Mott transition of two sublattices on the triangular kagome lattice and produces two novel phases called plaquette insulator with a clearly visible gap and a gapless Kondo metal. When the Coulomb interaction is stronger than the critical value Uc, a short range paramagnetic insulating state emerges before the ferrimagnetic order is formed independent of asymmetry. Furthermore, we discuss how to measure these phases in future experiments.

4:42PM R19.00012 Doniach Diagram in Disordered Electrons System. HYUNYONG LEE, Advanced Materials Science, Pohang University of Science and Technology (POSTECH), Pohang 790-784, South Korea, STEFAN KETTEMANN, School of Engineering and Science, Jacobs University Bremen, Bremen 28759, Germany — We have derived the quantum phase diagram of disordered electron systems with magnetic impurities. The competition between RKKY interaction, J_{RKKY}, and Kondo effect gives rise to a rich quantum phase diagram, or Doniach diagram. We present numerical results for disordered 2D electron systems which show that both Kondo temperature, T_K and J_{RKKY} are widely distributed and quantum critical point is extended to a critical region. We find a sharp cutoff in the distribution of their ratio, J_{RKKY}/T_K, and from that critical density of magnetic impurity below which Kondo always wins. We find that the spin coupled phase grows at the expense of Kondo phase as increasing disorder. The spin coupled phase shows a succession of 3 phases: 1. a Griffiths phase with anomalous power laws determined by distribution of J_{RKKY}, 2. spin glass phase, 3. long range magnetic ordered phase. We report the results on graphene where we find that spin coupled phase is more stable against Kondo screening, but is more easily destroyed by disorder into a paramagnetic phase [1].

4:54PM R19.00013 Transport properties of a two impurity system: a theoretical approach. IGNACIO J. HAMAD, Departamento de Fisica, PUC Rio de Janeiro, 22453-900, Brazil, LAERCIO COSTA RIBEIRO, Centro Federal de Educacao Tecnologica Celso Suckow de Fonseca (CEFET-RJ/UnED-NI), RJ, Brazil, GEORGE MARTINS, Department of Physics, Oakland University, Rochester, MI 48309, USA, ENRIQUE V. ANDA, Departamento de Fisica, PUC Rio de Janeiro, 22453-900, Brazil — Double magnetic-impurity systems have attracted great attention due to their rich physics and possible technological applications. A system of two interacting Co atoms has been studied in a recent STM experiments (Nature Physics 7, 901 (2011)). The precise control of the inter-impurity distance made it possible to explore in detail the transport properties of the system as a function of the impurities’ interaction each. We explain, for all the parameter range studied, the physics observed in the experiments using a microscopic model, based on the two impurity Anderson model, including a two-path geometry for charge transport. The many-body system is treated in the finite-U Slave Boson Mean Field Approximation. Other results obtained using the Logarithmic Discretization Embedded Cluster Approximation are also discussed. We physically characterize the system and show that, as in the experiments, the features observed in the transport properties depend on the presence of two impurities but also on the existence of two conducting channels for electron transport. In particular, we obtain a splitting in the differential conductance, compatible with the one observed in the experiments, as a result of the superposition of the many-body Kondo states of each impurity.
2:30PM R22.00001 Optimizing coherent Raman scattering with plasmonic nanoparticles, DMITRII VORONINE, XIA HUA, ALEXANDER SINYUKOV, CHARLES BALLMANN, ALEXEI SOKOLOV, MÅRLAN SCULLY, Texas A&M University — Two commonly used techniques that provide species-specific spectroscopic signals in the form of vibrational fingerprints are surface-enhanced Raman scattering (SERS) and coherent anti-Stokes Raman scattering (CARS) spectroscopies. In order to enhance the signal, SERS takes advantage of the electromagnetic near-field enhancement while CARS employs molecular coherence. We have combined these two techniques to achieve best-of-both-worlds maximum signal enhancement by using optimized laser pulse shaping and time-resolved detection. We applied this new time-resolved surface-enhanced coherent anti-Stokes Raman scattering (t-SE-CARS) technique to investigate various molecular complexes in a vicinity of gold nanoparticles. While large signal enhancement has previously been achieved in SERS, surface-enhanced coherent signals have shown lower values. We investigate the mechanisms of these effects by analyzing the spatial dependence of the coherent Raman spectra for different hot spots in aggregated plasmonic nanoparticles. Understanding coherence effects in surface-enhanced Raman scattering may lead to improved nanoscale sensors.

2:42PM R22.00002 Complex metallic nanostructures using self-assembled DNA templates for SERS and plasmonic applications, MAURICIO PILO-PAIS, ANNE WATSON, DUKE University, THOM LABEAN, North Carolina State University, GLEB FINKELSTEIN, DUKE University — We custom-tune the plasmonic resonance of complex metallic nanostructures based on “DNA origami” templates (~90x70nm). Briefly, 5 nm gold nanoparticles are attached at selected places within a DNA-origami “nano-breadboard” and later enlarged, and even fused, by electroplating and etching to form the size- and shape-specific plasmonic resonances of the resulting metallic nanostructures. We perform SERS measurements of various Raman molecules (i.e. 4-aminobenzenethiol), which are chosen based on the plasmonic resonance frequency of the structure. The flexibility of the design and multiply parallel nature of the method open the road for designing and fabricating optimum structures for a desired plasmonic application.

2:54PM R22.00003 Enhanced surface Raman scattering in gold thin films deposited on large array anti-nanoring template, CHI CHIH HO, Nanoscience and Technology Program, Taiwan International Graduate Program, Institute of Physics, Academia Sinica, Taipei, Taiwan, TZE YANG LEE, Department of Engineering and System Science, National TsingHua University, Hsinchhu, Taiwan, WEI LI LEE, Institute of Physics, Academia Sinica, Taipei, Taiwan, FAN GANG TSENG, Department of Engineering and System Science, National TsingHua University, Hsinchhu, Taiwan — To evenly distribute hot spots over large area is an important subject for realistic applications using surface enhanced Raman scattering (SERS) effect. Here, we utilized a monolayer polymer/nanosphere hybrid to prepare a large area and well-ordered anti-nanoring template for gold thin film deposition. The resulting gold nanostructured thin film, which comprises an antidot network with isolated nano-disk (ND) and nanoring (NR) in each antidot, can be employed as an efficient SERS substrate. From finite difference time domain (FDTD) simulation, hot spots occur at the space between isolated ND and NR giving rise to enhanced surface Raman scattering. We fabricated a series of such gold nanostructured thin films with different thickness and geometry. An optimum condition for maximum SERS was obtained in experiment. Detailed size effect on SERS and comparison to FDTD simulation will be discussed.

3:06PM R22.00004 Ultraviolet surface-enhanced Raman spectroscopy using aluminum plasmonic gratings, ADAM T. ROBERTS, Army Aviation & Missile RDEC, SERKAN BUTUN, KORAY AYDIN, Dept. of Electrical Engineering & Computer Science, Northwestern University, HENRY Q. EVERITT, MARK BLOEMER, Army Aviation & Missile RDEC, GIUSEPPE D’AGLIANNO, NADIA MATTIUCCI, Aegis Technologies — Surface-enhanced Raman scattering (SERS) has been widely studied both theoretically and experimentally for chemical and biological sensing, primarily in the visible and near-infrared wavelengths. Although in the ultraviolet (UV) plasmonic behavior is limited by metallic damping, we have theoretically shown that SERS enhancement factors as large as $10^5$ can be achieved when the laser is tuned to the plasmonic band edge of an Al metallic grating grown on a sapphire substrate. Using electron beam lithography, aluminum gratings were fabricated whose pitch (150-300 nm), slit widths (64 nm), and thickness (50 nm) were chosen to produce large enhancement factors at wavelengths in the UV. Analytes such as thiophenol were then deposited on the gratings, and UV-SERS spectroscopy was performed to measure the enhancement factors and compare with theoretical estimates. Enhancement factors were measured by comparing the strength of the Raman signal from the grating region with the strength of the Raman signal from adjacent regions without a grating. The dependence of the enhancement factor on laser wavelength relative to the plasmonic band edge for a given grating pitch was explored, as was the effect of using a tapered slit geometry that focuses the local field on the nanoscale.

3:18PM R22.00005 Surfed Enhanced Raman Spectroscopy in Nanojunctions with Anomalous Polarization Dependence, JOSEPH B. HERZOG, MARK W. KNIGHT, YAJING LI, KENNY EVANS, NAOMI J. HALAS, DOUGLAS NATELSON, Rice University — Several papers have been published on surfaced enhanced Raman spectroscopy (SERS) in nanojunctions, and polarization studies have shown that the strongest SERS enhancement is generated when the incident light is polarized so that the electric field is directed across the interelectrode nanoparticle. This polarization dependence is certainly true for mesoscopic structures as dimers, but this works show that this is not always the case. Here we create nanogap both by electromigration and a novel “self-aligned” process, which can be scaled for mass production. Polarization dependent SERS measurements were performed on these junctions and have determined that transverse polarization of incident light generates the strongest SERS enhancement. Cathodoluminescent experiments as well as finite element method calculations have confirmed these findings and together with the experimental results have determined that the enhancements are due to strong localized hybrid modes in the gap which couple to a resonant transverse plasmon mode. This new finding has increased device sensitivity by an order of magnitude and opens the possibility for improved plasmonically-active optoelectronic devices and other nanophotonic applications.

3:30PM R22.00006 Surface-enhanced Raman detection of a vibrational Stark effect in C60-containing molecular junctions, YAJING LI, Department of Physics and Astronomy, MS 61, Rice University, PETER DOAK, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, LEEOR KRONEK, Weizmann Institute of Science, Rehovot, Israel, DOUGLAS NATELSON, Department of Physics and Astronomy, MS 61, Rice University — Understanding the interplay of local electric fields and molecular vibrational degrees of freedom is of considerable interest. One nontrivial consequence of this coupling is the vibrational Stark effect, in which vibrational energies are altered through coupling to electric fields. With this in mind, we probe the vibrational Stark effect in Au/C60/Au monolayer junctions. Following electromigration, these metal nanostructures possess nanometer-scale interelectrode gaps that support highly localized surface plasmon resonances, resulting in SERS electromagnetic enhancements sufficient for single-molecule studies. These structures have also proven suitable for simultaneous single-molecule electronic transport experiments, in which we observed the vibrational modes of the molecules shift systematically as a function of applied bias. We will present measurements of the electrically driven vibrational energy shifts of C60 in such junctions and compare those with theoretical expectations obtained from DFT calculations.

3:42PM R22.00007 Fractal nanostructures with Hilbert curve geometry as a SERS substrate, ILYA GRIGORENKO, CityTech, CUNY — A new type of substrates for Surface Enhanced Raman Scattering measurements is proposed. The shape of the substrate is based on self-similar fractal space filling curves, which possess properties of both one dimensional and two dimensional geometries. Here I present theoretical studies of the dielectric response of thin film doped semiconductor nanostructures, where conducting electrons are trapped in an effective potential having the geometry of the Hilbert curve. It is found that the system may exhibit the induced charge distributions specific for either two dimensional or one dimensional systems, depending on the excitation frequency. It is also shown that with the increase of the depth of the trapping potential the resonance of the system demonstrates a counter-intuitive shift to lower frequencies.
higher-order diffraction modes at longer wavelengths and larger incident angles. This geometrical effect is further accompanied by a swing atoms and the surface-plasmon modes in a metallic slit array is found. For passive control, on the other hand, a geometrical effect is demonstrated for focused

3:54PM R22.00008 Exciton-plasmon interaction and photo-injection of plasmonic hot carriers in hybrid nanostructures, ALEXANDER GOVOROV, HUI ZHANG, Ohio University, MIN OUYANG, University of Maryland, College Park, YURIJ GUNKO, School of Chemistry, University of Dublin, Trinity College — We investigate theoretically the effects of exciton-plasmon interaction and plasmon-assisted carrier injection in a hybrid semiconductor-metal nanostructure under resonant optical excitation. We treat the coupling between the metal and semiconductor nanocrystals using a many-body Fano model and a quantum density-matrix formalism. Hot carriers have a characteristic energy distribution in the plasmon wave function in a metal nanocrystal and participate in tunnel and ballistic injection currents to the neighboring semiconductor nanostructure. The photo-current induced by hot plasmonic electrons in the nanostructure depends on the barrier height, excitation frequency, plasmon energy, relaxation rates, and geometry of a device. The Coulomb exciton-plasmon interaction may also play an essential role in the optical absorption and electron injection. The results obtained in this study can be used to design and describe a variety of plasmonic nanodevices with hot electron injection for photo-catalysis, light-harvesting, and solar cells.

4:06PM R22.00009 Photoconductance measurements of patterned nanocrystal films on gold nanojunctions, KENNETH EVANS, Applied Physics Ph.D. Program, Rice University, SRAVANI GULLAPALLI, MICHAEL WONG, Department of Chemical and Biomolecular Engineering, Rice University, DOUGLAS NATELSON, Department of Physics & Astronomy, Rice University — Large scale production of nanoscale absorbers and emitters based on single, or few, colloidal nanocrystals would be an important advancement for light-based electronics and investigating poorly understood quantum phenomena such as blinking. We present a method for integrating nanocrystals into plasmonic active gold nanoparticle review of patterned nanocrystal films. Initial photoconductance measurements in nanocrystal-based devices are compared with bare gold junctions and the possibility for plasmon-assisted absorption and emission is discussed.

4:18PM R22.00010 Coherent Oscillations in Spoof-Like Plasmonic Ag deposited by PEALD, RYAN COMPTON, Chemistry Division, Naval Research Laboratory, Washington, DC 20375, USA, NRC Postdoctoral Research Associate, SHARKA M. PROKES, OREST J. GLEMBOCKI, Electronic Science Division, Naval Research Laboratory, Washington, DC 20375, USA, JEFFREY C. OWRTUSKY, Chemistry Division, Naval Research Laboratory, Washington, DC 20375, USA — The spoof-like plasmonic properties of Ag thin films produced by plasma enhanced atomic layer deposition (PEALD) were investigated with static and transient spectroscopy. The PEALD process results in a film with cylindrical 2D structures separated by air gaps, giving rise to the plasmonic behavior. Films with thicknesses ranging from 10 to 32 nm were deposited and compared to films of similar thickness produced with traditional e-beam methods. Transmission spectra of the ALD films exhibit a strong surface plasmon resonance (SPR) band at approximately 700 nm, while the e-beam samples were devoid of band structure. The SPR band of the 10 nm ALD sample is blue-shifted (to 550 nm), suggesting morphological differences for the thinnest film. Transient absorption studies with a 400 nm probe revealed electron-phonon coupling times that are similar for both ALD and e-beam films. Transient measurements of the ALD Ag probed near the plasmon band (800 nm), however, feature coherent oscillations attributed to breathing of the cylindrical structures, whereas the e-beam films exhibit no oscillatory behavior. The oscillation period was found to be independent of ALD thickness, except in the 10 nm sample where no oscillations were observed.

4:30PM R22.00011 Optical analogue of quantum spin and dynamic localization in optical waveguides arrays, KIN CHUNG AU YEUNG, KIN WAH YU, The Chinese University of Hong Kong — We have discovered an optical analogue of quantum spin in optical waveguides. Quantum-optical analogy is recently a hot topic. By using special configuration of optical devices, some optical analogues of quantum systems can be realized. Stefano Longhi and coworkers proposed some classical realization of quantum phenomena like the two-site Fermi-Hubbard system [1] and Rabi oscillation [2]. In this work, we propose an optical waveguides arrays system with evanescent couplings according a symmetrized Kac matrix. The system can mimic the quantum spin under different operators like the rotation operator. Also by adding a suitable time-dependent applied potential to the system, dynamic localization of optical signal can be realized along the signal propagation. The system can be extended to mimic any arbitrary angular momentum by increasing the number of optical waveguides arrays. The occurrences of spin under rotation operator and dynamic localization are simulated by a field-evolution analysis using an input Gaussian beam.


4:42PM R22.00012 Comparison of Active and Passive Approaches for Controlling the Near-Field Optical Path of Guided-Light Wave, DANHONG HUANG, US Air Force Research Lab, MICHELLE EASTER, Hunter College of the City University of New York, DAVID WELLEMS, HENRY MOZER, US Air Force Research Lab, ALEXEI MARADUDIN, University of California-Irvine, GODFREY GUMBS, Hunter College of the City University of New York, DAVE CARDIMONA, US Air Force Research Lab — Both active and passive approaches are proposed and compared for controlling the optical path of p-polarized light wave guided through a surface-patterned metallic structure with sub-wavelength features. For active control, the dynamical role of photo-excited electrons in a slit-embedded atomic system with field-induced transparency (FIT) is demonstrated for modulating transmitted-light intensity in the near-field region. Additionally, the strong coupling between the optical transitions within slit-embedded FIT atoms and the surface-plasmon modes in a metallic slit array is found. For passive control, on the other hand, a geometrical effect is demonstrated for focused transmitted light passing through a Gaussian-shaped metallic lens embedded with an array of slits. This geometrical effect is further accomplished by a swing of the light-focusing pattern in the near-field region as the incident angle is increased, as well as by the reduction of an anomalous light refraction due to higher-order diffraction modes at longer wavelengths and larger incident angles.

This research was supported by the Air Force Office of Scientific Research (AFOSR)

4:54PM R22.00013 Gain/loss induced localization in low-dimensional PT-symmetric models, FELIX IZRAILEV, Instituto de Fisica, BUAP, Puebla, Mexico, and NSCL and Dept. of Physics and Astronomy, Michigan State University, USA, OMAR O. VASQUEZ-CANDANEDO, Instituto de Fisica, BUAP, Puebla, Mexico — We show that both loss (absorption) and gain (amplification) can induce the potential to the system, dynamic localization of optical signal can be realized along the signal propagation. The system can be extended to mimic any arbitrary angular momentum by increasing the number of optical waveguides arrays. The occurrences of spin under rotation operator and dynamic localization are simulated by a field-evolution analysis using an input Gaussian beam.

F.M.I. gratefully acknowledges the support of the SEP-CONACYT (Mexico) grant No.80715

4:54PM R22.00013 Gain/loss induced localization in low-dimensional PT-symmetric models, FELIX IZRAILEV, Instituto de Fisica, BUAP, Puebla, Mexico, and NSCL and Dept. of Physics and Astronomy, Michigan State University, USA, OMAR O. VASQUEZ-CANDANEDO, Instituto de Fisica, BUAP, Puebla, Mexico — We show that both loss (absorption) and gain (amplification) can induce the potential to the system, dynamic localization of optical signal can be realized along the signal propagation. The system can be extended to mimic any arbitrary angular momentum by increasing the number of optical waveguides arrays. The occurrences of spin under rotation operator and dynamic localization are simulated by a field-evolution analysis using an input Gaussian beam.

F.M.I. gratefully acknowledges the support of the SEP-CONACYT (Mexico) grant No.80715
5:06PM R22.00014 Generalizing speed-of-light limitations to arbitrary passive linear media
AARON WELTERS, STEVEN JOHNSON, Department of Mathematics, Massachusetts Institute of Technology — We prove that well-known speed of light restrictions on electromagnetic energy velocity can be extended to a new level of generality, encompassing even nonlocal chiral media in periodic geometries, while at the same time weakening the underlying assumptions to only passivity and linearity of the medium (along with a transparency window, which ensures well-defined energy propagation). Surprisingly, passivity alone is sufficient to guarantee causality and positivity of the energy density (with no thermodynamic assumptions), in contrast to prior work which typically assumed the latter properties. Moreover, our proof is general enough to include a very broad range of material properties, including anisotropy, bianisotropy (chirality), nonlocality, dispersion, periodicity, and even delta functions or similar generalized functions. The results in this talk are proved using deep results from linear-response theory, harmonic analysis, and functional analysis.

5:18PM R22.00015 The curvy photonics of squid camouflase
ALISON SWEENEY, AMANDA HOLT, University of Pennsylvania, MORSE DANIEL, University of California, Santa Barbara, DARIUSZ STRAMSKI, University of California, San Diego, Scripps Institute of Oceanography — Cephalopods (squids and octopuses) ubiquitously possess reflective structures in their skin composed of “reflectin” proteins. Although a few simple laminar, Bragg-stack type optical structures have been known in a handful of common squid species for some time, our extensive survey of optically active tissues of exotic deep-sea species has revealed complex, extended curvatures and topologies in dermal reflectors of these rarely-studied animals. Molecular deep-sequencing has revealed these structures also to be composed of reflectin-like proteins. Here we show a survey of some of these deep-sea reflector structures, and present evidence that each novel structure may be a transform of the radiation in the optical niche in the ocean where each of these species live, such that light reflecting off the sides of these animals in their specific ocean habitat resembles the light that would be transmitted through the animals if they were transparent, from many different viewing angles and possible ocean depths.

Wednesday, March 20, 2013 2:30PM - 5:30PM — Session R35 DCMP: Novel Superconductors I

343 - James Eckstein, University of Illinois at Urbana-Champaign

2:30PM R35.00001 The Introduction of substitutional and non-substitutional dopants into MgB2 in high pressure/Temperature or non-equilibrium regimes
MIKE SUMPTION, The Ohio State University — In an attempt to study the effect of doping of MgB2 under conditions leading to efficient doping, we used both an high temperature/high pressure induction furnace to dope into MgB2 bulks at temperatures up to 1600 C and 1500 Psi, and thin film, PLD multilayer and mixed layer film fabrication. The high temperature/high pressure formation was used to explore the solubility at high temperatures of various dopants, and the thin film formation was an attempt to use non-equilibrium conditions to inject dopants more effectively. The dopants used were C, Ti, and Zr. C was seen to reach a maximal level at 4 at% C site substituted into MgB2, as evidenced by EPMA and XRD results. Zr, of interest as a possible Mg site substitution in MgB2 was not seen to enter into the MgB2 phase (instead segregating) in the bulk high temperature/high pressure experiments, but was seen to enter in during PLD, as evidenced by STEM and XRD results. Ti additions were attempted in the high pressures and temperature regime, with some evidence for dopant introduction. Critical field measurements on the Zr doped samples where seen to suppress Bc2 for all except very low levels of Ti addition, presumably associated with the much greater doping efficiency.

2:42PM R35.00002 The Penetration Depth of MgB2 as measured by DC SQUIDs
DANIEL CUNNANE, KE CHEN, X.X. XI, Temple University — High-speed superconducting circuits may benefit from the high Tc and large superconducting gap of MgB2. Nb remains the state of the art for superconducting electronics partly because of its small penetration depth and its isotropic nature. A microscopic theory on the penetration depth of multiband superconductors states that a clean MgB2 sample is nearly isotropic while a sample in the dirty limit is anisotropic. We have made and measured DC SQUIDs using MgB2 Josephson junctions to determine the inductance of an MgB2 microstrip. The penetration depth along the c-axis, \( \lambda_c \), was calculated using the inductance value and dimensions of the microstrip. We have previously reported the absolute value of the penetration depth of our MgB2 films to be around 40 nm. Now we have made devices with film ranging from the clean limit to the dirty limit by adding defects during the deposition. The absolute value of \( \lambda_c \) at low temperature is compared to the cleanliness of the film. The temperature dependence was also measured which is non-trivial due to the two-gap nature of MgB2. These results are compared with theory that confirmed our previous results.

2:54PM R35.00003 Superconducting properties of aligned flexible networks and yarns of MgB2-CNT nanowires
JULIA BYKOVA, MARCIO DIAS LIMA, DERRICK TOLLY, CARTER HAINES, AUSTIN HOWARD, MYRON SALAMON, RAY BAUGHMAN, ANVAR ZAKHIDOV, University of Texas at Dallas — Magnesium diboride (MgB2) has attracted great interest due to its outstanding superconducting characteristics. Literature reports showed that addition of carbon nanotubes (CNT) to a MgB2 matrix significantly improves its properties: CNTs can carry extremely high currents and also provide electrical and mechanical connection between MgB2 grains. Here we present a new method to produce networks of aligned MgB2-CNT nanowires which can be spinned into flexible yarns. Free-standing, aligned CNT sheets were used as a starting network. A conformal layer of boron was deposited on CNTs by Laser Assisted Chemical Vapor Deposition. The resultant boron-CNT nanowires (thickness of 70±10 nm) were exposed to magnesium vapor and were converted into MgB2-CNT composites. The MgB2-CNT arrays are flexible and can be easily bent and even twisted. Critical temperature reaches 37 K and depends on thickness and crystalline structure of nanowires. Current critical and critical fields were shown to be comparable or even better than standard MgB2 wires. We discuss the correlation of observed two step behavior in electric transport curves with interconnects between MgB2-CNT nanowires and Josephson junction network formation.

3:06PM R35.00004 Enhancement of lower critical field in thin MgB2 films and MgB2/MgO multilayers
TENG TAN, EVAN JOHNSON, NARENDRA ACHARAYA, MICHAEL HAMBE, KE CHEN, Department of Physics, Temple University, ALEX KRICK, STEVEN MAY, Department of Materials Science and Engineering, Drexel University, XIAOXING XI, Department of Physics, Temple University — Magnesium diboride is a conventional superconductor with a high \( T_c \) of 39 K, a low residual resistivity of < 0.1 \( \mu \Omega \)cm (at 42 K), and higher thermodynamic critical field \( H_c \) values than Nb. These properties make MgB2 a promising superconductor as an alternative to Nb for future SRF cavities. However, the lower critical field \( H_{c1} \) of MgB2 is low, and vortex dissipation above \( H_{c1} \) can lead to degradation of the quality factor and low RF breakdown field. Here, we report an enhancement of \( H_{c1} \) in thin MgB2 films and MgB2/MgO multilayers. The value of \( H_{c1}(5K) \) is increased from 40 mT in a 300 nm-thick MgB2 film to 180 mT when the MgB2 layer thickness is 100 nm either in a single-layer film or in a MgB2/MgO multilayer with a total MgB2 layer thickness of 300 nm. Superconducting MgB2 thin films have been coated in-situ on the inner wall of a SRF cavity using the hybrid physical chemical vapor deposition (HPCVD) technique. The characterization of the coating will be presented.
3:18PM R35.00005 Thickness dependence of superconducting properties in magnesium diboride thin films. 

DOUGLAS BERINGER, The College of William and Mary, CESAR CLAVERO, Lawrence Berkeley National Laboratory, TENG TAN, XIAOXING XI, Temple University, ROSA LOHASZEW, The College of William and Mary — Thin film MgB$_2$ is a promising material currently researched for improvements in superconducting radio frequency (SRF) technology and applications. At present, bulk niobium SRF accelerating cavities suffer from a fundamental upper limit in maximally sustained accelerating gradients; however, a scheme involving multi-layered superstructures consisting of superconducting-insulating-superconducting (SIS) layers has been proposed to overcome this fundamental material limit of 50 MV/m. The SIS multi-layer paradigm is reliant upon implementing a thin shielding material with a suitably high H$_c1$ which may prevent early field penetration in a bulk material layer and consequently delay the high field breakdown. It has been predicted that for thin superconducting films — thickness less than the London penetration depth ($\sim$140 nm in the case of MgB$_2$) — the lower critical field H$_c1$ will be enhanced with decreasing thickness. Thus, MgB$_2$, with a high bulk H$_c1$ value is a prime candidate for such SIS structures. Here we present our study on the surface morphology and superconducting properties on a series of MgB$_2$ thin films and correlate the effects of film thickness and surface morphology on H$_c1$.

This work was supported in part by the U.S. Department of Energy (DE-SC0004410 and DE-AC05-06OR23177) and Defense Threat Reduction Agency (HDTRA1-10-1-0072).

3:30PM R35.00006 High resolution $^{11}$B NMR of MgB$_2$ using cryogenic magic-angle spinning.

RAIVO STERN, National Institute of Chemical Physics and Biophysics, Tallinn 12618, Estonia, PETER BECKETT, MARK S. DENNING, School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK, IVO HEINMBA, MUKESH C. DIMRI, National Institute of Chemical Physics and Biophysics, Tallinn 12618, Estonia, EDWARD A. YOUNG, Institute of Cryogenics, School of Engineering Sciences, University of Southampton, Southampton SO17 1BJ, UK, MARINA CARRAVELLA, School of Chemistry, University of Southampton, Southampton SO17 1BJ, UK — Static and magic-angle spinning (MAS) $^{11}$B NMR data at 4.7 T and 8.5 T have been obtained under cryogenic conditions on a diluted sample of magnesium diboride powder in the normal and superconducting state. We demonstrate that MAS NMR is possible on type-II superconductors despite the sample rotation. The data provide accurate information on the magnetic shift variation and longitudinal relaxation data down to a temperature of 8 K, with a resolution improvement over the entire temperature range. The onset of superconductivity is unaffected by the sample rotation, as revealed by a sharp variation of the magnetic shift just below the critical temperature.

1 Appeared in JCP 137, 114201, http://dx.doi.org/10.1063/1.4751476

3:42PM R35.00007 The full 3D electronic band structure of MgB$_2$ determined by soft x-ray ARPES.

YASMINE SASSA, MARTIN MANSSON, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland, BASTIAN M. WOJEK, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, MASAKI KOBAYASHI, Swiss Light Source, Erwin Scherrer Institute, CH-5232 Villigen PSI, Switzerland, OLOF GOTBERG, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, VLADIMIR STROCOV, Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland, NIKOLAI ZHIGADLO, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland, OSCAR TJERNBERG, Materials Physics, Royal Institute of Technology KTH, S-16440 Kista, Sweden, BERTRAM BATLOGG, Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland — Mg$_2$B$_6$ is a prototypical multi-band multi-gap superconductor with electron-phonon coupling driving $T_c$. We are able to measure the band dispersion not only in the k$_x$-k$_y$ plane, but also probe in detail the k$_z$ dependence and thus, the 3D nature of the bands. Furthermore, we have found the ARPES intensities are very polarization dependent and their analysis provides an excellent agreement with the orbital nature of the electronic states. The calculated electronic band structure captures very well all the features revealed in our experiment.

3:54PM R35.00008 Fragile Structure Transition in Mo3Sb7.

J.-Q. YAN, University of Tennessee, Oak Ridge National Laboratory, M.A. MCGUIRE, A.F. MAY, Oak Ridge National Laboratory, D.C. MANDRUS, University of Tennessee, Oak Ridge National Laboratory, B.C. SALES, Oak Ridge National Laboratory — Despite a relatively low superconducting transition temperature $T_c = 2.08$ K, the Zintl compound Mo$_3$Sb$_7$ has attracted considerable interest due to the possible involvement of magnetism in superconducting pairing, and promising thermoelectric performance with proper doping. Mo$_3$Sb$_7$ crystallizes in a $\text{Ir}_3\text{Ge}_2$-type cubic structure with space group Im3m at room temperature. A structure transition from cubic to tetragonal ($\text{I}4$/$\text{mmm}$) was observed at 53 K and this very low-temperature transition is accompanied by the opening of a 12$\mu$eV gap. Here we present the growth of Mo$_3$Sb$_7$ single crystals and our work in exploring the correlation between the low-temperature superconductivity, the structure transition, and the spin gap. The low-temperature superconductivity was observed in both the cubic and tetragonal phases. The structure transition was found to be extremely sensitive to Te or Ru substitution which shifts the Fermi level toward the valence band edge. Work at ORNL was supported by the U.S. Department of Energy, Basic Energy Sciences, Materials Sciences and Engineering Division.

4:06PM R35.00009 Crystal growth, complex phase diagram and high pressure studies of layer compound PdBi$_3$.

KUI ZHAO, Texas Center for Superconductivity and Department of Physics, University of Houston, XIYU ZHU, BING LV, YU YI XUE, PAUL CHU, Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002 — Among the different Pd-Bi Alloys, Pd-Bi$_2$, which is crystallized in a layered tetragonal ($\text{I}4$/$\text{mmm}$) structure, has been identified as a superconductor with transition temperature at $\sim 5.4K$. Band structure calculations indicate that the interlayer Bi-Bi bonds are weak but not negligible, which implies the 3D bonding character of this compound. In order to enhance or weaken the interlayer bonding and ultimately increase the Tc in this system, high pressure measurement, isovalent chemical substitution of Bi with Sb, and chemical intercalation using transition metal Cu and alkali metal Na, are applied to the system. Meanwhile, isovalent chemical substitution on the Bi site by Pb is also carried out. The magnetic, electrical, and calorimetric properties of these compounds are determined at ambient pressure and compared. The detailed high pressure results and the complete phase diagram of chemical substitution and intercalation will be presented and discussed.

Work in Houston is supported in part by US AFOSR, the State of Texas, L. L. Temple Foundation and John and Rebecca Moores Endowment.

Additional Affiliation: Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720

4:18PM R35.0010 Superconductivity with extremely large upper critical fields in Nb$_2$Pd$_{0.88}$S$_5$

QIU RUN ZHANG, GANG LI, DANIEL RHODES, ANDRAJIA KISWANDI, TIGLET BASARA, J SUNG, THEO SIEGRIST, National High Magnetic Field Laboratory, Tallahassee, FL, USA, MICHELLE JOHANNES, Center for Computational Materials Science, Naval Research Laboratory, Washington DC, USA, LUIS BALICAS, National High Magnetic Field Laboratory, Tallahassee, FL, USA — Here, we report the discovery of superconductivity in a new transition metal-chalcogenide compound, i.e. Nb$_2$Pd$_{0.88}$S$_5$, with a transition temperature $T_c = 6.6$ K. Despite its relatively low $T_c$, it displays remarkably high and anisotropic superconducting upper critical fields, e.g. $\mu_0H_{c2} (T \to 0 K) \approx 37$ T for fields applied along the crystallographic b-axis. This value is considerably larger than the value reported for the technologically relevant Nb$_2$Sbn compound ($\mu_0H_{c2} \sim 30$ T, with $T_c = 18$ K)\textsuperscript{1,2}. Its ratio of $\mu_0H_{c2} (T \to 0 K)$ to $T_c$ is also larger than those of the new Fe based superconductors, e.g. $\beta$-FeSe ($\sim 20$ T/8 K)\textsuperscript{3}, Ba$_2$Fe$_2$As$_2$ ($\sim 70$ T/28 K)\textsuperscript{4}, and even higher than the reported ratio for the Chevrel-phase PbMo$_2$S$_6$ ($\sim 13.3$ K)\textsuperscript{5} compound. For a field applied perpendicularly to the b-axis, $\mu_0H_{c2}$ shows a linear dependence in temperature which coupled to a temperature-dependent anisotropy of the upper critical fields, suggests that Nb$_2$Pd$_{0.88}$S$_5$ is a multi-band superconductor. This is confirmed by band structure calculations which reveal nearly cylindrical and quasi-one-dimensional Fermi surface sheets having hole and electron character, respectively.
4:30PM R35.00011 Synthesis, structure, chemical doping and high pressure studies of the SrPt$_3$P with unique structure features$^1$. BENMAAN JAWDAT, BING LV, XIYU ZHU, YUYI XUE, CHING CHU$^2$. Texas Center for Superconductivity and Department of Physics, University of Houston, Houston, TX 77204-5002 — Superconductivity up to 8.4 K was reported by Takayama et al in APT$_3$P (A=Sr, Ca and La) in 2012 with structural information based only on X-ray powder refinement. The compounds are suggested to crystallize in an antiperovskite-based structure closely related to that of the heavy fermion superconductor CePt$_3$Si but are nonparallel unlike CePt$_3$Si. Both small single crystals and polycrystalline samples of SrPt$_3$P, the compound with the highest T$_c$ of this class of materials, are synthesized through solid state reactions. In this presentation, full and detailed structural information will be revealed based on X-ray single crystal analysis. Different chemical doping on different sites and high pressure studies have been carried out on the compound of SrPt$_3$P. The results and its implication will be presented and discussed.

$^1$Research at Houston is supported in part by US AFOSR, the State of Texas, T.L.L. Temple Foundation and John and Rebecca Moores Endowment.

$^2$Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720

4:42PM R35.00012 Revealing the superconducting state of CaC$_6$ by angle-resolved photoelectron spectroscopy$. SHUOLONG YANG, JONATHAN SOBOTA, Stanford Institute for Materials and Energy Science; Geballe Laboratory for Advanced Materials, Department of Physics and Applied Physics, Stanford, CA; CHRIS PICKARD, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK; MAKOTO HASHIMOTO, DONGHUI LU, Stanford Institute for Materials and Energy Sciences, SLAC, CA; SUNG-KWAN MO, Advanced Light Source, Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA; MARK ELLERBY, London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London, UK; ZHI-XUN SHEN, Stanford Institute for Materials and Energy Science; Geballe Laboratory for Advanced Materials, Department of Physics and Applied Physics, Stanford, CA — We studied the electronic band structure of CaC$_6$ using angle-resolved photoelectron spectroscopy (ARPES). We were able to make direct connections to the DFT calculation and identify various electron- and hole-pockets both at the Γ and K-points. Most importantly, we convincingly observed the interlayer band, which was predicted to be responsible for superconductivity and to display a near-free-electron-like dispersion. The near-circular Fermi surface of the interlayer band is clearly separable from the carbon-derived bands, which enables a pocket-dependent superconducting gap analysis near the Γ-point. Distinct electron-photon coupling regimes were observed for the interlayer and the carbon-derived bands using self-energy analysis in agreement with previous studies.

4:54PM R35.00013 In laser-intercalated layered cobaltates: a functional RG treatment$. CHRISS TIAN PLATT, MAXIMILIAN KIESEL, WERNER HANKE, Institute for Theoretical Physics, University of Wuerzburg, RONNY THOMALE, Ecole Polytechnique Federale de Lausanne — The superconducting state of water-intercalated cobaltates is still poorly understood. Starting with an effective three orbital model which fits the experimentally observed Fermi surface, we apply the functional renormalization group and study the phase diagram of Na$_3$Co$_2$O$_7$ as a function of doping. Here, we find ferromagnetic and triplet-pairing tendencies near van-Hove filling as well as (d + id)-superconductivity for larger dopings. The calculated gap function in this (d + id)-phase reveals a near-nodal behavior, and an increased Co$_2$O$_7$ layer distance promotes the ferromagnetic and triplet-pairing channels. Our findings are consistent with recent experimental observations. The cobaltates thus establish a chiral singlet superconductor based on transition metal oxides.

5:06PM R35.00014 Evidence for phase separation between the co-existing Density Wave and Superconducting orders in (TMTSF)$_2$PF$_6$. ARJUNNARAYANAN, PETER HANSON, Physics Department, New York University — Resistance, Thermopower and Angular Dependent Magnetoresistance (AMRO) measurements were used to study the organic conductor (TMTSF)$_2$PF$_6$ at pressures where co-existence between Superconducting and Spin Density Wave orders occurs. While in other material families such as the cuprates, there has been much discussion about the existence of a phase in which these orders co-exist. We report direct evidence of such a phase in (TMTSF)$_2$PF$_6$ and show that it is formed by the competition between the two orders. We use the AMRO to identify the phase that is formed by the co-existence of superconductivity and spin density wave order.

5:18PM R35.00015 Electron correlations in C$_{60}$ and aromatic superconductors, YUSUKE NOMURA, KAZUMA NAKAMURA, RYOTARO ARITA, Department of Applied Physics, University of Tokyo — Recent discovery of superconductivity in fcc/A15 Cs$_3$C$_{60}$ under pressure and in aromatic compounds ($K$-alkali-doped picene) has stimulated a renewed interest in molecular superconductors such as K$_3$C$_{60}$ and Rb$_2$C$_{60}$. To clarify the mechanism of the superconductivity, it is essential to understand low-energy electronic structure of these systems. In the present study, we perform a systematic study for understanding the relation between electronic correlation and superconductivity in C$_{60}$ and aromatic compounds [1]. We derived, from first principles, extended Hubbard models for twelve compounds: fcc K$_3$C$_{60}$, Rb$_2$C$_{60}$, Cs$_3$C$_{60}$ (with three different lattice constants), A15 Cs$_3$C$_{60}$ (with four different lattice constants), doped solid picene, corocene, and phanthenene. We show that these compounds are strongly correlated and have similar energy scales of their bandwidths and interaction parameters. However, they have a different trend in the relation between the strength of the electronic correlation and superconducting transition temperature. While the C$_{60}$ compounds have a positive correlation, the aromatic compounds exhibit a negative correlation. [1] Y. Nomura, K. Nakamura, and R. Arita, Phys. Rev. B 85, 155452 (2012).

Wednesday, March 20, 2013 2:30PM - 5:30PM — Session R36 DCMP: Superconducting Proximity Effects: Mesoscopic and Related 344 - Zhiqiang Mao, Tulane University

2:30PM R36.00001 Nonlocal correlations in a proximity-coupled normal metal. TAEWAN NOH, SAM DAVIS, VENKAT CHANDRASEKHAR, Northwestern University — We report evidence of large, nonlocal correlations between two spatially separated normal metals in superconducting-normal-metal (SN) heterostructures, which manifest themselves as a nonlocal voltage generated in response to a driving current. Unlike prior experiments in SN heterostructures, the nonlocal correlations are mediated not by a superconductor, but by a proximity-coupled normal metal. The nonlocal correlations extend over relatively long length scales in comparison to the superconducting case. At very low temperatures, we find a reduction in the nonlocal voltage for small applied currents that cannot be explained by the quasiclassical theory of superconductivity. We believe is a signature of new long-range quantum correlations in the system.
2:42PM R36.00002 Superconducting proximity effect in MBE grown Nb-InAs junctions1, CARYL KAN, CHI XUE, STEPHANIE LAW, JAMES ECKSTEIN, University of Illinois, Urbana-Champaign — Several proposals for the realization of Majorana fermions rely on excellent quality proximity coupling between a superconductor and a high-mobility semiconductor. We examine the long-range proximity coupling between MBE-grown InAs and in situ grown superconducting overlayers by fabricating transport devices, and investigate the effect of substrate choice and growth conditions on the quality of the MBE InAs. GaAs is commonly available as a high quality insulating substrate. Overcoming its lattice mismatch with InAs using GaSb and AISb layers results in locally smooth terraced surfaces, but global spiral dislocation structures also appear and have a negative impact on the InAs mobility. Growing InAs on homoepitaxial GaSb results in improved morphology and increases the mean free path. We compare the proximity effect in devices made both ways.

1This material is based upon work supported by the U.S. Department of Energy, Division of Materials Sciences under Award No. DE-FG02 07ER46453, through the Frederick Seitz Materials Research Laboratory at the University of Illinois at Urbana-Champaign.

2:54PM R36.00003 Electrostatic Tuning of the Proximity-Induced Exchange Field in EuS/Al Bilayers1, TIIJANG LIU, JOSEPH PRESTIGIACOMO, PHILIP ADAMS, Louisiana State University, LOUISIANA STATE UNIVERSITY COLLABORATION — We demonstrate that the proximity-induced exchange field, $H_{ex}$ in ferromagnetic/paramagnetic bilayers can be modulated with an electric field. An electrostatic gate arrangement is used to tune the magnitude of $H_{ex}$ in the Al component of EuS/Al bilayers. We produced modulations of ~ 30 Oe in $H_{ex}$ with the application of perpendicular electric fields of the order of $\pm 10^4$ V/cm. Several possible mechanisms accounting for the electric field’s influence on the interfacial coupling between the Al layer and the ferromagnetic insulator EuS will be discussed.

1Authors gratefully acknowledge support from the U.S. DOE.

3:06PM R36.00004 Unbiased Analysis of Super/Ferro Bilayer Physics, THOMAS LEMBERGER, MICHAEL HINTON, JIE YONG, The Ohio State University, ADAM HAUSER, The Ohio State University, JULIA MEYER, SPSMS, UMR-E CEA — S/F bilayer physics has been studied for some time now. With a large number of unknown and seemingly-known parameters, some values are traditionally and understandably assumed to be fixed quantities. In particular, the exchange energy, $E_{ex}$, is believed to be comparable to the Curie temperature. We analyze the data assuming only that the Fermi velocity $v_F$ in F and the density of states, $2N_S(0)$, in S are known. Fitting $T_c$ vs. $d_F$ with the dirty-limit theory, we determine the interface resistance, $R_0$, the ratio $E_{ex}/\rho_F$, and the ferromagnetic coherence length $\xi_F$. For physically plausible values of $\rho_F$ $v_F$, the dephasing rate of Cooper pairs in F is 10 times smaller than expected from the known Curie temperature of F. We propose that dephasing is mitigated by spin-orbit scattering. We also find that the transmission probability for electrons striking the F/S interface is much less than unity.

3:18PM R36.00005 Exploring the mini-gap state and magnetoresistance in platinum nanowires1, DANIEL SLOTCAVAGE, MEENAKSHI SINGH, THOMAS MALLOUK, MOSES CHAN, The Pennsylvania State University — Periodic oscillations in differential magnetoresistance and a superconducting mini-gap state were found in single-crystal gold nanowires [Wang et al., PRL 102, 247003 (2009)]. The oscillations were attributed to motion of individual vortices in the nanowire. We have studied proximity-induced superconductivity in polycrystalline platinum nanowires grown using template-based electrodeposition. Systematic studies of the dependence of the mini-gap state on temperature, magnetic field, and sample morphology and geometry were conducted. We found the mini-gap state to persist in polycrystalline samples. The presence of the mini-gap state in polycrystalline samples demonstrates its robustness with respect to sample morphology. On the other hand, the differential magnetoresistance oscillations was not found in these wires. Future work will focus on determining the conditions required for the occurrence of these oscillations.

1This work is supported by the National Science Foundation (DMR 0820404) and a Summer Discovery Grant from The Pennsylvania State University.

3:30PM R36.00006 Unconventional quantum oscillations in mesoscopic rings of spin-triplet superconductor Sr$_2$RuO$_4$1, XINXIN CAI, YIQUN YING, NEAL STALEY, The Pennsylvania State University, YAN XIN, NHMFL, Florida State University, DAVID FOBES, TIJIANG LIU, ZHIQIANG MAO, Tulane University, YING LIU, The Pennsylvania State University — Spin-triplet superconductor Sr$_2$RuO$_4$ has been found to feature exotic vortex physics including the formation of vortex lattices at low fields and most recently, evidence for half-flux quanta trapped in a doubly connected sample. We carried out the magnetoresistance measurements in mesoscopic ring samples of Sr$_2$RuO$_4$ fabricated on mechanically exfoliated single crystals of Sr$_2$RuO$_4$ by photolithography and focused ion beam. With the magnetic field applied perpendicular to the in-plane direction, thin-wall rings of Sr$_2$RuO$_4$ were found to exhibit a large number of full-flux quantum oscillations with pronounced amplitudes unexpected from the conventional Little-Parks effect. Furthermore, in thick-wall, two distinct periods were observed in both resistance and critical current oscillations, which we attribute to the effect of vortices, namely, the “lock-in” effect of a vortex lattice in Sr$_2$RuO$_4$. No evidence for half-flux-quantum oscillations were identified in any sample measured so far without the presence of an in-plane field. The measurements with an in-plane field are being pursued.

1This work is supported by DOE under grant DE-FG02-04ER46159

3:42PM R36.00007 Analytic Description of Superconducting-Ferromagnetic Proximity Systems1, THOMAS E. BAKER2, Department of Physics & Astronomy University of California, Irvine, CA 92617, OVIDIU E. ICREEVERZI, ADAM K. MOKE, ANDREAS BILL, Department of Physics & Astronomy California State University Long Beach, Long Beach, CA 90840 — We present the exact analytic solution of the Usadel equations for a proximity system made of a superconductor and a ferromagnet in the wide dirty limit, including spin-flip scattering. The solution was found by mathematical analogy to the Jacobi elliptic function description of a classical mechanics system known as the bead on a hoop [1]. We highlight the parallels between the two systems and present an analysis of the solution with special attention to long rage triplet effects and the inverse Fulde-Ferrell-Larkin-Ovchinnikov state. We determine the Josephson critical current and the variation of the critical temperature with spin-flip scattering.


1We gratefully acknowledge the support of the National Science Foundation (DMR-0907242), the CSU Long Beach Graduate Research Fellowship, The Research Corporation, and the Army Research Laboratory.

2Also, Department of Physics & Astronomy California State University, Long Beach, CA 90840
3:54PM R36.00008 Microscopic Study of c-axis Proximity Effect in Cuprate-Manganese Heterostructures1. H. ZHANG, I. FRIDMAN, University of Toronto, N. GAUQUELIN, G.A BOTTON, Canadian Centre for Electron Microscopy and McMaster University, J. Y.T. WEI, University of Toronto and Canadian Institute for Advanced Research — Recent studies have reported long ranged proximity effect in epitaxial thin-film heterostructures of ferromagnetic manganites and superconducting cuprates, with possible origins in novel spin-triplet correlations [1]. A key evidence for this effect is the suppression of the superconducting $T_c$ observed in multilayer films of La$_{2/3}$Ca$_{1/3}$MnO$_3$ / YBa$_2$Cu$_3$O$_{7-\delta}$ (LCMO/YBCO). However, scanning tunnelling spectroscopy on c-axis LCMO/YBCO bilayers have not seen direct evidence for proximity-induced pairing down to 5nm LCMO thickness [2]. We re-examine the $T_c$ suppression by performing atomically-resolved transmission electron microscopy and resistivity measurements on c-axis YBCO/LCMO films grown by pulsed laser deposition, and relating the microstructure in YBCO with the layer thickness and $T_c$. The microscopy revealed double CuO-chain intergrowths forming non-stoichiometric YBCO-247 regions that do not appear in x-ray diffraction, but can be related to the $T_c$ suppression. We attribute these intergrowths to heteroepitaxial strain, by comparing all the lattice parameters and symmetries involved. [1] Z. Sefrioui et al., PRB 67, 214511 (2003); C. Visani et al, Nat. Phys. 8, 539 (2012). [2] Fridman et al, PRB 84, 104522 (2011).

1Work supported by NSERC, CFI/OIT and CIFAR

4:06PM R36.00009 ABSTRACT WITHDRAWN

4:18PM R36.00010 New structural features in solution-derived YBCO nanocomposite films responsible for a successful novel pinning mechanism, J. GAZQUEZ, R. GUZMAN, ICMAB-CSIC, Spain, J. SALAFRANCA, Universidad Complutense de Madrid, Spain, R. MISHRA, Vanderbilt University, USA, M. VARELA, Materials Science and Technology Division, ORNL, USA, A. PALAU, V. ROUCO, M. COLL, A. LLORDES, ICMAB-CSIC, Spain, G. DEUTSCHER, Tel Aviv University, Israel, X. OBRADORS, T. PUIG, ICMAB-CSIC, Spain — The optimization of high temperature superconductors calls for a detailed knowledge about the effects of materials’ manipulations on the subnanometer scale, since the subtle interplay of a variety of nanoscale defect structures that pin the magnetic flux lattice will dictate the performance of these materials. The outstanding properties of solution deposited YBa$_2$Cu$_3$O$_{7-\delta}$ nanocomposites arise from the strains associated to the network of YBa$_2$Cu$_3$O$_{7-\delta}$ intergrowths emerging from the spontaneously segregated oxide nanoparticles, and a novel pinning mechanism coupling this lattice strain with superconducting pairing [1]. However, YBa$_2$Cu$_3$O$_{7-\delta}$ intergrowths involve the addition of an extra CuO chain and their ubiquity may lead to an off-stoichiometry that could jeopardize the superconducting properties of the film. Conversely, we will show, by means of aberration corrected scanning transmission microscopy in combination with electron energy loss spectroscopy, how the system balance this deficiency of Cu through new structural features, previously unforseen, that may constitute new and effective pinning centers and may be responsible for the novel pinning mechanism proposed.


4:30PM R36.00011 Crossover from Peierls distortion to one-dimensional superconductivity in arrays of (5,0) carbon nanotubes, TING ZHANG, MING YUAN SUN, ZHE WANG, WU SHI, PING SHENG, the Hong Kong University of Science and Technology — We consider the electronic instabilities in (3,3)@(8,8) and (5,0)@(15,0) metallic double wall carbon nanotubes. Using 2rd order renormalization group method, we find that in the single wall (3,3) and (5,0) CNTs, the Peierls transition dominates, while if dressed with metallic outer shell, namely the (8,8) CNT and (15,0) CNT to form double wall carbon nanotube system(DWNT), the screening effect greatly reduces the Coulomb interaction of inner tubes, and superconductivity(SS) instability is identified to be the groud state, although the crossover temperature of which SS response functions take over could be very low.

4:42PM R36.00012 1D to 3D Crossover Transition in a System of Weakly Coupled Superconducting Nanowires, QIHONG CHEN, MING YUAN SUN, ZHI LIN HOU, TING ZHANG, ZHE WANG, WU SHI, ROLF W. LORTZ, PING SHENG, the Hong Kong University of Science and Technology — Recent Results have shown the existence of superconductivity in quasi-one-dimensional systems, e.g., the 1D superconducting carbon nanotubes embedded in the aligned, linear pores of the aluminophosphate-fiv (AFI) zeolite. In order to understand theoretically the experimental observations on the thermal specific heat and the electrical resistance variation as a function of temperature, we have carried out Monte Carlo simulations on a Ginzburg-Landau (GL) model of Josephson-coupled superconducting nanowires. The results show that the competition between 1D fluctuations and the weak transverse Josephson coupling between the nanowires can give rise to a 1D-3D crossover transition at a temperature $T_c$ below the mean field $T_c^0$ of the wires. The electrical resistance can experience a sharp drop at $T_c$, at which point the nanowires become phase coheerent. The simulated specific heat exhibits a rounded peak between $T_c^0$ and $T_c^0$, whereas the phase correlation length within the ab plane diverges at $T_c$ from above, in a manner that is consistent with the occurrence of a BKT-transition in the ab plane. These Monte Carlo simulated behaviors are in excellent agreement with the experimental data.

4:54PM R36.00013 Phase slip in large array superconducting anti-dot thin films1, WEI-LI LEE, HSANG-HSI KUNG, TING-HUI CHEN, CHIA-TSO HSIEH, CHI-CHIH HO, KENG-HUI LIN, WEN-TAU JUAN, Institute of Physics, Academia Sinica — Phase slip is one of the most intriguing phenomena in superconducting nanostructure, which gives rise to a finite resistance below superconducting transition temperature. By using a special technique we developed previously for the preparation of a monolayer polymer/nanosphere hybrid, we fabricated a series of large array niobium antidot thin films with niobium line width ranging from about 36 nm to 90 nm. From the resistance and magnetization measurement, we found that the transition to the superconducting state is enhanced with increasing magnetic field applied along the normal direction of the antidot thin film, which becomes more significant in samples with smaller niobium line width. We argue that this phenomenon provides an evidence for the existence of thermal activated phase slip effect that was discovered for the first time in superconducting antidot thin film structure. Detailed results and analysis will be discussed.

1This work is supported by the Academia Sinica nano program.

5:06PM R36.00014 p-wave Superconductor in a Mesoscopic Size Grain, SUNGKIT YIP, BOR-LUEN HUANG, Institute of Physics, Academia Sinica — Motivated by the claim that Sr$_2$RuO$_4$ is a p-wave superconductor with broken time-reversal symmetry in the bulk, and many recent experimental studies of superconductors in mesoscopic size grains, we study theoretically a two-component p-wave superconductor in confined geometries, considering circular disks and rectangular samples, using both Ginzburg-Landau (GL) and quasiclassical (QC) Green function theories. For GL theory with parameters near the weak-coupling limit, we find that a sufficiently small circular disk remains normal. For zero field and intermediate sizes, a disk with sufficiently smooth boundary is in a time-reversal symmetric state, where the order parameter can be represented by a real vector forming a vortex-like structure. Only for larger grains and at lower temperatures can a broken time-reversal state be recovered. For intermediate sizes but with finite external magnetic field, the system can have possibly re-entrant phase transitions. For rectangular samples with sufficiently large aspect ratios, the superconductor near its transition temperature at zero fields has its order parameter vector parallel to the long side of the sample. Within a critical aspect ratio however, the order parameter vector forms a vortex-like structure, much like for the disk.
5:18PM R36.00015 Superconductivity and anomalous magnetic phase in LuGe$_2$ single crystals

NAKHEON SUNG, B.K. CHO, Gwangju Institute of Science and Technology (GIST), Y.J. JO, Kyungpook National University, S.K. CHO, A.I. COLDEA, University of Oxford, H. KIM, R. PROZOROV, Ames Laboratory and Iowa State University — LuGe$_2$ single crystals (ZrSi$_2$-type orthorhombic structure, $C_{nmm}$) were synthesized by the high temperature metal flux method. LuGe$_2$ was found to be the type-II superconductivity below superconducting transition temperature, $T_c = 2.3$ K. An anomalous magnetic and electric phase below $T^* = 4$ K was found only along $b$-axis in electrical transport measurement, and confirmed additionally by magnetization and heat capacity measurement. From the heat capacity data, LuGe$_2$ was found to be the weak coupling BCS type superconductivity at $T_c$, whereas the anomalous phase above $T^*$ seems to have a close correlation with the superconducting state below $T_c$. Upper critical field, $H_{c2}(T)$, of the superconductivity exhibits significant anisotropy either along $b$-axis or along $a$ (and $c$)-axis. Recently, a possible second superconducting state in superconducting YbSb$_2$ single crystals, which has the same structure as LuGe$_2$, was reported. [1] Thus, we will discuss in detail on the anisotropic superconducting properties and the anomalous phase above $T_c$ in terms of the possible second superconductivity as in YbSb$_2$.


Thursday, March 21, 2013 8:00AM - 11:00AM –
Session T1 DCMP: Invited Session: Superfluids under Nanoscale Confinement
Ballroom I - Jeevak Parpia, Cornell University

8:00AM T1.00001 Topological superfluids confined in a nanoscale slab geometry
1. JOHN SAUNDERS, Department of Physics, Royal Holloway University of London — Nanofluidic samples of superfluid $^3$He provide a route to explore odd-parity topological superfluids and their surface, edge and defect-bound excitations under well controlled conditions. We have cooled superfluid $^3$He confined in a precisely defined nano-fabricated cavity to well below 1 mK for the first time. We fingerprint the order parameter by nuclear magnetic resonance, exploiting a SQUID NMR spectrometer of exquisite sensitivity. We demonstrate that dimensional confinement, at length scales comparable to the superfluid Cooper-pair diameter, has a profound influence on the superfluid order of $^3$He. The chiral A-phase is stabilized at low pressures, in a cavity of height 650 nm. At higher pressures we observe $^3$He-B with a surface induced planar distortion. $^3$He-B is a time-reversal invariant topological superfluid, supporting gapless Majorana surface states. In the presence of the small symmetry breaking NMR static magnetic field we observe two possible B-phase states of the order parameter manifold, which can coexist as domains. Non-linear NMR on these states enables a measurement of the surface induced planar distortion, which determines the spectral weight of the surface excitations. The expected structure of the domain walls is such that, at the cavity surface, the line separating the two domains is predicted to host fermion zero modes, protected by symmetry and topology. Increasing confinement should stabilize new p-wave superfluid states of matter, such as the quasi-2D gapped A phase, which breaks time reversal symmetry, has a protected chiral edge mode, and may host half-quantum vortices with a Majorana zero-mode at the core. We discuss experimental progress toward this phase, through measurements on a 100 nm cavity. On the other hand, a cavity height of 1000 nm may stabilize a novel “striped” superfluid with spatially modulated order parameter.

In collaboration with L.V. Levitin, R.G. Bennett, A.J. Casey, B. Cowan, J. Parpia, E.V. Surovtsev

1Supported by EPSRC (UK) GR/J022004/1 and European Microkelvin Consortium, FP7 grant 228464

8:36AM T1.00002 Probing Chirality in Superfluid $^3$He-A: Free surface as an ideal boundary condition
1. KIMITOSHI KONO, Low Temperature Physics Laboratory, RIKEN — Superfluid $^3$He is known as a typical topological superfluid. A recent theoretical investigation suggests Majorana surface states at the free surface of superfluid $^3$He-B phase [1]. On the other hand, superfluid $^3$He-A is known as a chiral superfluid. The scattering of quasiparticle from small object is predicted to be skew with respect to an anisotropy axis [2]. We have developed an experimental technique to study transport properties of ions under the free surface of superfluid $^3$He [3]. By using this technique, we can investigate interaction between elementary excitations in superfluid $^3$He and small objects under well-controlled conditions. For example, in $^3$He-B interaction with Majorana surface states, although no interaction is expected, will be investigated, whereas in $^3$He-A skew scattering of quasiparticle from electron bubbles will be probed. In this paper, we present the recent results of transport properties of electron bubbles trapped below the free surface of superfluid $^3$He. In particular, experimental evidences of the skew scattering and chirality of superfluid $^3$He-A will be presented. The skew scattering of quasiparticle in $^3$He-A from electron bubble results in a bubble transport analogous to the Hall effect, where the anisotropy vector of $^3$He-A behaves as if it was a magnetic field in the Hall effect. Under experimental conditions, the effect is observed as an analogue of edge magnetoplasmon effect. After the analysis of data, we obtained a reasonable qualitative agreement with the theory [2].


3This work is done in collaboration with Hiroki Ikegami.

9:12AM T1.00003 Surface Majorana cone of the topological superfluid $^3$He B phase
1. RYUJI NOMURA, Tokyo Institute of Technology — Topological superfluids and superconductors are characterized by a non-trivial topological number in the gapped bulk state and gapless edge states on their surfaces. The surface states are proposed to be Majorana fermions as they satisfy the Majorana condition, i.e., a particle and its antiparticle are equivalent, and their linear dispersion is called Majorana cone. It is an urgent issue in condensed matter physics to confirm the existence of such Majorana fermions. Superfluid $^3$He is a suitable system to reach a definite conclusion since the spin-triplet p-wave symmetry is well established in the bulk state. We measured transverse acoustic impedance of the superfluid $^3$He B phase changing the boundary condition of a wall from a diffusive scattering up to practically specular limit by coating the wall with thin layers of superfluid $^3$He. A growth of low-energy peak in the transverse acoustic impedance was observed at higher specularities, which is the clear evidence of low-lying quasiparticle states in the vicinity of the wall. A self-consistent theoretical calculation reproduces the experimental results well and shows that the observed growth of the peak is the reflection of the linear dispersion of the surface Andreev bound states. Thus, we experimentally confirmed Majorana fermions on the surface of the superfluid $^3$He B phase and showed that the superfluid $^3$He B phase is truly a topological superfluid with the bulk-edge correspondence.

5:18PM R36.00015 Superconductivity and anomalous magnetic phase in LuGe$_2$ single crystals
the isoelectronic family of MoS$_2$ — Atomic monolayers of transition metal dichalcogenides have emerged as an interesting class of 2-dimensional (2D) crystals beyond graphene. In particular, the symmetry protected topological order [1]. Due to the symmetry protected topological order, helical surface Majorana fermions in the B phase remain gapless and their Ising spin character persists. I unveil that the competition between the Zeeman magnetic field and dipole interaction involves an anomalous quantum phase transition where a topological phase transition takes place together with spontaneous breaking of symmetry. Based on the quasiclassical theory, I illustrate that the phase transition is accompanied by anisotropic quantum criticality of spin susceptibilities on the surface, which is detectable in NMR experiments [1,2].


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Thursday, March 21, 2013 8:00AM - 11:00AM –
Session T2 DCMP: Invited Session: Valley Polarization Physics: Transition Metal Dichalcogenides and Other Ballroom II - Tony Heinz, Columbia University

8:00AM T2.00001 Valley optoelectronics and spin-valley coupling: from graphene to monolayer group-VI transition metal dichalcogenides1, WANG YAO, The University of Hong Kong — The Bloch bands in many crystals have a degenerate set of energy extrema in momentum space known as valleys. The band-edge carriers then have an extra valley index which may also be used to encode information for device applications provided that dynamic control of valley index is possible. In this talk, we show that, when inversion symmetry is broken, a pair of valleys which are equivalent by time-reversal are distinguishable by their magnetic moment and Berry curvature. These quantities give rise to valley Hall effect and circularly-polarized valley optical transition selection rule both in graphene (where inversion symmetry can be broken in a controlled way in gated bilayers), and in monolayer group-VI transition metal dichalcogenides (where the 2D crystal has inherent structural inversion asymmetry). Moreover, in monolayer dichalcogenides, we find the electrons and holes at the band edges are described by massive Dirac Fermions with strong spin-valley coupling, which further results in valley and spin dependent optical selection rule, and coexistence of valley and spin Hall effects. These phenomena make possible dynamic control of valley and spin by electric and optical means for device applications in monolayer dichalcogenides. We will report photoluminescence studies on dichalcogenide thin films, which show the first evidence on valley optical selection rule and optical valley pumping, and signature of the spin-valley coupling.

3The work was supported by the Research Grant Council of Hong Kong (HKU706412P). The author acknowledges collaborations with Guibin Liu, Zhirui Gong, Hongyi Yu, Xiaodong Cui, Di Xiao, Qian Niu and Xiaodong Xu.

8:36AM T2.00002 Optical control of exciton valley polarization in MoS$_2$, KIN FAI MAK, Cornell University — Atomic monolayers of transition metal dichalcogenides have emerged as an interesting class of 2-dimensional (2D) crystals beyond graphene. In particular, the isoelectronic family of MoS$_2$, MoSe$_2$, WS$_2$, and WSe$_2$ monolayers are direct band gap semiconductors[1] Unlike graphene, because of the lack of inversion symmetry and the presence of strong spin-orbit interactions, the fundamental energy gaps of these compounds are located at two inequivalent high-symmetry valleys in the Brillouin zone (K and K') with coupled valley and spin degrees of freedom. This electronic property makes them unique from conventional semiconductors. In this talk, we will discuss the properties of MoS$_2$ atomic layers as a prototype. Through characterization of the optical properties of the material as a function of thickness, we show that quantum confinement effects lead to a crossover in MoS$_2$ from a bulk indirect gap semiconductor to a direct gap semiconductor at monolayer thickness[2]. With this basic property established, we show that complete valley polarization of the excitons in monolayer MoS$_2$ can be achieved by optical pumping with circularly polarized light[3]. Furthermore, this polarization can be retained for longer than 1ns. Our results thus highlight the great potential of this material family for studies of valley and spin Hall physics.

3Ibid.
4Mak, PRL 105, 2010
ANDRAS KIS, EPFL — After quantum dots, nanotubes and nanowires, two-dimensional materials in the shape of sheets with atomic-scale thickness represent the newest addition to the diverse family of nanoscale materials. Single-layer molybdenum disulphide (MoS$_2$), a direct-gap semiconductor is a typical example of these new graphene-like materials that can be produced using the adhesive-tape based cleavage technique originally developed for graphene. The presence of a band gap in MoS$_2$ allowed us to fabricate transistors that can be turned off and operate with negligible leakage currents. Furthermore, our transistors can be used to build simple integrated circuits capable of performing logic operations and amplifying small signals. I will report here on our latest 2D MoS$_2$ transistors with improved performance due to enhanced electrostatic control, showing improved currents and transconductance as well as current saturation. We also record electrical breakdown of our devices and find that MoS$_2$ can support very high current densities, exceeding the current carrying capacity of copper by a factor of fifty. Furthermore, I will show optoelectronic devices incorporating MoS$_2$ with sensitivity that surpasses similar graphene devices by several orders of magnitude.

Financially supported by grants from Swiss National Science Foundation, EU-FP7, EU-ERC and Swiss Nanoscience Institute.

9:48AM T3.00004 Novel electronic degrees of freedom emerging from symmetry breaking of honeycomb lattices. JI FENG, International Center for Quantum Materials, Peking University — Electrons are central to the society-transforming information technologies. The intrinsic degrees of freedom of an electron, namely, its charge and spin, have been extensively explored in electronic and spintronic devices. As we are approaching the limit of device miniaturization, the exploration of novel electronic degrees of freedom, in terms of theoretical development and materials discovery, is of current interest. In this talk, we will focus on two strategies to break the symmetry of a Fermionic honeycomb lattice that lead to novel degrees of freedom of Bloch electrons. The essential idea in these approaches is to lift the isospin degeneracy a honeycomb lattice by introducing contrasting identities (chemical or magnetic) to the two sublattices. The new indices of Bloch electrons will then arise, corresponding to contrasting responses to external fields, such as in optical selectivity and anomalous electronic transport. Using combined computational, theoretical and experimental approaches, we go on to demonstrate that the proposed physics can be realized in real material systems. In particular, our results indicate that monolayer transition metal chalcogenides, such as non-magnetic MoX$_2$ and antiferromagnetic MnPX$_3$ (X = S, Se), can indeed exhibit selective circular dichroism. The associated Berry curvature-supported quantum transport will also be discussed.

Thursday, March 21, 2013 8:00AM - 11:00AM – Session T3 DCMP DBIO: Invited Session: From Cells to Tissues: The Material Properties of Living Matter Ballroom III - Aaron Mertz, Yale University

8:00AM T3.00001 Spreading and spontaneous motility of multicellular aggregates on soft substrates, FRANCOISE BROCHARD-WYART, Institut Curie-UPMC — We first describe the biomechanics of multicellular aggregates, a model system for tissues and tumors. We first characterize the tissue mechanical properties (surface tension, elasticity, viscosity) by a new pipette aspiration technique. The aggregate exhibits a viscoelastic response but, unlike an inert fluid, we observe aggregate reinforcement with pressure, which for a narrow range of pressures results in pulsed contractions or shivering. We interpret this reinforcement as a mechanism sensitive to the acto-myosin cortex. Such an active behavior has previously been found to cause tissue pulsation during dorsal closure of Drosophila embryo. We then describe the spreading of aggregates on rigid glass substrates, varying both intercellular and substrate adhesion. We find both partial and complete wetting regimes. For the dynamics, we find a universal spreading law at short time, analogous to that of a viscoelastic drop. At long time, we observe, for strong substrate adhesion, a precursor film spreading around the aggregate. Depending on aggregate cohesion, this precursor film can be a dense cellular monolayer (liquid state) or consist of individual cells escaping from the aggregate body (gas state). The transition from liquid to gas state appears also to be present in the progression of a tumor from noninvasive to metastatic, known as the epithelial-mesenchymal transition. Finally, we describe the effect of the substrate rigidity on the phase diagram of wetting. On soft gels decorated with fibronectin and strongly cohesive aggregates, we have observed a wetting transition induced by the substrate rigidity: on ultra soft gels, below an elastic modulus Ec the aggregates do not spread, whereas above Ec we observe a precursor film expending with a diffusive law. The diffusion coefficient D(E) presents a maximum near Ec. A maximum in the substrate rigidity has also been observed for single cells. Near Ec, we observe a new phenomenon: a cell monolayer expands outward from the aggregate apparently under tension. In this tense monolayer, holes nucleate, and lead to a symmetry breaking as the entire aggregate starts to move in a similar fashion as a giant fish keratocyte.

8:36AM T3.00002 Modeling cell-matrix traction forces in Keratinocyte colonies, SHILADIYA BANERJEE, Department of Physics, Syracuse University — Crosstalk between cell-cell and cell-matrix adhesions plays an essential role in the mechanical function of tissues. The traction forces exerted by cohesive keratinocyte colonies with strong cell-cell adhesions are mostly concentrated at the colony periphery. In contrast, for weak cadherin-based intercellular adhesions, individual cells in a colony interact with their matrix independently, with a disorganized distribution of traction forces extending throughout the colony. In this talk I will present a minimal physical model of the colony as contractile elastic media linked by springs and coupled to an elastic substrate. The model captures the spatial distribution of traction forces seen in experiments. For cell colonies with strong cell-cell adhesions, the total traction force of the colony measured in experiments is found to scale with the colony’s geometrical size. This scaling suggests the emergence of an effective surface tension of magnitude comparable to that measured for non-adherent, three-dimensional cell aggregates. The physical model supports the scaling and indicates that the surface tension may be controlled by acto-myosin contractility.

Supported by the NSF through grant DMR-1004789. This work was done in collaboration with Aaron F. Mertz, Eric R. Dufresne and Valerie Horsley (Yale University) and M. Cristina Marchetti (Syracuse University).

9:12AM T3.00003 May the force be with you: Surface tension predicts tissue rearrangement, RAMSEY FOTY, D.University of Medicine and Dentistry of New Jersey, Robert Wood Johnson Medical — No abstract available.
8:00AM T5.00001 Polarization dependence of Raman 2D band in bilayer graphene. JAE-JUNG LEE, NGOR MBAYE SECK, Department of Physics, Sungog University, Seoul, Korea, DUHEE YOON, Electrical Engineering Division, Engineering Department, University of Cambridge, Cambridge, UK, HYEONSIK CHEONG, Department of Physics, Sungog University, Seoul, Korea — The Raman intensity of the double-resonance 2D band in single-layer graphene has a strong polarization dependence (Yoon et al. Nano Lett.). The intensity is maximum when the excitation and detection polarization are parallel and minimum when they are orthogonal, whereas that of G band is isotropic. This strong polarization dependence is the consequence of the inhomogeneous optical absorption and emission mediated by electron-phonon interactions. Here, the polarization dependence of the Raman 2D band in bilayer graphene. The 2D band of bilayer graphene can be decomposed to 4 Lorentzian peaks corresponding to different scattering process involving 2 conduction and 2 valence bands. The 2D band in bilayer graphene shows a similar polarization dependence as that of single layer. Furthermore, the excitation energy dependence was investigated by using 4 different excitation laser wavelengths. The polarization ratio of each of the 4 Lorentzian peaks seems to reflect the features of the electronic band structure of bilayer graphene in the energy range of the excitation laser.

8:12AM T5.00002 Undetectable Raman Spectrum of Graphene on Platinum Surface. A. ZETTL, QIN ZHOU, Department of Physics, University of California at Berkeley; Materials Sciences Division, Lawrence Berkeley National Laboratory — Raman spectroscopy is often used as a quick and convenient tool to evaluate the growth quality of graphene. Recently there has been growing interest in platinum mediated graphene CVD growth for producing high-quality, large grain size, and highly flat graphene layers. Surprisingly, no Raman signal of graphene can be detected in the as-grown state on platinum substrates, despite using different laser wavelengths from 488 nm to 785 nm. This phenomenon is brieﬂy mentioned in earlier literature and has been attributed to strong platinum-graphene interaction. We investigate the disappearance of graphene Raman signatures on metal substrates, by performing Raman spectrum measurements on graphene layers transferred onto various substrates.

8:24AM T5.00003 Raman spectroscopy of single layer graphitic carbon nitride. JOEL THERRIEN, YANCEN LI, ECE Dept UMass Lowell, DANIEL SCHMIDT, Plastics Engineering Dept UMass Lowell, ADAM COLLARD, Physics U. Texas Austin, DANIEL FINKENSTADT, TAYLOR YUST, US Naval Academy — Single layer graphitic carbon nitride (referred to as melon) has been synthesized by our group in sizes up to 50 μm across. Raman spectroscopy has been performed on single layer melon and multi layer samples. Much like melon, graphene shows a unique raman spectrum when in single layer form. These experimental results have been compared to theoretical calculations for possible melon structures. Bond counts for feasible structures of hexagonal carbon nitride have been calculated and some possible structures have been eliminated from consideration based on these efforts. Periodic supercells have been built to make sheets based on structures to be modeled via density-functional theory, as implemented using VASP, to calculate energy dependence was investigated by using 4 different excitation laser wavelengths. The polarization ratio of each of the 4 Lorentzian peaks seems to reflect the features of the electronic band structure of bilayer graphene in the energy range of the excitation laser.

9:48AM T3.00004 Biophysical aspects of embryonic development. LARS HUFNAGEL, European Molecular Biology Laboratory - EMBL, Heidelberg — No abstract available.

10:24AM T3.00005 Forces, waves and emergent dynamics during collective cell migration. XAVIER TREPAT, Institute for Bioengineering of Catalonia — A broad range of biological processes such as morphogenesis, tissue regeneration, and cancer invasion depend on the collective motion of cell groups. For a group of cells to migrate cohesively, it has long been suspected that each constituent cell must exert physical forces not only upon its extracellular matrix but also upon neighboring cells. I will present novel techniques to measure these distinct force components. Using these techniques, we unveiled an unexpectedly rich physical picture in which the distribution of physical forces is dominated by heterogeneity, cooperativity, and jamming. I will show, moreover, that these essential features of inter-cellular force transmission enable the propagation of a new type of mechanical wave during tissue growth. Finally, I will demonstrate that both in epithelial and endothelial cell sheets, forces and waves are mechanically linked to cell velocities through a newly discovered emergent mechanism of innately collective cell guidance: plithotaxis.

Thursday, March 21, 2013 8:00AM - 11:00AM — Session T5 DCMP: Graphene: Transport and Optical Phenomena: Raman and Phonons 301 - Francois Peeters, University of Antwerp

8:00AM T5.00004 Magneto-Raman experiments in single- and multi-layer graphene. F.M. ARDITO, UNICAMP - Univ. Estadual de Campinas, T.G. MENDES DE SA, UFMG - Univ. Federal de Minas Gerais, P.F. GOMES, UNICAMP - Univ. Estadual de Campinas, E. NERY, D.L. MAFRA, UFMG - Univ. Federal de Minas Gerais, F. IKAWA, M.J.S.P. BRASIL, UNICAMP - Univ. Estadual de Campinas, L.M. MALARD, F. PLENTZ, M.A. PIMENTA, R.G. LACERDA, UFMG - Univ. Federal de Minas Gerais, E. GRANADO, UNICAMP - Univ. Estadual de Campinas — Micro-Raman experiments as a function of magnetic field up to 15 T were performed on a set of natural graphene flakes on Si/SiO$_2$ substrates and multilayer epitaxial graphene. Raman signals were observed for graphene at multiple Landau levels observed in epitaxial graphene. Calculated phonon energy and broadening oscillations obtained from the phonon’s Green function show good agreement with the results obtained for SiC samples, in line with a previous report [1]. For graphene flakes, the field evolution of the G-band is strongly sample-dependent, and may also depend on the position of the focal spot. A splitting of G-band in two peaks was observed in some cases for $B < 10$ T. Our results suggest the large sensitivity of graphene electron-phonon interaction to both magnetic field and local conditions. [1] C. Faugeras et al., Phys. Rev. Lett. 103, 186803 (2009).

8:36AM T5.00005 Transport and Raman measurements in Graphene: Interaction strength and scattering mechanisms. SEBASTIAN REMI, ANNA SWAN, BENNETT GOLDBERG, Boston University — Among the most common techniques for characterization of graphene materials have been electronic transport and Raman measurements, for instance both can be easily tuned by changing the charge carrier density and electronic screening. In each situation the underlying physics is connected to the interactions and relaxation mechanisms in the material. However it is well known that the electronic scattering time does not necessarily describe the broadening observed in Raman measurements. Here we present micro Raman and transport measurements of single layer graphene field effect devices. We discuss interaction and scattering mechanisms and how these are connected in the different measurements.

9:00AM T5.00006 Raman scattering of 2D materials. TING YU, Division of Physics and Applied, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371 2, RICHIRO SAITO, Department of Physics, Tohoku University, Sendai, Miyagi 9808578, Japan, MILDRED DRESSELHAUS, Department of Electrical Engineering and Computer Science, Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 — Motivated by graphene, two-dimensional (2D) materials become the center of current Nanoscience and Nanotechnology. In this talk, I will report our recent works on Raman scattering study of 2D materials such as graphene and MoS$_2$. In detail: the in-plane and out-of-plane arrangement of carbons in graphene layers are identified by both Raman and HRTEM with atomic resolution; the structure evolution of molecules anchored on the surface of graphene is studied by Raman; the behavior of Dirac Fermions of graphene in a magnetic field is probed; the strain effects on MoS$_2$ and the identification of crystallographic orientation of MoS$_2$ are also discussed. The results presented here are highly relevant to the fundamental and applications of graphene and other 2D transition metal dichalcogenides (TMDs).
9:12AM T5.00007 Temperature-dependent photoluminescence and Raman spectroscopy of single-layer MoS$_2$. J.R. SIMPSON, Towson University, R. YAN, Notre Dame, S. BERTOLAZZI, A. KIS, J. BRIVIO, EPFL, M. WATSON, Towson University, H.C. XINC, Notem Dame, A.R. HIGHT WALKER, NIST — We report the temperature-dependent photoluminescence (PL) and Raman spectra of single-layer MoS$_2$. Mechanical exfoliation from bulk MoS$_2$ provides single-layer flakes which are then transferred to either sapphire (with and without ALD HfO$_2$ overcoating) or suspended over holes in a Si/Si$_3$N$_4$ substrate. We measure the temperature dependence of PL and Raman spectra from (100 to 400) K using HeNe 632.8 nm (PL) and Ar$^{+}$ ion 514.5 nm (Raman) laser excitations coupled to a microscope and grating spectrometer. PL shows a single, narrow peak corresponding to a direct-band transition at 1.9 eV with a width of 50 meV. The PL peak redshifts and broadens with increasing temperature. Raman spectra reveal two strong phonon vibrational modes, the planar $E_{2g}^r$ and out-of-plane $A_{1g}$, both of which soften linearly with increasing temperature as a result of anharmonic effects. We extract a linear temperature coefficient for both Raman modes comparable to the G-mode of graphene. A comparison with the dependence of phonon peak position on incident optical power for the suspended sample shows moderate heat flux efficiency. The impact of dielectric and substrate environment on extraction of thermal conductivity will be discussed.

9:24AM T5.00008 Observation of polaronic effects in electron transport in graphene by infrared spectroscopy, KELIANG HE, LIANG ZHAO, JIE SHAN, Case Western Reserve University, KIN FAI MAK, NICK PETRON, JAMES HONE, TONY F. HEINZ, Columbia University, G. LARRY CARR, NSLS, Brookhaven National Laboratory — Polaronics, quasi-particles consisting of electrons and the accompanying lattice polarization, are generally considered to be unimportant for the electrical transport properties of nonpolar crystals such as graphene. The distinctive linear dispersion relation found in graphene and the drastically reduced screening of Coulomb interactions associated with the material’s reduced dimensionality, however, lead to strong coupling between Dirac electrons and high-energy phonons in graphene. In this work, we apply the infrared absorption spectroscopy to investigate the optical conductivity of graphene as a function of electrostatic doping density. We have observed a phonon side band in the intraband optical conductivity with a significant spectral weight transfer from the Drude response, indicating the importance of the polaronic effects. The effects can also be tuned by doping. The conductivity spectra have been analyzed in the framework of the extended Drude model to yield the spectral dependence of the mass enhancement factor (band structure renormalization) and the scattering rate (with an onset for phonon scattering) at different doping levels. Our results are in good agreement with many-body calculations for graphene conductance with polaronic corrections.

9:36AM T5.00009 Electron-phonon bound states in graphene, JUSTIN ZHU, SAMVEL M. BADALYAN, FRANCOIS PEETERS, Department of Physics, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium — We investigate the fine structure of the energy spectrum in graphene induced by electron-optical phonon coupling. Despite the small electron-phonon coupling, perturbation theory is inapplicable in the part of spectrum near the optical phonon emission threshold. In zero magnetic field [1] we derive new dispersion equation, which in the immediate neighborhood below the threshold describes an electron-phonon bound state. We find that the singular vertex corrections beyond perturbation theory strongly enhance the electron-phonon binding energy scale. In quantizing magnetic fields [2], our findings beyond perturbation theory show that the true spectrum near the phonon emission threshold is completely governed by new branches of the spectrum, corresponding to bound states of an electron and an optical phonon with a binding energy of the order of $\omega_B$ where $\omega_B$ is the electron-phonon coupling and $\omega_0$ the phonon energy.


9:48AM T5.00010 Graphene thermal conductivity from first principles, LUCAS LINDSAY, TOM REINECKE, Naval Research Laboratory, Washington, D.C., DAVID BROIDO, Department of Physics, Boston College — Previous theoretical work based on optimized Tersoff interatomic potential found that the thermal conductivity of graphene is dominated by out-of-plane phonons in part due to reflection symmetry of the graphene sheet [1,2]. Since empirical potentials can have questionable predictive power, here we present calculations of the thermal conductivity of graphene using interatomic forces determined from first principles coupled with a numerical solution to the Peierls-Boltzmann transport equation. We find good agreement with experiment for the calculated phonon dispersion and thermal conductivity of graphene and validate earlier theoretical results which used the optimized empirical potential. [1] J.H. Seol, et al, Science 328, 213 (2010). [2] L. Lindsay, et al, Phys. Rev. B 82, 115427 (2010).

10:00AM T5.00011 Thermal transport in low-dimensional systems: the case of Graphene and single layer Boron Nitride, LUIZ FELIPE PEREIRA, DAVIDE DONADIO, Max Planck Institute for Polymer Research — Low-dimensional systems present unusual transport properties in comparison to bulk materials. In contrast with the three-dimensional case, in one- and two-dimensions heat transport models predict a divergence of the thermal conductivity with system size. In reality, in a low-dimensional system the mean-free-path of heat carriers is typically much shorter than the system size on the simulation results. Equilibrium molecular dynamics predicts a convergence of the thermal conductivity with system size, even for systems between theory and experiments for such low-dimensional systems. We perform extensive molecular dynamics simulations of heat transport in graphene and single layer BN, in order to clarify the behavior of the thermal conductivity in realistic low-dimensional systems. In particular, we address the influence of system size on the simulation results. Equilibrium molecular dynamics predicts a divergence of the thermal conductivity with system size, even for systems with less than one hundred nanometers and thousands of atoms. Meanwhile, large scale non-equilibrium molecular dynamics shows a divergence of the thermal conductivity with system size up to the micrometer scale. We analyse the discrepancy between methods in terms of perturbations in phonon populations induced by the non-equilibrium regime.

10:12AM T5.00012 Phonon-limited transport coefficients in extrinsic graphene$, ENRIQUE MUNOZ, Departamento de Fisica, Pontificia Universidad Catolica de Chile — The effect of electron-phonon scattering processes over the thermoelectric properties of extrinsic graphene was studied. Electron-phonon interaction is formulated in the second quantization language, for chiral Dirac spinor fields and phonon Bose fields, within the deformation potential approximation. Electrical and thermal resistivity, as well as the thermopower, were calculated within the Bloch theory approximations. Analytical expressions for the different transport coefficients were obtained from a variational solution of the Boltzmann transport equation. The phonon-limited electrical resistivity $\rho_{\text{el-phon}}$ shows a linear in temperature dependence at high temperatures, and follows a $n-\frac{1}{2}$ dependence at low temperatures, in agreement with experiments. The phonon-limited thermal resistivity at low temperatures exhibits a $\sim T$ dependence and achieves a nearly constant value at high temperatures. The predicted Seebeck coefficient at very low temperature is $S(T) \sim \pi^2 k_B T / (3 e E_F)$, which shows a $n-\frac{1}{2}$ dependence with the carrier density, in agreement with experiments.


$^1$E M aknowledges financial support from Fondecyt Grant 11100064.
Hallucinations detected.
10:24AM T10.00005 Scaling up with superconducting qubits — ALEXANDRE BLAIS, Universite de Sherbrooke — There have been significant developments in the field of superconducting qubits since the first observation, almost 15 years ago, of coherent oscillations in a superconducting electrical circuit. One key number could summarize this progress: the coherence time. Indeed, this quantity has increased by about 5 orders of magnitude since the first experiments. Characterizing this progress with a single number is, however, too simplistic. It does not capture the many improvements that the field has witnessed and, in the same way, hides many of the challenges that lie ahead. Indeed, with many ingredients having to come together and work just right, quantum computation is about more than long coherence times. A much better (yet incomplete) measure is the error rate of single- and two-qubit logical gates. Recent experiments show this rate approaching the level required for fault-tolerant quantum computation, a requirement for a scalable quantum computer architecture. In parallel, much effort has been invested in using superconducting qubits as artificial atoms to explore quantum optics with microwaves and in unconventional parameter ranges. With an emphasis on theoretical work, in this talk I will present an overview of the recent achievements in the field and present some challenges that will have to be overcome.

Thursday, March 21, 2013 8:00AM - 10:48AM — Session T19 DCMP: Metal-Insulator Transitions I

8:00AM T19.00001 Importance of subleading corrections for the Mott critical point — A.-M.S. TREMBLAY, Universite de Sherbrooke, Quebec, Canada, and Canadian Institute for Advanced Research, PATRICK SEMON, Universite de Sherbrooke — The interaction-induced metal-insulator transition should be in the Ising universality class. Experiments on layered organic superconductors suggest instead that we observe critical end points of the first-order Mott transition in $d = 2$ does not belong to any of the known universality classes for thermal phase transitions. In particular, it is found that $\delta = 2$. Given the quantum nature of the two phases involved in the transition, we use dynamical mean-field theory and a cluster generalization to investigate whether the new exponents could arise as transient quantum behavior preceding the asymptotic critical behavior. In the cluster calculation, a canonical transformation that minimizes the sign problem in continuous-time quantum Monte Carlo simulations allows previously unattainable precision. Our results show that there are important subleading corrections in the mean-field regime that can lead to an apparent exponent $\delta = 2$. Experiments on optical lattices could verify our predictions for double occupancy. P. Sémon and A.-M.S. Tremblay, Phys. Rev. B 85, 201101(R)/(R)1-5 (2012).

1Supported by NSERC, Canada Research Chair, CIFAR, CFI, MELS, Calcul Quebec, Compute/Calcul Canada

8:12AM T19.00002 Quantum critical Mott transition in triangular lattice Hubbard model — YI YANG MENG, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University, KUANG SHING CHEN, Department of Physics and Astronomy, Louisiana State University, UNJONG YU, GIST-college, Kwangju Institute of Science and Technology, Korea, SHUXIANG YANG, Department of Physics and Astronomy, Louisiana State University, — We numerically study electric transport near the Mott metal-insulator transition for the half-filled Hubbard model on a triangular lattice, with the interaction strength ($U/t$) and temperature as control parameters. We compute spectral and transport properties and estimate the Mott transition to occur at the critical interaction strength $U/t_c=8.5\pm0.5$. From the metallic side, the van Hove singularity in the density of states moves towards the Fermi level with increasing $U/t$ and eventually collapses at the Mott transition, above which the Mott gap opens. In the quantum critical region above the transition point, the system exhibits a marginal Fermi liquid behavior. Due to the competition between electronic correlations and geometric frustrations, we observe non-trivial transport properties across the transition such as a universal jump in the resistivity, consistent with recent quantum field theory proposals. Implications for experiments on the layered triangular lattice organic material k-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ and EtMe$_3$Sb[Pd(emit)$_2$]$_2$ are also discussed.

8:24AM T19.00003 Mott criticality in electric transport of triangular lattice Hubbard model — TOSHIHIRO SATO, KAZUMASA HATTORI, HIROKAZU TSUNETSUGU, Institute for Solid State Physics, University of Tokyo — We numerically study electric transport near the Mott metal-insulator transition for the half-filled Hubbard model on a triangular lattice. Our approach is a cellular dynamical mean field theory (CDMFT) with a continuous-time QMC solver and we calculate optical conductivity including vertex corrections. The main issue is the variation of optical conductivity upon controlling Coulomb repulsion $U$ for various temperatures. Near the Mott critical end point, a Drude peak on the metallic side smoothly continues to an “ingap” peak emerging within the Hubbard gap on the insulating side. We find a critical power-law behavior in their $U$-dependence near the critical point. The obtained critical exponent $1/\delta = 0.15$ of the optical weight differs from the exponent $1/\delta = 1/3$ of the order parameter (double occupancy) in the CDMFT calculations. This discrepancy suggests that conductivity does not have the same scaling behavior as that for the order parameter $[1]$. $1$T. Sato, K. Hattori, and H. Tsunetsugu, J. Phys. Soc. Jpn. 81, 083703 (2012).

8:36AM T19.00004 Self-localization of a single hole in Mott antiferromagnets — ZHENG ZHU, Institute for Advanced Study, Tsinghua University, Beijing, China, HONG-CHEN JIANG, Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA, 93106-4030, U.S.A., YANG QI, CHUN-SHUN TIAN, ZHENG-YU WENG, Institute for Advanced Study, Tsinghua University, Beijing, 100084, China — Anderson localization - quantum suppression of carrier diffusion due to disorders - is a basic notion of modern condensed matter physics. Here, we report a novel localization phenomenon totally contrary to this common wisdom. Strikingly, it is purely of strong interaction origin and occurs without the assistance of disorders. Specifically, by combined numerical (density matrix renormalization group) method and analytic analysis, we show that a single hole injected in a quantum antiferromagnetic ladder is generally self-localized even though the system respects the translational symmetry. The localization length is found to monotonically decrease with the increase of leg number, stronger self-localization in the two-dimensional limit. We find that a peculiar coupling between the doped charge and the quantum spin background causes quantum interference among different hole paths. The latter brings the hole’s itinerant motion to a halt, a phenomenonologly analogous to Anderson localization. Our findings are opposite to the common belief of the quasiparticle picture for the doped hole and unveil a completely new paradigm for lightly doped Mott insulators.

8:48AM T19.00005 Emergent Metal in Disordered Two Dimensional Mott Insulator$^1$ — ONIAM NGANBA MEETEI, NANDINI TRIVEDI, Ohio State University, ELIAS LAHOU, AMIT KANIHEL, Technion - Israel Institute of Technology — We show that disordered a two dimensional Mott insulator leads to an insulator-metal transition, even in the absence of any doping. For disorder strengths comparable to the interaction, the Mott gap closes and extended states develop at the chemical potential. Further increase in disorder drives the emergent metal into a gapless localized insulating phase. We make detailed comparisons of our theoretical predictions on the emergent metal with transport and APRES data on 1T-TaS$_2$ intercalated by Cu. The parent compound 1T-TaS$_2$ is a Mott insulator at low temperature ($T < 1800$K). In the commensurate charge density wave (CCDW) phase, the “star of David” unit cells with 13 Ta atoms form a commensurate triangular lattice with a single half filled band crossing the Fermi energy. Strong interaction produces a Mott gap in the half filled band. Disorder introduced by intercalating Cu atoms between TaS$_2$ layers closes the Mott gap and drives the material into a metallic phase without destroying the CCDW order in good agreement with theory. Our work presents the first evidence of such an insulator-metal transition in a disordered two-dimensional Mott insulator.

$^1$This work was supported by DOE grant number DE-FG02-07ER46423 (ONM and NT) and by Israeli Science Foundation (EL and AK).
Mean-Field Theory for the Hubbard Model

The presence of some form of long-range correlations in the on-site energies. One of the most widely used examples are disorder potentials generated by potentials correlations of the screened disordered potential, a so-far neglected mechanism to suppress the role of Anderson localization (interference) effects.

non-Gaussian form for the spatial that this effect, which cannot be captured by a simple renormalization of the disorder strength, instead reflects a peculiar studies of the interaction-localization problem.

DOBROSAVLJEVIĆ, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL — We perform variational used to define the localization length. Furthermore, we check for the validity of single parameter scaling (SPS), and its dependence on the Levy index.

Levy-type. We numerically compute the Lyapunov exponent and its variance. This exponent is a self-averaging quantity whose inverse in certain cases can be

MAYETT, JENNIFER SCHWARZ, Syracuse University — Abstract: Quantum transport through disordered systems has been the subject of extensive research

justification for the systematic extension of the single site typical medium theory to a momentum coarse grained Dynamical Cluster Approximation where the and review two quantities that measure the localization transition: the inverse participation ratio and the typical (geometrically averaged) density of states. We with “resonant states” becoming significant in the tails of the density of states. In this work, we present exact diagonalization results of the Anderson model

RELL, Louisiana State University — The ensemble averaged density of states is commonly used as an order parameter to distinguish between a metal and insulator. However, for disordered electronic systems this is not the case: the disorder averaged density of states exhibits no singular behavior as the mobility edge between extended and localized states is crossed. In addition, recent work on rare events in the Anderson model further complicates this characterization with “resonant states” becoming significant in the tails of the density of states. In this work, we present exact diagonalization results of the Anderson model and review two quantities that measure the localization transition: the inverse participation ratio and the typical (geometrically averaged) density of states. We also examine the log-normal distribution of the local density of states in real and momentum space. In particular, the results in momentum space provide a justification for the systematic extension of the single site typical medium theory to a momentum coarse grained Dynamical Cluster Approximation where the non-local effects can be included systematically.

Supported by NSF-MWN/CIAM and NSF-PIRE.

9:24AM T19.00008 Spontaneous symmetry breaking in matrix models

FABIO FRANCHINI, Massachusetts Institute of Technology & SISSA — Matrix models with rotational invariant weights provide, in the large $N$ limit, a robust universality of correlated eigenvalues. Here, we want to argue that a weight that breaks the eigenvalue distribution into disjoint supports, further induces a spontaneous breaking of the rotational symmetry. This SSB of the $U(N)$ can potentially be used as a toy model to study the eigenstate distribution at the Anderson Metal/Insulator Transition.

1Supported by a Marie Curie International Outgoing Fellowship (FP7/2007-2013) under the grant PIOF-PHY-276093.

9:36AM T19.00009 Puzzle in the Anderson transition with long-range correlated potentials

GREG PETERSEN, NANCY SANDLER, Ohio University — The conditions for an Anderson transition in 1D systems has been an open question since it’s discovery a half century ago. Although scaling theory predicts localization in this case, it has been shown that a transition exists in the presence of some form of long-range correlations in the on-site energies. One of the most widely used examples are disorder potentials generated by $1/k^\alpha$ spectral densities [1] that, with an appropriate short range cutoff, result in vanishing correlation functions in the thermodynamic limit. However, these results are in direct contradiction to work by Kotani et. al. [2] that argues for the existence of a metallic state only when infinite range correlations are non-zero. In this talk we will show that there is no contradiction between the two results as the correlation function generated from numerical techniques is staunchly different from analytic expectations. Furthermore, we will present the exact analytic expression for the correlation function in the thermodynamic limit. Finally, we will discuss the role played by short- and long-range features of the correlation function in the Anderson transition.

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9:48AM T19.00010 Momentum Space Signatures of Anderson Localization

CONRAD MOORE, CHINEDU EKUMA, Louisiana State University, HANNA TERLETSKA, Brookhaven National Laboratory, ZIYANG MENG, JUANA MORENO, MARK JAR-RELL, Louisiana State University — The ensemble averaged density of states is commonly used as an order parameter to distinguish between a metal and insulator. However, for disordered electronic systems this is not the case: the disorder averaged density of states exhibits no singular behavior as the mobility edge between extended and localized states is crossed. In addition, recent work on rare events in the Anderson model further complicates this characterization with “resonant states” becoming significant in the tails of the density of states. In this work, we present exact diagonalization results of the Anderson model and review two quantities that measure the localization transition: the inverse participation ratio and the typical (geometrically averaged) density of states. We also examine the log-normal distribution of the local density of states in real and momentum space. In particular, the results in momentum space provide a justification for the systematic extension of the single site typical medium theory to a momentum coarse grained Dynamical Cluster Approximation where the non-local effects can be included systematically.

2This work is supported by NSF Award No. LA-SIGMA EPS - 1003897

10:00AM T19.00011 Anderson localization in one-dimension with Levy-type disorder

DAN MAYETT, JENNIFER SCHWARZ, Syracuse University — Abstract: Quantum transport through disordered systems has been the subject of extensive research since Anderson’s seminal theory of localization. Motivated by experimental realizations of light transport across media exhibiting Levy-type fluctuations, we study the one-dimensional Anderson model where the random site energies are governed by a probability distribution with a broad tail, otherwise known as Levy-type. We numerically compute the Lyapunov exponent and its variance. This exponent is a self-averaging quantity whose inverse in certain cases can be used to define the localization length. Furthermore, we check for the validity of single parameter scaling (SFS), and its dependence on the Levy index.

10:12AM T19.00012 Interactions produce strongly non-Gaussian spatial correlations of the screened random potential

H. JAVAN MARD, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, E.C. ANDRADE, Technische Universitaet Dresden, Dresden, Germany, E. MIRANDA, Univ. of Campinas,Campinas,SP,Brazil, V. DOBROSAVLJEVIĆ, Department of Physics and National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL. — We perform variational studies of the interaction-localization problem by using both the Hartree-Fock and the Gutzwiller (slave boson) approximations to describe the interaction-induced renormalizations of the effective (screened) random potential seen by quasiparticles. Here we present results of careful finite-size scaling studies for the conductance of disordered Hubbard chains at half-filling and zero temperature. While our results indicate that quasiparticle wavefunctions remains exponentially localized even in presence of moderate to strong repulsive interactions, we find surprisingly strong enhancement of the conductance of finite size systems. In particular, we show that interactions produce a strong decrease of the characteristic conductance scale $g^* \sim \sin$ the offsetting the signal of strong localization. We show that this effect, which cannot be captured by a simple renormalization of the disorder strength, instead reflects a peculiar non-Gaussian form for the spatial correlations of the screened disordered potential, a so-far neglected mechanism to suppress the role of Anderson localization (interference) effects.

the importance of the hydrodynamic limit and the limitations of current approaches. Technics used often involve simplified models or calculational tricks, which can obscure some of the underlying physical processes. Here we use a Boltzmann systems driven out of equilibrium is a field in which we are still searching for general principles and universal results. Quantum critical systems are useful in quantum-phase transition from the conventional superconductor to an uncondensed state driven by the Fermi surface anisotropy. At strong anisotropy we find no sign of an ordering transition down to very low temperature suggesting existence of a direct in the thermodynamic limit. For the relevant regime of intermediate coupling strength our data show that the Fermi surface mismatch indeed suppresses numeric results obtained with Diagrammatic Monte Carlo, a new technique for correlated fermionic systems based on sampling Feynman diagrammatic series. Supported by the Johns Hopkins Institute for Quantum Matter, under Grant No. DE-FG02-08ER46544 from the US Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

References:
1) E.J.W. Verwey, Nature 144, 327 (1939)

Thursday, March 21, 2013 8:00AM - 11:00AM
Session T22 DCMP: Strongly Correlated Electron Theory III

8:00AM T22.00001 Lifshitz Transition in the Two Dimensional Hubbard Model. KUANG-SHING CHEN, Department of Physics and Astronomy, Louisiana State University, ZIYANG MENG, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University, THOMAS PRUSCHKE, Institute for Theoretical Physics, University of Göttingen, Germany, JUANA MORENO, MARK JARRELL, Department of Physics and Astronomy, Center for Computation and Technology, Louisiana State University — Using large-scale dynamical cluster quantum Monte Carlo simulations, we study the Lifshitz transition of the two dimensional Hubbard model with next-nearest-neighbor hopping (′), chemical potential and temperature as control parameters. At = 0, we identify a line of Lifshitz transition points associated with a change of the Fermi surface topology at zero temperature. In the overdoped region, the Fermi surface is complete and electron-like; across the Lifshitz transition, the Fermi surface becomes hole-like and develops a pseudogap. At (or very close to) the Lifshitz transition points, a van Hove singularity in the density of states crosses the Fermi level. The van Hove singularity occurs at finite doping due to correlation effects, and becomes more singular when ′ becomes more negative. The resulting temperature dependence on the bare d-wave pairing susceptibility close to the Lifshitz points is significantly different from that found in the traditional van Hove scenarios.

8:12AM T22.00002 Density Matrix Embedding Theory of Strongly Correlated Models. QIAONI CHEN, GERALD KNIJA, GARNET KIN-LIC CHAN, Princeton University — We apply the recently developed density matrix embedding theory(DMET), to the honeycomb Hubbard model and the cuprate p-d model. DMET is based on the density matrix ratio than the Green’s function, thus all couplings are frequency independent and of much lower cost than in DMFT. In DMFT large clusters can be treated with similar accuracy but lower cost than in DMFT. (i) In the honeycomb Hubbard model, QMC calculations show a spin-liquid between a metal and insulator, but suffered from potential finite size errors. Using cluster DMET we find only a second-order phase transition near = 3.3 between the metal and insulator, with no spin-liquid. Our thermodynamic data allow a direct comparison to QMC calculations, highlighting the finite size errors. (ii) Three band model calculations with large cluster DMFT are infeasible, however cluster DMET calculations are very affordable. Earlier DMFT calculations place the metal-insulator transition at an unphysical d-occupancy. Using cluster DMET treatments, we show that the transition between metal and insulator shifts into the physical regime due to our ability to include large cluster correlations.

8:24AM T22.00003 Diagrammatic Monte Carlo for Fermions with Spin-Dependent Hopping Anisotropy. JAN GUKELBERGER, Theoretische Physik, ETH Zurich, EVGENY KOZIK, CPHET, Ecole Polytechnique, LODE POLLET, Department Physik, LMU Munich, KRIS VAN HOUCKE, Department of Physics and Astronomy, Ghent University, NIKOLAY PROKOF’EV, BORIS SVISTUNOV, Department of Physics, University of Massachusetts, MATTHIAS TROYER, Theoretische Physik, ETH Zurich — We study attractively interacting fermions on a square lattice whose Fermi surfaces exhibit a spin-dependent anisotropy. Such a system was proposed to harbor several exotic phases, most notably a Cooper-pair Bose-metal featuring a gap for fermionic excitations but gapless, uncondensed pair excitations along a Bose surface in momentum space. We present unbiased numeric results obtained with Diagrammatic Monte Carlo, a new technique for correlated fermionic systems based on sampling Feynman diagrammatic series directly in the thermodynamic limit. For the relevant regime of intermediate coupling strength our data show that the Fermi surface mismatch indeed suppresses the BCS transition to superfluidity. At strong anisotropy we find no sign of an ordering transition down to very low temperature suggesting existence of a quantum-phase transition from the conventional superconductor to an uncondensed state driven by the Fermi surface anisotropy.

8:36AM T22.00004 Non-Equilibrium Conductivity at Quantum Critical Points. ANDREW BERRIDGE, London Centre for Nanotechnology, M.J. BHASEEN, King’s College London, A.G. GREEN, London Centre for Nanotechnology — The behaviour of quantum systems driven out of equilibrium is a field in which we are still searching for general principles and universal results. Quantum critical systems are useful in this search as their out of equilibrium steady states may inherit universal features from equilibrium. While this has been shown in some cases, the calculational techniques used often involve simplified models or calculational tricks, which can obscure some of the underlying physical processes. Here we use a Boltzmann transport approach to study the steady-state non-equilibrium properties - conductivity and current noise, of the Bose-Hubbard model head-on. We must explicitly consider heat-flow and rate limiting processes in the establishment of the steady-state to show that it can indeed be universal. Our analysis reveals the importance of the hydrodynamic limit and the limitations of current approaches.
9:00AM T22.00006 Electric polarization in correlated insulators, REZA NOURAFKAN, GABRIEL KOTLIAR, Department of Physics & Astronomy, Rutgers University, Piscataway, NJ 08854-8019, USA, CONDENSED MATTER THEORY TEAM — We derive a formula for the electric polarization of interacting insulators, expressed in terms of the full Green’s functions of the system. We use the formula to investigate changes in the electric polarization of the half-filled ionic Hubbard model. Correlations work in favor of covalency and a small lattice deformation can trigger substantial changes in the electric polarization. At the onset of the anti-ferromagnetic phase, a small lattice distortion suppresses the staggered magnetization and simultaneously the electric polarization has a higher variation. This behavior is absent when the anti-ferromagnetic phase is fully established. We also find that the quasi-particle approximation is a reliable approximation for weak to intermediate interaction strengths.

9:12AM T22.00007 Multiple energy scales and emerging quasiparticles in a doped Mott insulator, WENHUI XU, GABRIEL KOTLIAR, Department of Physics and Astronomy, Rutgers University — We recognize two temperature scales relevant to formation of quasiparticles but distinct from the Brinkman-Rice scale in a doped Mott insulator. \( T_{\text{qp}} \) marks the formation of incoherent quasiparticles, while a smaller scale \( T_{\text{FL}} \) indicates the onset of Fermi-liquid coherence. Below \( T_{\text{qp}} \), the scattering rate evolves linearly with temperature and the quasiparticle weight is also strongly \( T \)-dependent. Furthermore, the imaginary part of self energy is particle-hole asymmetric at low energy. These facts lead to non-Fermi liquid behaviors in transport properties. The Fermi liquid scale \( T_{\text{FL}} \) is characterized by a smooth saturation of quasiparticle weight and emerging particle-hole symmetry in self energy. We compute transport properties and find that non-Fermi liquid behavior of longitudinal and Hall resistivity persist down to well below \( T_{\text{FL}} \) while Hall angle and Nernst effect have revealed Fermi-liquid behavior above \( T_{\text{FL}} \). We also discuss the validity of relaxation time approximation in interpreting non-Fermi liquid behaviors.

9:24AM T22.00008 Strongly enhanced thermal transport in a lightly doped Mott insulator\(^1\), VELIKO ZLATIC, Institute of Physics, Zagreb, JIM FREERICKS, Physics Department, Georgetown University — We discuss the charge and heat transport of a “bad metal” described by the Falicov-Kimball model near half-filling, using DMFT. For a lightly doped Mott insulator, the exact solution gives transport coefficients of a universal form at low, \( T \lesssim T_0 \), and high temperatures, \( T \gtrsim T_0 \). These characteristic temperatures are such that, for \( T \lesssim T_0 \), transport is not affected by the excitations across the gap and that, for \( T \gtrsim T_0 \), the chemical potential is at the center of the gap. At intermediate temperatures, \( T_0 \lesssim T \lesssim T_\text{FL} \), the chemical potential moves in the gap and the Wiedemann-Franz law doesn’t hold. Here, the increased asymmetry of the electron and hole currents can manifest itself to enhance the thermopower \( S(T) \) and the figure of merit \( ZT \). At small doping and \( U>1 \) we find \( ZT \gtrsim 100 \). Above \( T_\text{FL} \), the electron-hole symmetry is restored and \( S(T) \) drops to small values. For \( U>1 \) and moderate doping, there is a broad temperature interval in which \( ZT \gtrsim 1 \), even though the electronic thermal conductivity and the effective Lorenz number are not small. In this regime, the phonons might be less adverse to ZT. Large ZT is also obtained for a three-dimensional cubic lattice. Similar effects could not be obtained with non-interacting electrons or a Fermi liquid.

\(^1\)This work is supported by the NSF grant No. DMR-1006605. V.Z. acknowledges support by Croatian MZOS Grant No.0035-0352843-2849

9:36AM T22.00009 Strongly Correlated Transport in the Falicov Kimball Model, GREG BOYD, JIM FREERICKS, Georgetown University, VELIKO ZLATIC, Institute of Physics, Zagreb, Croatia — Many materials like the cuprates, heavy fermions, and strongly correlated oxides, are non-Fermi liquid “bad metals”, with linear or quasi-linear resistivity as a function of temperature. The low-energy excitations are quasiparticle-like near the Fermi surface, but their lifetimes are short, so they are not coherent or free-particle-like, as in conventional Fermi-liquids (whose quasi-particle lifetimes diverge at the Fermi energy). It turns out that this kind of behavior is ubiquitous in a wide range of different strongly correlated models, as long as the temperature is above the Fermi-liquid scale. To illustrate this, we investigate the strongly correlated transport in the Falicov-Kimball model using dynamical mean-field theory (DMFT) — which is exactly solvable in the limit of infinite coordinate number. We show results for the resistivity as a function of temperature, the quasiparticle lifetime, and the spectral function. These results are quite similar to those recently found for the Hubbard model, illustrating that this high temperature behavior is seen in many different models of strong electron correlations.

9:48AM T22.00010 Charge density wave melting in a correlated system: real-time dynamics in the Hubbard-Holstein model, BRIAN MORITZ, Northern Illinois University and the University of North Dakota, CHENG-CHIEN CHEN, MICHEL VAN VEENENDAAL, Northern Illinois University and the Advanced Photon Source, Argonne National Laboratory — Strongly correlated materials exhibit an intricate interplay between multiple degrees of freedom that can lead to competing phases with distinct broken symmetry. We study this interplay via the real-time dynamics in the photo-induced melting of the charge density wave state of the Hubbard-Holstein model. Using small cluster sparse matrix exact diagonalization and Krylov subspace techniques, we simulate the temporal evolution of the many-body wavefunction to reveal both the charge and lattice dynamics. To understand the nature of the electron-hole interaction strength, we study the behavior in proximity of the transition to the competing antiferromagnetic phase and comment on the character of the photo-induced transient state.

10:00AM T22.00011 Variational Monte Carlo Study of Heisenberg Model in Honeycomb Lattice with Six Spin Interactions, NILADRI SENGUPTA, Louisiana State University, SANDEEP PATHAK, UC Santa Cruz, KA-MING TAM, JUANA MORENO, MARK JARRELL, Louisiana State University — We inverted the possibility of the spin liquid phase proposed by Quantum Monte Carlo simulation on the Hubbard model in a honeycomb lattice. We consider the effective spin half Heisenberg model including the nearest neighbors, next nearest neighbors and six sites exchange interactions. Variational Monte Carlo simulations are performed by using the Gutzwiller projected BCS or resonating valence bond wavefunction. Different kind of symmetries (s,p±ip,d,d±id) in the pairing function are considered in order to investigate the effects of higher order exchange interactions.

10:12AM T22.00012 Representing vertex function in inhomogeneous frequency grid and its application in parquet formalism, KA-MING TAM, SHUXIANG YANG, JUANA MORENO, MARK JARRELL, Louisiana State University — Representing two-particle vertices has always been a central issue in computational methods such as the parquet formalism, a self-consistent two-particle field theory. Despite the great effort over the past two decades, its application is very limited. This is predominately due to two crucial factors—the stability of the iteration and the size of the memory allocation for representing the vertex. We previously demonstrated that the stability problem may be alleviated by explicitly restoring the crossing symmetry, making simulations beyond weak coupling for the Hubbard model feasible [1,2]. The next step for the practical applications of the parquet formalism is to compress the memory required to represent the vertex. In this work, we elaborate a scheme which invokes an inhomogeneous frequency grid replacing the homogeneous Matsubara frequency grid, and thereby reducing the memory by over a order of magnitude. This may represent a crucial step towards the practical applications of the parquet formalism for large cluster sizes.


Effect of Electron-Phonon Interaction Range for a Half-Filled Band in One Dimension. MARTIN HOHENADLER, University of Würzburg, FAKHER ASSAAD, University of Würzburg, HOLGER FEHRENKE, University of Greifswald — We demonstrate that fermion-boson models with nonlocal interactions can be simulated at finite band filling with the continuous-time quantum Monte Carlo method. We apply this method to explore the influence of the electron-phonon interaction range for a half-filled band in one dimension, covering the full range from the Holstein to the Fröhlich regime. The phase diagram contains metallic, Peierls, and phase-separated regions. Nonlocal interactions suppress the Peierls instability, and thereby lead to almost degenerate power-law exponents for charge and pairing correlations.

Fluctuation-induced pair density wave state in itinerant ferromagnets near to quantum criticality. ANDREW G. GREEN, London Centre for Nanotechnology, GARETH CONDUIT, TCM, Cavendish Laboratory, University of Cambridge, CHRISTOPHER P. PEDDER, London Centre for Nanotechnology — Magnetic fluctuations near to itinerant ferromagnetic quantum criticality can have profound effects. It has long been realised - since the understanding of superfluidity in helium-3 - that ferromagnetic fluctuations can drive p-wave superconductivity. Near to quantum criticality, fluctuations lead to characteristic scaling with temperature and, ultimately, to a reconstruction of the phase diagram by the fluctuation-driven formation of spatially modulated magnetic order. Here, we show that near to the putative quantum critical point, these two effects become intertwined leading to a fluctuation-driven pair density wave. Moreover, describing this physics from the quantum order-by-disorder perspective reveals a fundamentally common origin of the two effects.

Thursday, March 21, 2013 8:00AM - 10:48AM – Session T30 DCMP: Disordered and Glassy Systems (non-polymeric) 338 - Nicolas Giovambattista, Brooklyn College

8:00AM T30.00001 Two-State “Hopping” Dynamics in Molecular Liquids and Glasses1, MARCUS CICERONE, QIN ZHONG, MADHUSUDAN TYAGI, JOSEPH CURTIS, National Institute of Standards and Technology, DEVIN AVERETT, University of Wisconsin-Madison, JUAN DE PABLO, University of Chicago — Hopping has long been suspected as an important mode of transport in supercooled liquids at temperatures below Tc. It has been observed in model systems, but until now, has not been directly observed in molecular liquids. We show that incoherent quasi-elastic neutron scattering (QENS) reveals a two-state scenario where, on a 1 ps timescale, molecules are either confined to motion on a lengthscale of 0.05 nm, or free to undergo motion on a much larger lengthscale of roughly 0.3 nm, where r_H is the hydrodynamic radius. The motion executed by the least-constrained molecules fits the description of hopping motion observed in model simulations and colloid experiments. The population free to hopping at low temperature where the mobile states are long-lived. We show also that this two-state scenario holds well above Tc, where the mobile state lifetime exhibits apparently universal behavior, and transport appears to proceed by both small-step diffusion and larger-step “hopping” processes. Our interpretation of the neutron scattering data is confirmed by atomistic MD simulations, which reveal additional richness, and suggest that this very short-time two-state behavior may be the precursor to dynamic heterogeneity as observed on longer timescales.

1This work was partially funded by NIH/NIBIB under grant R01 EB006398-01A1, and utilized facilities supported in part by the National Science Foundation under Agreement No. DMR-0454672.

8:12AM T30.00002 Models of two level systems for anisotropic glassy materials1, DRAGOS-VICTOR ANGHEL, IRINA MIHAELA DUMITRU, ALEXANDRU GEORGE NEMNES, Horia Hulubei National Institute of Physics and Nuclear Engineering, DMITRII CHUROCHKIN, Faculty of Mathematical and Physical Sciences, University of Chile — We use an extended version of the standard tunneling model to explain the sound absorption in anisotropic glassy materials and heat transport in mesoscopic slabs and bridges. The glassy properties are determined by an ensemble of two level systems (TLS). In our model a TLS is characterized by a 3 × 3 symmetric tensor, [T], which couples to the strain field. [S], through a 3 × 3 × 3 × 3 tensor of coupling constants, [[R]]. The structure of [[R]] reflects the symmetry of the host lattice. We also propose microscopic theoretical models and models of TLS by which we test some of the most well known models of glassy materials, together with our own model.

1The work was supported by the Romanian National Authority for Scientific Research projects PN-II-ID-PCE-2011-3-0960 and PN09370102/2009

8:24AM T30.00003 ABSTRACT WITHDRAWN

8:36AM T30.00004 Configurational excitations of simple liquids. TAKUYA IWASHITA, University of Tennessee, TAKESHI EGAMI, University of Tennessee and Oak Ridge National Laboratory — The dynamics of glass-forming liquids has not been fully understood at the atomic-scale level, even for normal liquids because the basic mechanism regarding to liquid dynamics remain unknown. An elementary process of liquids, in which an atom loses or gains one of its nearest neighbors, was studied using MD simulations of various metallic liquids at high temperatures. The result was presented in terms of Maxwell relaxation time, represented by viscosity/Γ, and the lifetime of local topology of atomic connectivity. Above crossover temperature, TA, the Maxwell relaxation time is almost equal to the lifetime of local topology, suggesting the topological excitation as the elementary excitation in high temperature liquid metal. We also showed that the TA may be associated with the propagation of transverse sound wave beyond an atomic shell. Below TA the Maxwell relaxation time becomes larger than the lifetime of local topology. This result implies an importance of the interaction between local configurational excitations in the supercooled state.

8:48AM T30.00005 Supercooled Liquids with Enhanced Orientational Order1, MICHAEL WÜbbenhorst, SIMONA Capponi, KU Leuven, Belgium, SIMONE NAPOLITANO, Universite Libre de Bruxelles, Belgium — The nature of the glass transition, the transformation of a liquid into a disordered solid, still remains one of the most intriguing unsolved problems in materials science. Recent models rationalize crucial features of vitrification with the presence of medium-range ordered regions coexisting with the isotropic liquid. In lines with this prediction, here we report an extraordinary enhancement in bond orientational order (BOO) in ultrathin films of supercooled polyols, grown by physical vapour deposition. By varying the deposition conditions and the molecular size, we could tune the kinetic stability of the liquid phase enriched in BOO towards conversion into the ordinary liquid phase. We observed a strong increase in the dielectric strength with respect to the ordinary supercooled liquid and slower structural dynamics, suggesting the existence of a metastable liquid phase with improved orientational correlations[1]. [1] J. S. Capponi, S. Napolitano, and M. Wübbenhorst, Nat. Commun. doi: 10.1038/ncomms2228 (2012).

1The authors acknowledge financial support from the Research Council of the K.U. Leuven, projects No. OT/06/30 and OT/11/065, and financial support from FWO (Fonds Wetenschappelijk Onderzoek - Vlaanderen) within the project G.0642.08
9:00AM T30.00006 The Kinetics of the Glass Transition and Physical Aging in Germanium Selenide Glasses1, HOAYU ZHAO, YUNG KOH, SINDEE SIMON, Texas Tech University, SABYASACHI SEN, UC Davis, MAREK PYDA COLLABORATION — The kinetics associated with the glass transition is investigated using differential scanning calorimetry (DSC) for germanium selenide glasses with Ge content ranging from 0 to 30 at. % Ge and mean coordination numbers ranging from 2.0 to 2.6. As Ge content increases, the glass transition region broadens and the step change in heat capacity at Tg decreases. As a result of physical aging, enthalpy overshoots are observed in DSC heating scans and the corresponding change in enthalpy can be calculated as a function of aging time. The enthalpy loss on aging linearly increases with the logarithm of aging time and then levels off at an equilibrium value that increases with decreasing aging temperature. The time required to reach equilibrium increases with decreasing aging temperature and, at a given temperature, with decreasing germanium content. The results indicate that all samples show expected physical aging behavior, and no evidence for a Boolchand intermediate phase characterized by high stability and absence of physical aging is found.

1Funding from the National Science Foundation CHE-1112416 is gratefully acknowledged

9:12AM T30.00007 Dynamical and structural heterogeneities close to liquid-liquid phase transitions: The case of gallium1, ALEX ANTONELLI, SAMUEL CAJAHUARINGA, MAURICE DE KONING, Universidade Estadual de Campinas — Liquid-liquid phase transitions (LLPT) have been proposed in order to explain the thermodynamic anomalies exhibited by some liquids. Recently, it was found, through molecular dynamics simulations, that liquid elemental gallium, described by a modified embedded-atom model, exhibits a LLPT between a high-density liquid (HDL) and a low-density liquid (LDL), about 60 K below the melting temperature. In this work [1], we studied the dynamics of supercooled liquid gallium close to the LLPT. Our results show a large increase in the plateau of the self-intermediate scattering function (β-relaxation process) and in the non-Gaussian parameter, indicating a pronounced dynamical heterogeneity upon the onset of the LLPT. The dynamical heterogeneity of the LDL is closely correlated to its structural heterogeneity, since the fast diffusing atoms belong to high-density domains of predominantly 9-fold coordinated atoms, whereas the slow diffusing ones are mostly in low-density domains of 8-fold coordinated atoms. The energetics suggests that the reason for the sluggish dynamics of LDL is due to its larger cohesive energy as compared to that of the HDL. [1] S. Cajahuaringa, M. de Koning, and A. Antonelli, J. Chem. Phys. 136, 064513 (2012).

1Work supported by FAPESP, CNPq, CAPES, and FAEPEX/UNICAMP

9:24AM T30.00008 Pressure Dependence of the Glass Transition Temperature in the Fragile Glass Former Cumene, TIM RANSOM, WILLIAM OLIVER, University of Arkansas Department of Physics — The glass transition temperature, Tg, is one of the most important characteristics of glassy systems. While Tg has been measured for many systems at atmospheric pressure, direct measurement of the glass transition is difficult at high pressures due to small sample sizes and long time scales. Tg(P) measurements to date mostly involve extrapolations of high-pressure viscosity or relaxation data to η = 10−14 P or t = 100 s, respectively. In this study we present direct measurement of Tg at pressures up to several GPa through a combination of pressure gradient tracking and observation of increases in the thermal expansion coefficient upon heating from the glass to the viscous liquid state. High pressures are attained through the use of a diamond anvil cell and precise temperatures are maintained via custom heating and cryogenic systems. By directly mapping this phase boundary, we can compare models for Tg(P). In addition, high-pressure analysis requiring knowledge of Tg at pressure will be greatly aided.

9:36AM T30.00009 Average Oscillator Strength Per State of a one-dimensional disordered Frenkel exciton system in the Coherent Potential Approximation1, ABDELRKRIM BOUKAHLI, Physics Department, University of Wisconsin-Whitewater, Whitewater, WI 53190, ROBERT SIEMANN, Department of Mathematics, University of Wisconsin-Whitewater, Whitewater, WI 53190, DAVID HUBER, Physics Department, University of Wisconsin-Madison, Madison, WI 53706 — We report the results of studies of the low energy side of the Average Oscillator Strength Per State, F(E) = F(E)/ρ(E), where F(E) is the line shape function and ρ(E) is the density of states function of one dimensional Frenkel excitons in the Coherent Potential Approximation (CPA). A Gaussian distribution of the transition frequencies with rms width σ (0.07 ≤ σ ≤ 0.4) is used. Our CPA theory predicts that on the low energy side of the peak the tails are short and independent of the disorder parameter σ; implying a behavior consistent with the Urbach rule. Our CPA results are in excellent agreement with previous investigations.

1AB acknowledge support from the college of L&S.

9:48AM T30.00010 Atomistic Modeling of Mechanical Loss in Amorphous Oxides1, RASHID HAMDAN, JONATHAN TRINASTIC, HAI-PING CHENG, University of Florida — The mechanical and optical loss in amorphous solids, described by the internal friction and light scattering susceptibility are investigated using classical, atomistic molecular dynamics simulation. We implemented the trajectory bisection method and the non-local ridge method in DL-POLY molecular dynamics simulation software. These methods were used to locate the different local potential energy minima that a system visits through an MD trajectory and the transition state between any two consecutive minima. From the distributions of the barrier energy minima that a system visits through an MD trajectory and the transition state between any two consecutive minima. From the distributions of the barrier height and asymmetry, and the relaxation time of the different transition states we calculated the internal friction of pure amorphous silica and mixed oxides.

1Acknowledgment: NSF/PHYS

10:00AM T30.00011 The nature of the β-peak in the loss modulus of amorphous solids, YOSSI COHEN1, Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, SMARAJIT KARMAKAR, Dept of Physics, Universita di Roma La Sapienza, Piazzale Aldo Moro 2, Rome, Italy, ITAMAR PROCACCIA, Department of Chemical Physics, The Weizmann Institute of Science, Rehovot 76100, Israel, KONRAD SAMWER, Dept of Physics, University of Gottingen, Germany — Glass formers exhibit, upon an oscillatory excitation, a response function whose imaginary and real parts are known as the loss and storage moduli respectively. The loss modulus typically peaks at a frequency known as the α frequency which is associated with the main relaxation mechanism of the super-cooled liquid. In addition, the loss modulus is decorated by a smaller peak, shoulder or wing which is referred to as the β-peak. The physical origin of this secondary peak had been debated for decades, with proposed mechanisms ranging from highly localized relaxations to entirely cooperative ones. Using numerical simulations, we expose a clear and unique cooperative mechanism for the said β-peak which is distinct from that of the α-peak.

1Current affiliation: Lorenz Center and the Department of Earth Atmospheric and Planetary Sciences, MIT, Cambridge, MA, USA.
10:12AM T30.00012 Density of Surface States in a-Si/Ge Using a Two Parameter Hamiltonian
ELIEZER RICHMOND, Retired — To rigorously investigate the contribution of surfaces to the density of electronic states of a-Si/Ge and the effect of the topology on the density of surface states (DOS), a surface for amorphous homopolar tetrahedral solids is defined. The density of unsaturated bonds is 0.106 bonds/Å². Reconstruction enables a 88% reduction in the density of unsaturated bonds. The effects on the DOS in the valence band and energy gap is investigated using a two parameter Hamiltonian. The local and configuration DOS are computed for the unsaturated bond and the four back bond hybrids. The ring structure effects the DOS in the valence band, but not the more localized energy gap states. The spectral feature due to surface atoms with only one unsaturated bond is affected by the topology. The antibonding spectral feature in the energy gap deriving from surface atoms with 2 or 3 unsaturated bonds is independent of all topological effects while the bonding spectral feature from these same surface atoms is not. Comparison with empirical results verifies the contribution of the unsaturated bonds to ESR signals and elucidates the origin of the subtle valence band features in UPS spectra.

10:24AM T30.00013 Fluctuating Mobility Generation and Transport in Glasses
APIWAT WSITSORASAK, PETER WOLYNES, Rice University — Complex spatiotemporal structures developing in glasses during aging and heating processes involve the interplay between fluctuating mobility generation and transport. To understand these structures, we extend mode-coupling theory to inhomogeneous system and combine the theory with activated events within the framework of Random-First Order Transition theory of glasses. We explore using numerical methods the process of fluctuating mobility generation and transport in glasses as the glasses age after cooling and as they rejuvenate after heating. This scheme allows us to investigate the dynamical heterogeneity in glasses below the glass transition temperature. We found a growing length scale and an increasing relaxation time upon the aging process. On the contrary, in the rejuvenating process, the mobility propagates from the high mobility at free surfaces into the bulks which resembles flame front propagation in combustion theory.

10:36AM T30.00014 Many-body localization in one dimension as a dynamical renormalization group fixed point
RONEN VOSK, EHUD ALTMAN, Weizmann Institute of Science — We formulate a dynamical real space renormalization group approach to describe the time evolution of a random spin-1/2 chain, or interacting fermions, initialized in a state with fixed particle positions. Within this approach we identify a many-body localized state of the chain as a dynamical infinite randomness fixed point. Near this fixed point our method becomes asymptotically exact, allowing analytic calculation of time dependent quantities. In particular we explain the striking universal features in the growth of the entanglement seen in recent numerical simulations: unbounded logarithmic growth delayed by a time inversely proportional to the interaction strength. Lack of true thermalization in the long time limit is attributed to an infinite set of approximate integrals of motion revealed in the course of the RG flow, which become asymptotically exact conservation laws at the fixed point. Hence we identify the many-body localized state with an emergent generalized Gibbs ensemble. Within the RG framework we show that long range resonances are irrelevant at strong randomness, and formulate a criterion for when they do become relevant and may cause a delocalization transition.

Thursday, March 21, 2013 8:00AM - 11:00AM
Session T36 DCMP: Ruthenates, Iridates, and p-wave Superconductivity

8:00AM T36.00001 Theoretical study of novel superconductivity in Ir oxides with large spin-orbit coupling
HIROSHI WATANABE, TOMONORI SHIRAKAWA, SEIJI YUNOKI, RIKEN, CREST, COMPUTATIONAL MATERIALS SCIENCE LABORATORY, RIKEN ASI TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM, COMPUTATIONAL CONDENSED MATTER PHYSICS LABORATORY, RIKEN ASI TEAM, CREST, JAPAN SCIENCE AND TECHNOLOGY AGENCY TEAM, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM, RIKEN AICS TEAM — Recently, the Ir 5d electronic system has attracted much attention. In this material, three Ir 5d orbitals of Ir atoms are hybridized with each other by the spin-orbit coupling of 5d electrons. As a result of the quantum entanglement of spin and orbital degrees of freedom, an anomalous \( J_{4\phi} = |J - s| = 1/2 \) state is realized, which causes interesting properties. To clarify the properties of this system, we have studied the ground state of the three-orthogonal Hubbard model with a spin-orbit coupling term using variational Monte Carlo method. Here, we study the electronic states when carriers are doped in this three-orthogonal system and discuss the possibility of superconductivity. The obtained ground state phase diagram reveals the antiferromagnetic order is stable around the electron density \( n = 5/3 \), is destabilized by carrier doping and the ground state turns to be superconducting under a certain condition. Similar to the high-Tc cuprates, a large asymmetry between electron doping (\( n > 5 \)) and hole doping (\( n < 5 \)) is also observed. Due to the large spin-orbit coupling, the spin is no longer a good quantum number. Instead, the pseudospins form a Cooper pair and a \( d_{x^2-y^2} \)-wave "pseudospin-singlet" superconductivity is realized.

8:12AM T36.00002 Observation of strong spin-orbital entanglement in \( \text{Sr}_2\text{RuO}_4 \)
ANDREA DAMASCHELLI, C.N. Veenstra, Z.-H. Zhu, B. Ludbrook, A. Nicolaou, M. Raichle, I.S. Elfimov, Quantum Matter Institute, UBC, Canada, M.W. Haverkort, MPI, Stuttgart, Germany, B. Slomski, G. Landolt, J. H. Dil, PSI, Switzerland, S. Kittaka, Y. Maeno, Kyoto University, Japan — \( \text{Sr}_2\text{RuO}_4 \) stands out even amongst the unconventional superconductors. The relativistic spin orbit interaction causes a momentum dependent entanglement of orbital and spin quantum numbers. Using circularly polarized light combined with spin and angle resolved photoemission spectroscopy, we directly observe this entanglement in good agreement with relativistic band-structure calculations. The presence of spin-charge entangled states inherently has a profound influence on the description of the superconducting state. These entangled states are not well described by a product of an orbital and spin wave-function, thereby blurring the distinction between triplet and singlet states.

8:24AM T36.00003 Dislocations and the enhancement of superconductivity in odd-parity superconductor \( \text{Sr}_3\text{RuO}_4 \)
YIQUN YING, NEAL STALEY, XINXIN CAI, YING LIU, Department of Physics and Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA, YAN XIN, National High Magnetic Field Laboratory, Florida State University, Tallahassee, Florida 32306, USA, KAI SUN, Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA, DAVID FOBES, TJJUAN LIU, ZHIQIANG MAO, Department of Physics, Tulane University, New Orleans, Louisiana 70118, USA — We investigated the 3-K phase of spin-triplet, odd-parity superconductor \( \text{Sr}_3\text{RuO}_4 \), which was usually referred to the eutectic phase of Ru and \( \text{Sr}_2\text{RuO}_4 \) and has attracted much attention. In this material, three \( t_{2g} \) orbitals of Ru atoms are hybridized with each other by the spin-orbit coupling of 5d electrons. As a result of the quantum entanglement of spin and orbital degrees of freedom, an anomalous \( J_{4\phi} = |J - s| = 1/2 \) state is realized, which causes interesting properties. To clarify the properties of this system, we have studied the ground state of the three-orthogonal Hubbard model with a spin-orbit coupling term using variational Monte Carlo method. Here, we study the electronic states when carriers are doped in this three-orthogonal system and discuss the possibility of superconductivity. The obtained ground state phase diagram reveals the antiferromagnetic order is stable around the electron density \( n = 5/3 \), is destabilized by carrier doping and the ground state turns to be superconducting under a certain condition. Similar to the high-Tc cuprates, a large asymmetry between electron doping (\( n > 5 \)) and hole doping (\( n < 5 \)) is also observed. Due to the large spin-orbit coupling, the spin is no longer a good quantum number. Instead, the pseudospins form a Cooper pair and a \( d_{x^2-y^2} \)-wave "pseudospin-singlet" superconductivity is realized.

\[ \text{The work is supported by DOE under Grant No. DE-FG02-04ER4615} \]
8:36AM T36.00004 Numerical study of the stability of half-quantum vortices in superconducting Sr$_2$RuO$_4$.
KEVIN ROBERTS, RAFFI BUDAKIAN, MICHAEL STONE, University of Illinois at Urbana-Champaign — We numerically solve the coupled Landau-Ginzburg-Maxwell equations for a model of a $\pi_x + i\pi_y$ superconductor in which whole or half-quantas of flux threads through a hole. We recover the pattern of stable and unstable regions for the half-flux observed in the experiments of Jang et al [1].


8:48AM T36.00005 Unravelling the Surface-to-Bulk Progression of the Electronic Structure in Sr$_2$RuO$_4$.
CHRISTIAN N. VEENSTRA, Z.-H. ZHU, B. LUDBROOK, M. CAPSONI, G. LEVY, A. NICOLAOU, J.A. ROSEN, R. COMIN, I.S. ELFIMOV, A. DAMASCHELLI, Quantum Matter Institute, UBC, Canada, S. KITTAKA, Y. MAENO, Kyoto University, Japan — We revisit the normal-state electronic structure of Sr$_2$RuO$_4$ by angle-resolved photoemission spectroscopy (ARPES) with improved data quality, as well as ab-initio band structure calculations in the local-density approximation (LDA) with the inclusion of spin-orbit coupling (SO). We find that the current model of a single surface layer ($\sqrt{2} \times \sqrt{2}$)R45$^\circ$ reconstruction does not explain all detected features. The observed depth-dependent signal degradation, together with the close quantitative agreement with LDA+SO slab calculations based on the surface crystal structure as determined by low-energy electron diffraction (LEED), reveal that at a minimum – the subsurface layer also undergoes a similar although weaker reconstruction. This model accounts for all features - a key step in understanding the electronic structure - and indicates a surface-to-bulk progression of the electronic states driven by structural instabilities, with no evidence for other phases stemming from either topological bulk properties or the interplay between SO and the broken symmetry of the surface.

9:00AM T36.00006 Quantifying covalency and metallicity in pyrochlore ruthenates undergoing metal-insulator transitions.
ASHISH CHAINANI, RIKEN Harima Institute, AYAKO YAMAMOTO, RIKEN Advanced Science Institute, MASAHARU MATSUNAMI, RITSUKO EGUCHI, MINETAKA TAGUCHI, YASUTAKA TAKATA, RIKEN Harima Institute, HIDENORI TAGA, RIKEN Advanced Science Institute, SHIK SHIN, YOSHINORI NISHINO, MAKINA YABASHI, KENJI KENJI TAMASAKU, TETSUYA ISHIKAWA, RIKEN Harima Institute — We use bulk-sensitive hard x-ray photoelectron spectroscopy to investigate the electronic structure of the cubic pyrochlore ruthenates Ti$_2$Ru$_2$O$_7$ and Hg$_2$Ru$_2$O$_7$, which show first-order temperature(T)-dependent metal-insulator transitions (MITs). Ru 3d core-level spectroscopy shows drastic changes as a function of T. The metallic-origin features in core-level spectra get quenched upon gap formation in valence band spectra. The results establish temperature-driven Mott-Hubbard transitions in three-dimensional ruthenates and reveals three energy scales: (a) ultrasoft electronic changes happen on the largest (~eV) energy scale, (b) the band gap energy/charge gap (E$_g$ ~ 160-200 meV) are intermediate, and (c) the lowest energy scale corresponds to the transition temperature T$_{MIT}$ (< 10 meV), which is also the gap energy of Ti$_2$Ru$_2$O$_7$ and the magnetic-ordering temperature of Hg$_2$Ru$_2$O$_7$. The results identify and quantify the role of covalency and metallicity in the pyrochlore ruthenates undergoing T-dependent metal-insulator transitions.

9:12AM T36.00007 Weak-coupling analysis of quasiparticle excitations in strontium ruthenate.
JOHN DEISZ, TIM KIDD, Department of Physics, University of Northern Iowa — We report FLEX calculations for the quasiparticle properties of pure and electron-doped strontium ruthenate. Through self-consistent calculations of energy- and band-dependent linewidths and effective masses, the specific heat coefficient and superconducting $T_c$, we assess the effectiveness of this weak coupling approach for consistently describing the electron-electron correlations in this material. We also analyze the impact of the momentum dependence of the electron self-energy in describing the significant correlation effects observed in strontium ruthenate.

9:24AM T36.00008 Theory of edge currents in Sr$_2$RuO$_4$: effects of topology and gap anisotropy.
SAMUEL LEDERER, SRINIVAS RAGHU, Stanford University — Substantial experimental evidence suggests that Sr$_2$RuO$_4$ is a chiral p-wave superconductor. Depending on bandstructure, such a system may exhibit topologically protected edge modes, and in general would exhibit intrinsic edge currents. The latter, however, have not been observed in sensitive scanning probe measurements. A possible resolution to this apparent contradiction has been offered by Raghuv et al.[1]. They show that, in weak coupling, superconductivity is dominant not on the 2D $\gamma$ band as commonly believed, but on the quasi-1D $\alpha$ and $\beta$ bands, leading to a topologically trivial state, presumably with suppressed currents. They also show that the favored order parameter has sharp gap minima on the Fermi surface. We present calculations of edge currents incorporating these features using two different methods: self-consistent Bogoliubov-de Gennes equations, and Ginsburg-Landau theory. We find that, contrary to expectation, the existence and character of topological edge modes have no effect on edge currents. Multiband effects and gap anisotropy yield quantitative reductions, but order 1 edge currents are a generic consequence of chiral p-wave superconductivity at low temperature in Sr$_2$RuO$_4$.


9:36AM T36.00009 Superconductivity in Weyl Semimetals.
VIVEK AJI, HUAZHOU WEI, University of California Riverside, SUNG-PO CHAO, NTHU Taiwan — Weyl fermions are linearly dispersing massless particles in three dimensions. They are chiral in that the projection of their spin along their momenta is a conserved quantum number. Interest in these particles in the condensed matter context was piqued by the possibility of their emergence in the low energy sector of Pyrochlore lanates. Since then a number of other systems have been suggested that also support such excitations. We discuss the nature of the superconducting phases that arise for chemical potential at the Weyl nodes. Among the possibilities are the finite momentum pairing state (FFLO) and the conventional BCS state.

9:48AM T36.00010 Quantum quench in a p+ip superfluid: non-equilibrium topological gapless state.
MATTHEW FOSTER, Rice University, MAXIM DZERO, Kent State University, VICTOR GURARIE, University of Colorado at Boulder, EMIL YUZBASHYAN, Rutgers University — Ground state “topological protection” has emerged as a main theme in quantum condensed matter physics. A key question is the robustness of physical properties including topological quantum numbers to perturbations, such as disorder or non-equilibrium driving. In this work we investigate the dynamics of a p+ip superfluid following a zero temperature quantum quench. The model describes a 2D topological superconductor with a non-trivial (trivial) BCS (BEC) phase. We work with the full interacting BCS Hamiltonian, which we solve exactly in the thermodynamic limit using classical integrability. The non-equilibrium phase diagram is obtained for generic quenches. A large region of the phase diagram describes strong to weak-pairing quenches wherein the order parameter vanishes in the time-long time, due to pair fluctuations. Despite this, we find that the topological winding number survives for quenches in this regime, leading to the prediction of a gapless topological state. We speculate on potential realizations, including a proximity effect quench on the surface of 3D topological insulator.
10:00AM T36.00011 Phases in two dimensional $p_x + ip_y$ superconducting systems with interactions beyond nearest-neighbor1, ANTONIO RUSSO, SUDIP CHAKRAVARTY, University of California, Los Angeles — A $p_x + ip_y$ superconducting system with longer range hopping and pairing terms is considered. Chern numbers are calculated numerically, and in a simple, visual way by considering weak superconductor order parameter which is still in the same topological phase. Using nearest, second nearest, and third nearest hoppings and pairings, we find Chern numbers 0 through 4, including 3 which, unlike the other Chern numbers, must be thought of in terms of combinations of different range interactions. These Chern numbers are interpreted as phases, with different properties, in particular, the number of edge states created when a cut is introduced. We also explore the effect of introducing magnetic flux (in the extreme type-II limit) through flux tubes (which are vortices in the 2D system). In particular, we look at the effect of varying distances between these vortices on the lowest excitation energies of the system.

1This work is supported by NSF under Grant No. DMR-1004520.

10:12AM T36.00012 Intra-valley Spin-triplet p+ip Superconducting Pairing in Lightly Doped Graphene1, JIANHUI ZHOU, Carnegie Mellon University, TAO QIN, International School for Advanced Studies, Italy, JUNREN SHI, Peking University, China — We analyze various possible superconducting pairing states and their relative stabilities in lightly doped graphene. We show that, when inter-sublattice electron-electron attractive interaction dominates and Fermi level is close to Dirac points, the system will favor intra-valley spin-triplet $p + ip$ pairing state. Based on the novel pairing state, we further propose a scheme for doing topological quantum computation in graphene by engineering local strain fields and external magnetic fields.

1MOST 973 program No.2009CB929101, China

10:24AM T36.00013 Edge currents in multiband chiral p-wave superconductors1, WEN HUANG, McMaster University, CATHERINE KALLIN, McMaster University and Canadian Institute for Advanced Research, EDWARD TAYLOR, McMaster University — The superconducting phase of Sr$_2$RuO$_4$ is believed to be a time-reversal symmetry breaking state with spontaneous supercurrents at the edge or domain walls of the sample. Yet Scanning SQUID and related probes have so far failed to detect any signature of such edge currents. Recent theoretical work suggests that the active superconducting bands in Sr$_2$RuO$_4$ are the two quasi-1D bands associated primarily with the $d_{xz}$ and $d_{yz}$ orbitals of Ru$^{4+}$. This contrasts with the more conventional picture in which chiral p-wave superconductivity is primarily a single-band effect, with the $\gamma$ band being the active superconducting band. Based on Bogoliubov-de Gennes calculations for tight-binding models, we study the implications of two-band chiral p-wave order on the edge current. The two-band model includes inter-orbital hopping and spin-orbit coupling. In general, the two-band model predicts a net edge current that is at least about an order of magnitude smaller than that from the one-band model. In particular, comparable magnitudes of inter-orbital hopping and spin-orbit coupling lead to substantial reduction of edge current. Also presented are finite temperature calculations involving all three bands.

1NSERC, CIFAR, CRC

10:36AM T36.00014 Low-lying electronic structure and possible intrinsic gap control in J = 1/2 Mott insulating perovskite iridate Sr$_3$Ir$_2$O$_7$1, CHANG LIU, SU-YANG XU, NASSER ALIDoust, MADHAB NEUPANE, M. ZAHID HASAN, Joseph Henry Laboratory and Department of Physics, Princeton University, Princeton, New Jersey 08544, USA, TAY-RONG CHANG, HORNG-TAY JENG, Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan, HSIN LIN, ROBERT MARKIEWICZ, ARUN BANSIL, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA, CHETAN DHITAL, SOVIT KHADKA, YOSHINORI OKADA, VIDYA MADHAVAN, STEPHEN WILSON, Department of Physics, Boston College, Chestnut Hill, Massachusetts 02467, USA — Using angle resolved photoemission spectroscopy, the ground state of perovskite iridate Sr$_3$Ir$_2$O$_7$ is found to be in close vicinity to a metal-to-insulator transition. Photoemission data reveal two bands extending up to surprisingly small binding energies around the Brillouin zone corner X, followed by a van Hove-like flat portion at the top of the valence bands. One of these bands form a saddle point while the other shows apparent spectral weight suppression along the in-plane antiferromagnetic vector direction $(\Gamma-\Sigma)$, signaling a possible electronic response to the additional long range order. The energy scale of the Mott insulating gap shows considerable sample-to-sample variation, which points to possible intrinsic control of low temperature resistivity by apical oxygen deficiency - a process suggested by transport experiments and, importantly, similar to the doping process of the cuprates that gives rise to high temperature superconductivity.

1DOE Grant No. DE-FG02-05ER46200

10:48AM T36.00015 Orbital angular momentum textures in perovskite oxide materials, WONSIG JUNG, WONSIG KYUNG, YOONYOUNG KOH, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, YOSHIIKU YOSHIDA, National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8568, Japan, Y.J. CHOI, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea, MASASHI ARITA, KENYA SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima, Hiroshima 739-0046, Japan, C. KIM, Institute of Physics and Applied Physics, Yonsei University, Seoul 120-749, Korea — We measured electronic structures of perovskite oxide materials Sr$_2$MO$_4$ (M=Rh, Ru, Ir) with angle-resolved photoemission spectroscopy using circular dichroism (CD) method to investigate orbital characters. We observe large CD which shows complicated orbital structures of Sr$_2$MO$_4$. CD signal comes from orbital angular momentum induced from inversion symmetry breaking at cleaved surfaces. We compare results from various orbitals of 3-, 4- and 5-d.

Thursday, March 21, 2013 8:00AM - 10:48AM
Session T39 DCMP: Metals Alloys and Metallic Structures 348 - David Parker, Oak Ridge National Laboratory

8:00AM T39.00001 Spin-lattice coupling in BCC iron, JUNQI YIN, MARKUS EISENBACH, DON NICHOLSON, Oak Ridge National Laboratory — For empirical iron potentials, the magnetic contribution is usually implicitly considered, and the spin-lattice coupling is simply neglected. From first principle calculations, we proposed a Heisenberg type of exchange for BCC iron that couples the spin and lattice degrees of freedom. The parameterization is based on quantities already employed in embedded-atom potentials. Therefore, the model is a natural augmentation of the existing iron potentials, and is applicable to molecular dynamics simulations. Our model built on Dudarev potential can reproduce iron’s specific heat from the Curie temperature down to about 400K, and the estimate of the spin-lattice contribution indicates that it is significant near the transition. We applied our model to studying a < 111 > screw dislocation in BCC iron, and found evidences that the dislocation core has a local transition temperature different from the bulk one. Work is sponsored by the U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (M. E., D. M. N.), and by Office of Advanced Scientific Computing Research (J. Y.). This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC05-00OR22725.
The periodic quadrupole approach was applied to model the core dislocation structure, core interaction with Cr solute atoms and to estimate their effect on Peierls stress and barrier. The binding energy of Cr impurity atoms with a screw dislocation and its effect on the dislocation core structure are discussed and the importance of magnetism in the effects of Cr on screw dislocation mobility is demonstrated. This work was supported by the Center for Defect Physics, an Energy Frontier Research Center funded by the US Department of Energy, Office of Science, Office of Basic Energy Sciences.

A computational study of high entropy alloys YANG WANG, Pittsburgh Supercomputing Center, Carnegie Mellon University, MICHAEL GAO, National Energy Technology Laboratory, MICHAEL WIDOM, Department of Physics, Carnegie Mellon University, JEFF HAWK, National Energy Technology Laboratory — High entropy alloys (HEAs) exhibit a wide variety of excellent material properties, including high strength, reasonable ductility with appreciable work-hardening, corrosion and oxidation resistance, wear resistance, and outstanding diffusion-barrier performance, especially at elevated and high temperatures. In this talk, we will explain our computational approach to the study of HEAs that employs the Korringa-Kohn-Rostoker coherent potential approximation (KKR-CPA) method. The KKR-CPA method uses Green’s function technique within the framework of multiple scattering theory and is uniquely designed for the theoretical investigation of random alloys from the first principles. The application of the KKR-CPA method will be discussed as it pertains to the study of structural and mechanical properties of HEAs. In particular, computational results will be presented for AlCoCrCuFeNi (x = 0, 0.3, 0.5, 0.8, 1.0, 1.3, 2.0, 2.8, and 3.0), and these results will be compared with experimental information from the literature.

First-principles Calculations on the Stability of High Entropy Alloy1 M. CLAUDIA TROPARSKY, Department of Materials Science and Engineering, the University of Tennessee, PAUL KENT, JAMES R. MORRIS, G. MALCOM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — High entropy alloys (HEAs) constitute a new class of materials comprised of four or more elements in equimolar or near equimolar ratio, which tend to form simple solid solutions, mainly FCC or BCC. Despite extensive attention due to their potential applications as structural materials little is known about why these compounds are stable with respect to phase separation. We study the structural and thermodynamic properties of HEAs composed of Cr, Pd, Mn, Fe, Co, and Ni using density functional theory. We investigate the minimum energy structures of several alloys as well as the competing intermetallic compounds in an effort to assess the stability of the HEAs with respect to phase separation. We find that the enthalpy of formation of the alloys is frequently insufficient to explain their stability and that the entropy of mixing can in some cases account for the stability of these compounds. However, for some five-component alloys this does not appear to be sufficient. In this presentation, we will discuss the degree to which the entropy of mixing can stabilize these alloys.

Non-local first-principles calculations in Cu-Au, Ag-Au and Cu-Ag YONG-SHENG ZHANG, Department of Materials Science & Engineering, Northwestern University, GEORG KRESSE, Faculty of Physics, Center for Computational Materials Science, Universität Wien, CHRISTOPHER WÖLVERTON, Department of Materials Science & Engineering, Northwestern University — Cu-Au is the prototypical alloy system used to exemplify ordering and compound formation, and serves as a testbed for all new alloy theory methods. Yet, despite the importance of this system, conventional density functional theory (DFT) calculations with semi-local approximations (GGA) have two dramatic failures in describing the energies of this system: 1) DFT predicts incorrect ordered ground states for Au-rich compositions, and 2) DFT formation energies of the observed CuAu and CuAu compounds are nearly a factor of two smaller in magnitude than experimental values. Here, we show how modern extensions of DFT based on non-local interactions can rectify both of these failures. Using the self-consistent non-local HSE06 functional, the formation energies of Cu3Au and CuAu are −71 and −91 meV/atom, respectively, which are in excellent agreement with the experimental measurements. The semi-local GGA predicted CuAu is not a stable phase in the HSE06 calculations, and CuAu with the Li2 structure is theoretically predicted as a stable phase. For Ag-Au, both semi-local GGA and non-local HSE06 functionals give similar formation energies. The electronic structures are used to explain these different phenomena in Cu-Au and Ag-Au.

Stress dependent defect energetics in Tungsten from first-principles MD. HOSSAIN, California Institute of Technology, JAIME MARIAN, Lawrence Livermore National Laboratory — Tungsten (W) is an important material for high temperature applications due to its refractory nature. However, like all transition metals from the VI-A group, W suffers from low-temperature brittleness and lack of ductility, which poses serious questions for its use as a structural material. Tungsten’s mechanical properties can be enhanced by alloying with elements with d-electrons, such as Re, which has resulted in successful commercial alloys. In this work, we obtain the formation and migration energetics of Re solute atoms in terms of their interaction with vacancies and dislocations. To explore the influence of external stresses on Re transport properties, we examine the role of hydrostatic and shear deformation on the vacancy formation energy (VFE) and migration energy barrier (Em) in BCC W from first-principles calculations by developing a pseudopotential with 6s2, 6p0, 5d4, and 5f0 electronic states for the valence electrons. We find that under hydrostatic deformation, increase or decrease of vacancy formation energy depends on the type of deformation – tensile or compressive, while for shear deformation it decreases irrespective of the magnitude of applied deformation. On the other hand, migration energy barrier always decreases under hydrostatic deformation, but shows path-length dependent behavior under shear deformation. This talk will discuss the underlying principles and possible routes for enhancing mechanical strength from a physics perspective.

8:48AM T39.00005 First-principles Calculations on the Stability of High Entropy Alloy1 M. CLAUDIA TROPARSKY, Department of Materials Science and Engineering, the University of Tennessee, PAUL KENT, JAMES R. MORRIS, G. MALCOLM STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — High entropy alloys (HEAs) constitute a new class of materials comprised of four or more elements in equimolar or near equimolar ratio, which tend to form simple solid solutions, mainly FCC or BCC. Despite extensive attention due to their potential applications as structural materials little is known about why these compounds are stable with respect to phase separation. We study the structural and thermodynamic properties of HEAs composed of Cr, Pd, Mn, Fe, Co, and Ni using density functional theory. We investigate the minimum energy structures of several alloys as well as the competing intermetallic compounds in an effort to assess the stability of the HEAs with respect to phase separation. We find that the enthalpy of formation of the alloys is frequently insufficient to explain their stability and that the entropy of mixing can in some cases account for the stability of these compounds. However, for some five-component alloys this does not appear to be sufficient. In this presentation, we will discuss the degree to which the entropy of mixing can stabilize these alloys.

8:48AM T39.00006 Non-local first-principles calculations in Cu-Au, Ag-Au and Cu-Ag YONG-SHENG ZHANG, Department of Materials Science & Engineering, Northwestern University, GEORG KRESSE, Faculty of Physics, Center for Computational Materials Science, Universität Wien, CHRISTOPHER WÖLVERTON, Department of Materials Science & Engineering, Northwestern University — Cu-Au is the prototypical alloy system used to exemplify ordering and compound formation, and serves as a testbed for all new alloy theory methods. Yet, despite the importance of this system, conventional density functional theory (DFT) calculations with semi-local approximations (GGA) have two dramatic failures in describing the energies of this system: 1) DFT predicts incorrect ordered ground states for Au-rich compositions, and 2) DFT formation energies of the observed CuAu and CuAu compounds are nearly a factor of two smaller in magnitude than experimental values. Here, we show how modern extensions of DFT based on non-local interactions can rectify both of these failures. Using the self-consistent non-local HSE06 functional, the formation energies of Cu3Au and CuAu are −71 and −91 meV/atom, respectively, which are in excellent agreement with the experimental measurements. The semi-local GGA predicted CuAu is not a stable phase in the HSE06 calculations, and CuAu with the Li2 structure is theoretically predicted as a stable phase. For Ag-Au, both semi-local GGA and non-local HSE06 functionals give similar formation energies. The electronic structures are used to explain these different phenomena in Cu-Au and Ag-Au.

8:48AM T39.00007 Stress dependent defect energetics in Tungsten from first-principles MD. HOSSAIN, California Institute of Technology, JAIME MARIAN, Lawrence Livermore National Laboratory — Tungsten (W) is an important material for high temperature applications due to its refractory nature. However, like all transition metals from the VI-A group, W suffers from low-temperature brittleness and lack of ductility, which poses serious questions for its use as a structural material. Tungsten’s mechanical properties can be enhanced by alloying with elements with d-electrons, such as Re, which has resulted in successful commercial alloys. In this work, we obtain the formation and migration energetics of Re solute atoms in terms of their interaction with vacancies and dislocations. To explore the influence of external stresses on Re transport properties, we examine the role of hydrostatic and shear deformation on the vacancy formation energy (VFE) and migration energy barrier (Em) in BCC W from first-principles calculations by developing a pseudopotential with 6s2, 6p0, 5d4, and 5f0 electronic states for the valence electrons. We find that under hydrostatic deformation, increase or decrease of vacancy formation energy depends on the type of deformation – tensile or compressive, while for shear deformation it decreases irrespective of the magnitude of applied deformation. On the other hand, migration energy barrier always decreases under hydrostatic deformation, but shows path-length dependent behavior under shear deformation. This talk will discuss the underlying principles and possible routes for enhancing mechanical strength from a physics perspective.

9:24AM T39.00008 ABSTRACT WITHDRAWN —
9:36AM T39.00009 First Principles Calculation of Elastic Properties of Early-Late Transition Metal Alloys, WILLIAM HUHN, MICHAEL WIDOM, Carnegie Mellon University — Amorphous metals are of practical interest in applications requiring high strength materials. We choose to examine the elastic properties of crystalline phases to understand the elastic properties of amorphous solids. In this talk, we discuss our work using first principles methods to calculate elastic properties for crystalline alloys in various chemical families containing transition metals, specifically early (Ta, W) and late (Fe, Co, Rh, Ni, Cu, Zn) due to their good glass forming ability, as well as select borides. Certain Laves phases, which are known to have local chemical ordering similar to amorphous solids, are focused on. We analyze trends in the elastic properties of chemical families based on computed enthalpies of formation, elastic properties of pure elemental phases, and electronic and structural information. In particular, we use effective medium theories and enthalpies of formation to predict trends in bulk moduli. This information can be used to predict future candidate systems for high-strength amorphous metals.

9:48AM T39.00010 Structural transformations in the physical mixture of Pd and Cu nanoparticles, VINEETHA MUKUNDAN, Purdue University, JUN YIN, CHUAN-JIAN ZHONG, SUNY, Binghamton, OANA MALIS, Purdue University — Pd-Cu bimetallic nanoparticles have the potential to replace palladium, the second most active metal having important applications as a catalyst in fuel cell and hydrogen storage reactions. We investigated the temperature-induced transformations in physical mixtures of Pd and Cu nanoparticles, using in-situ real-time synchrotron based x-ray diffraction. These nanoparticle mixtures undergo coalescence and structural phase transformations at relatively low temperature, and sinter at higher temperature. They form alloys with ordered bcc (B2) structure at low temperature (300°C). At higher temperature (450°C), it transforms into a disordered fcc (alloy) structure. The structural parameters probed are size, phase, composition and morphology. Grain growth was modeled with growth laws proposed for nanocrystalline materials and the diffusion mechanism driving sintering was explored. The effect of elemental compositions, different substrates and annealing atmospheres on the evolution of the PdCu alloy nanoparticles was also explored.

10:00AM T39.00011 Twinning in nanocrystalline fcc and bcc metals, VLADIMIR S. BOYKO, ROMAN YA. KEZERASHVILI, Physics Department, New York City College of Technology, The City University of New York — The deformation twinning in nanocrystalline (nc) face-centered cubic (fcc) metals, body-centered cubic (bcc) metals, and in nc Si is analyzed. The phenomenological approach is used to make a bridge between microscopic mechanisms of twin nucleation and macroscopical characteristics of twinning with different crystal structures and to calculate the grain size range of the twinning propensity, the requisite external stresses for twinning propagation in nc polycrystals, the grain size at which the slip begins to prevail over the twinning. The developed approach allows to derive analytical expressions and estimate lower and upper limits of grain sizes at which a twinning propensity is occurred. Results of calculations for the nc fcc metals Al, Cu, Ni, Pd, Au, nc bcc metals Ta, Fe, Mo, W, Nb, and nc diamond-cubic Si are compared with the experimental data, otherwise predictions are made.

10:12AM T39.00012 Irradiation-induced formation of nano-crystallites with C15 Laves phase structure in bcc iron, MIHAI-COSMIN MARINICA, FRANÇOIS WILLAIME, JEAN-PAUL CROCOMBETTE, CEA Saclay — The thermal diffusion of defects as vacancies or interstitials is the main process which drives the material towards equilibrium after or in parallel to the damage production. A three dimensional periodic structure is proposed for self-interstitial clusters in body-centered-cubic metals, as opposed to the conventional two dimensional loop morphology [1]. The underlying crystal structure corresponds to the C15 Laves phase. The new three dimensional structures generalize previous observations [1, 2]. By systematic exploration of the energy landscape performed using an Eigenvector Following method [3] and Density Functional Theory calculations, we demonstrate that in α-iron these C15 aggregates are highly stable and immobile and that they exhibit large antiferromagnetic moments. These clusters form directly in displacement cascades and they can grow by capturing self-interstitials. This new morphology of self-interstitial clusters thus constitutes an important element to account for when predicting the microstructural evolution of iron base materials under irradiation.


10:24AM T39.00013 Composition fluctuation, local clustering, and crystallization in multi-component systems, MINGLEI WANG, KAI ZHANG, STEFANOS PAPANIKOLAOU, JAN SCHROERS, COREY S. O'HERN, Yale University — We perform molecular dynamics simulations of model multi-component metallic liquids to study mechanisms for non-polymorphic crystallization. We measure local concentration fluctuations, nucleation rates, and clustering as a function of the cooling rate for different size ratios, stoichiometries, and attraction strengths. In preliminary studies, we find that over a wide range of particle size ratios and cooling rates, small particles cluster in the interstices of contact networks formed by the large particles. These studies are important for understanding which systems are prone to crystallization and which are good glass-formers.

10:36AM T39.00014 Ab-initio study of the structure and dynamics of bulk liquid Cadmium and its liquid-vapour interface1, DAVID J. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN, LAZARO CALDERIN, Materials Research Institute and Research Computing and Cyberinfrastructure, The Pennsylvania State University, Pennsylvania 16802, USA, LUIS E. GONZALEZ, Dpt. Fisica Teorica, Universidad de Valladolid, Valladolid, SPAIN — Several static and dynamic properties of bulk liquid cadmium at a thermodynamic state near its triple point have been calculated by ab-initio molecular dynamics simulations. The calculated static structure shows a very good agreement with the available experimental data. The dynamical structure reveals collective density excitations with an associated dispersion relation which points to a small positive dispersion. Results are also reported for several transport coefficients. Additional simulations have also been performed in order to study the structure of the free liquid surface. The ionic density profile shows an oscillatory behavior with two different wavelengths as the spacing between the outer and first inner layer is different from that between the other inner layers. The calculated reflectivity shows a marked maximum whose origin is related to the surface layering along with a shoulder located at a much smaller wave-vector transfer.

1We acknowledge the support of MCINN(grant FIS2011-22957) and JCyL (grant VA104A11-2)

Thursday, March 21, 2013 11:15AM - 2:15PM –
Session U1 DCMP DCP: Invited Session: Hidden Order in URu2Si2 and Possibly Related Compounds
Ballroom I - John Mydosh, Kamerlingh Onnes Lab
11:15 AM U1.00001 Symmetry Breaking in the Hidden-Order Phase of URu$_2$Si$_2$. TAKASADA SHIBAUCHI, Department of Physics, Kyoto University — In the heavy fermion compound URu$_2$Si$_2$, the hidden-order transition occurs at 17.5K, whose nature has posed a long-standing mystery. A second-order phase transition is characterized by spontaneous symmetry breaking, and thus the nature of the hidden order cannot be determined without understanding which symmetry is being broken. Our magnetic torque measurements in small pure crystals reveal the emergence of an in-plane anisotropy of the magnetic susceptibility below the transition temperature [1], indicating the spontaneous breaking of four-fold rotational symmetry of the tetragonal URu$_2$Si$_2$. In addition, our recent observation of cyclotron resonance allows the full determination of the electron-mass structure of the main Fermi-surface sheets, which implies an anomalous in-plane mass anisotropy [2] consistent with the rotational symmetry breaking. These results impose strong constraints on the symmetry of the hidden order parameter.


11:51 AM U1.00002 Neutron scattering study of URu$_2$Si$_2$ magnetic properties: from hydrostatic pressure to uniaxial stress. FREDERIC BOURDAROT, SPSMS, UMR-E 9001, CEA-INAC/ UJF-Grenoble 1, MDN, 17 rue des Martyrs, F-38054 Grenoble, France — Since the discovery of the unusual magnetic and superconducting properties of URu$_2$Si$_2$ in 1985 by Palstra [1], this heavy fermion has been extensively studied. A “Hidden Order” evidences by bulk properties like specific heat, has been found below $T_D=17.8$K. Neutron scattering in this case is an efficient probe for the study of this compound as large magnetic excitations and an irreproducible tiny antiferromagnetic moment are present in this sample. Even though the tiny antiferromagnetic moment aligned along the c-axis at $Q\parallel (0,0,1)$, the magnetic excitations seem to be associated to a large magnetic moment of $\sim 1.5 \mu_B$ and show two minimums at $Q_0=(1.0,0,0)$ but also $\sim \mu_B=(0.6,0,0)$. These magnetic responses have been intensively studied in normal conditions by Broholm [2,3] and our group[4], but also versus magnetic field [5], and more recently under hydrostatic pressure [6]. The result of these experiments seem to indicate that the Hidden Order is linked to the excitation at $Q_0$ and not to the excitation at $Q_1$. We will present the revisited magnetic properties of URu$_2$Si$_2$ under uniaxial stress along the a-axis [7,8]. Both elastic and inelastic contributions have been measured versus the constraints. In the HO state, as the constraint increases, the AF gap excitation at $Q_0$ decreases and the tiny moment increases: it seems also that there is a relation between both parameters. On the other hand, the excitation gap at $Q_1$ is slightly increasing. From our measurement we infer a critical pressure of $\sim 0.33$ GPa, with a large increase of the antiferromagnetic moment. This behavior is very similar to results under hydrostatic pressure. Combining hydrostatic pressure, uniaxial stress along the a-axis and neutron Larmor diffraction measurements, that gives the lattice distribution of our URu$_2$Si$_2$ crystal, we conclude that the magnetic exchange integrals are dominated by the lattice parameter $a$ and not the ratio $c/a$ as usually believed.


12:27PM U1.00003 The hidden order phase in URu$_2$Si$_2$: Remarkable nesting and spin-orbital hybridization. PETER OPPENEER, Dept. of Physics and Astronomy, Uppsala University, Uppsala — Aspects of Fermi surface (FS) nesting properties of URu$_2$Si$_2$ are analyzed with particular focus on their implication for the mysterious hidden order phase which occurs at 17.5 K. We show that there exist two Fermi surfaces that exhibit unusually strong nesting at the antiferromagnetic wavevector, $Q_0=(0,0,1)$. The corresponding energy dispersions fulfill the relation $\varepsilon_{uj}(k) = -\varepsilon_{uj}(k \pm Q_0)$ at eight FS hotspot lines on the surfaces. Notably, the spin-orbital characters of the involved $5f$ states are different: $j_z=\pm 5/2$ vs. $\pm 3/2$, and hence the occurring degenerate Dirac crossings are symmetry protected in the nonmagnetic normal state. Pairing of electrons in these two FSs can commence through interaction with a quasiparticle with wavevector $Q_0$ and exchange of longitudinal angular momentum $\Delta j_z$. Dynamical symmetry breaking through an Ising-like spin-orbital excitation mode at $Q_0$ with $\Delta j_z=\pm 1$ induces a hybridization of the two states, causing substantial FS gapping. Concomitant spin and orbital currents in the uranium planes can give rise to a rotational symmetry breaking. The existence of such specifically nested FSs in URu$_2$Si$_2$ is confirmed in recent experiments.

This work has been performed with S. Elgazzar, J. Rusz, Q. Feng, T. Durakiewicz and J.A. Mydosh.

1:03PM U1.00004 A Hund’s rule mechanism for Hidden Spin-Orbital Density Wave in URu$_2$Si$_2$. PETER RISEBOROUGH, Temple University — It is proposed that the “Hidden Order” state of URu$_2$Si$_2$ corresponds to a combined spin-orbital density wave state, which is stabilized by the inter-orbital Hund’s rule coupling. The electronic system is described by the underscreened Anderson Lattice Model, in which there are two-fold degenerate $f$ bands which hybridize with a single conduction band. In the normal state, the bands at the Fermi-energy have $3s$ character and thus $j_z=\pm 5/2$. The magnetic excitations of Okazaki et al. [1] are consistent with the magnetic torque experiments of Okazaki et al. [2]. The similarity of the interband nesting and the intraband nesting conditions leads to an adiabatic continuity between the “Hidden Order” and Antiferromagnetic phases for small values of the hybridization. The presence of a nearly hybridized density gap results in an asymmetric form of the pseudogap caused by the “Hidden Order” transition. Precursor fluctuations of the hidden order parameter, above $T_HO$, lead to the formation of “hot spots” on the Fermi-surface and a depletion of the density of states in the vicinity of the Fermi-energy as is seen by point contact and optical spectroscopies. The amplitude of the precursor fluctuations increase as $T_HO$ is driven towards zero, however, the order of the transition switches from second-order to first-order pre-empting the quantum critical point. These results in accord with the change in the order of the transition inferred by Jaime et al. from measurements of the specific heat in an applied magnetic field. This model might also be applicable to the enigmatic pseudo-gap phases seen in high-temperature superconductors.

This work was supported by the US Department of Energy, Office of Basic Energy Science, Materials Science through grant DEFG02-ER45872.

1This work was supported by the US Department of Energy, Office of Basic Energy Science, Materials Science through grant DEFG02-ER45872.
Fermions become massive. At the same time, the weak antilocalization behavior is found to weaken in the gapped phase due to the loss of $\pi$. The metallic surface transport abruptly diminishes below the critical thickness of thin films, we revealed a systematic evolution of the surface conductance as a function of thickness and found a striking manifestation of the topological protection of the surface state with a massless Dirac dispersion. Field effect transistors consisting of thin (3-20 nm) $\text{Bi}_2\text{Se}_3$ samples are used to study the transport properties of topological insulators. We focus on the efforts to use quantum interference phenomena, such as weak anti-localization and the Aharonov-Bohm effect, to verify in a transport experiment the Dirac nature of the surface state and its defining properties.

Quantum transport in topological insulator nanowires and thin films. JENS H. BARDAISON, University of California, Berkeley — Topological insulators have an insulating bulk but a metallic surface. In the simplest case, the surface electronic structure of a 3D topological insulator is described by a single 2D Dirac cone. The transport properties of such a surface state are of considerable current interest; they have some similarities with graphene, which also realizes Dirac fermions, but have several unique features in their response to magnetic fields. In this talk, I give an overview of some of the main quantum transport properties of topological insulator surfaces. I focus on the efforts to use quantum interference phenomena, such as weak anti-localization and the Aharonov-Bohm effect, to verify in a transport experiment the Dirac nature of the surface state and its defining properties.

The strong, weak and anomalous sides of weak topological insulators. ZOHAR RINGLEN, Weizmann Institute of Science — Disorder and topology can be thought of as two counter-driving forces. While the former pushes electron wave functions to localize in space, the latter requires them to remain coherent over the entire system. We study the interplay between these two on the surface of a “weakly” topological phase- the Weak Topological Insulator. Using arguments based on flux-insertions and locality, we show that such surfaces cannot exhibit a localization transition even when the surface is strongly disordered. We also present a numerical study which further quantifies this result. We then reformulate the same notions, in field theory language, using a novel $\mathbb{Z}_2$-charge-anomaly. This anomaly generalizes the $\mathbb{Z}$-charge-anomaly associated with edges of the Integer Quantum Hall Effect. Besides unifying various aspects of Topological Insulators, the anomaly allows us to calculate new topological properties of TIs in the presence of electric fields.

Surface conduction of topological Dirac electrons in bulk insulating $\text{Bi}_2\text{Se}_3$. MICHAEL FUHRER, School of Physics, Monash University — The three dimensional strong topological insulator ($\text{STI}$) is a new phase of electronic matter which is distinct from ordinary insulators in that it supports on its surface a conducting two-dimensional surface state whose existence is guaranteed by topology. I will discuss experiments on the STI material $\text{Bi}_2\text{Se}_3$, which has a bulk bandgap of 300 meV, much greater than room temperature, and a single topological surface state with a massless Dirac dispersion. Field effect transistors consisting of thin (3-20 nm) $\text{Bi}_2\text{Se}_3$ are fabricated from mechanically exfoliated from single crystals, and electrochemical and/or chemical gating methods are used to move the Fermi energy into the bulk bandgap, revealing the ambipolar gapless nature of transport in the $\text{Bi}_2\text{Se}_3$ surface states. The minimum conductivity of the topological surface state is understood within the self-consistent theory of Dirac electrons in the presence of charged impurities. The intrinsic finite-temperature resistivity of the topological surface state due to electron-phonon scattering is measured to be 60 times larger than that of graphane largely due to the smaller Fermi and sound velocities in $\text{Bi}_2\text{Se}_3$, which will have implications for topological electronic devices operating at room temperature. As samples are made thinner, coherent coupling of the top and bottom topological surfaces is observed through the magnitude of the weak anti-localization correction to the conductivity, and, in the thinnest $\text{Bi}_2\text{Se}_3$ samples (3 nm), in thermally-activated conductivity reflecting the opening of a bandgap.
Thursday, March 21, 2013 11:15AM - 2:15PM –
Session U3 DCOMP DCMP: Invited Session: Application of the First-Principles and Atomistic Methods to Nuclear Detection Materials
Ballroom III - David Beach, Department of Energy, National Nuclear Security Administration

11:15AM U3.00001 Point Defect Properties of Cd(Zn)Te and TlBr for Room-Temperature Gamma Radiation Detectors1, VINCENTZ LORDI, Lawrence Livermore National Laboratory — The effects of various crystal defects in CdTe, Cd1-xZn,xTe (CZT), and TlBr are critical for their performance as room-temperature gamma radiation detectors. We use predictive first principles theoretical methods to provide fundamental, atomic scale understanding of the defect properties of these materials to enable design of optimal growth and processing conditions, such as doping, annealing, and stoichiometry. Several recent cases will be reviewed, including (i) accurate calculations of the thermodynamic and electronic properties of native point defects and point defect complexes in CdTe and CZT; (ii) the effects of Zn alloying on the native point defect properties of CZT; (iii) point defect diffusion and binding related to Te clustering in Cd(2)Te; (iv) the profound effect of native point defects—principally vacancies—on the intrinsic material properties of TlBr, particularly electronic and ionic conductivity; (v) tailored doping of TlBr to independently control the electronic and ionic conductivity; and (vi) the effects of metal impurities on the electronic properties and device performance of TlBr detectors.

1Prepared by LLNL under Contract DE-AC52-07NA27344 with support from the National Nuclear Security Administration Office of Nonproliferation and Verification Research and Development NA-22.

11:51AM U3.00002 First-principles calculations of self-trapping of carriers and excitons in NaI and SrI2, DANIEL ABERG, Lawrence Livermore National Laboratory — While the general potential of scintillators as radiation detectors has been demonstrated, one of the current goals is to develop materials with improved energy resolution sufficient to detect fissile materials with a low probability of errors at ports, borders, and airports. The poor resolution has been linked to the non-linear response to the gamma ray energy. Fundamental understanding of this requires detailed knowledge of elementary electronic excitation processes. In particular, in most metal halide scintillators charge carriers and excitations localize and create self-trapped species associated with large effective masses and slow diffusivities. First-principles modeling is essential for providing quantitative understanding of the involved microscopic processes. Here, we present comprehensive ab-initio calculations, with techniques ranging from hybrid DFT+exact exchange to self-consistent GW and Bethe-Salpeter approach, for modeling the electronic structure and mobilities of self-trapped carriers and excitons in metal halides with particular attention given to sodium and strontium iodide.

12:27PM U3.00003 Multiscale Modeling of Crystal Growth and Microstructural Evolution of CdZnTe, CHARLES HENAGER, JR., PNNL, Richland, WA 99352 — Crystal growth models and modeling tools for CdTe and CZT along with experimental melt growth experiments will be presented and discussed. The emphasis will be on an evolving multiscale modeling framework that can be applied to solve portions of the crystal quality and reproducibility problem of CZT crystals grown for high-resolution radiation detection. The growth models and methods include ab initio models of CdTe, ab initio molecular dynamics (MD) models CdTe, MD of solidification of CdTe, equilibrium growth defects in CdTe, and development of coarser-scale microstructural evolution models using phase field methods. These model and theory results will be discussed in terms of designing a multiscale approach to two relevant problems in CZT crystal growth, namely solid-liquid interface (SLI) stability and concurrent defect generation in the hot but cooling CZT solid. This dovetails with recent experimental research focused on the growth of CdTe from Te-rich melts with an emphasis on SLI instability. Experimental data on SLI instabilities will be featured as well as results of transmitted IR data on Te-particle distributions in as-grown CZT. A new mechanism of Te-particle genesis and spatial arrangement in CdTe and CZT is discussed in terms of a Rayleigh instability mechanism coupled with crystallographic SLI instabilities during growth. However, there are gaps in our capabilities at every length and time scale, plus gaps in building coarse-grained models from fine-scale models, in statistical representations of complex equilibria, and in understanding the complexities of solidification in ternary alloy systems where coupled thermal, concentration, stress, liquid flow, and SLI morphological fields exist. The talk concludes with an assessment of methods and approaches to address desired models and simulations of CZT solidification from the melt.

3This research was supported by the U.S. Department of Energy under Contract No. DE-AC05-76RL01830.

1:03PM U3.00004 First-principles Electronic Structure Calculations for Scintillation Phosphor Nuclear Detector Materials1, ANDREW CANNING, Lawrence Berkeley National Laboratory & UC Davis — Inorganic scintillation phosphors (scintillators) are extensively employed as radiation detector materials in many fields of applied and fundamental research such as medical imaging, high energy physics, astrophysics, oil exploration and nuclear materials detection for homeland security and other applications. The ideal scintillator for gamma ray detection must have exceptional performance in terms of stopping power, luminosity, proportionality, speed, and cost. Recently, trivalent lanthanide dopants such as Ce, Eu have received greater attention for fast and bright scintillators as the optical 5d to 4f transition is relatively fast. However, crystal growth and production costs remain challenging for these new materials so there is still a need for new higher performing scintillators that meet the needs of the different application areas. First principles calculations provide a useful insight into the chemical and electronic properties of such materials and hence can aid in the search for better new scintillators. In the past there has been little first-principles work done on scintillator materials in part because it means modeling f electrons in lanthanides as well as complex excited state and multi-particle processes. In this talk I will present an overview of the scintillation process and show how first-principles calculations can be applied to such systems to gain a better understanding of the physics involved. I will also present work on a high-throughput first principles approach to select new scintillator materials for fabrication as well as present more detailed calculations to study trapping process etc. that can limit their brightness. This work in collaboration with experimental groups has lead to the discovery of some new bright scintillators.

1Work supported by the U.S. Department of Homeland Security and carried out under U.S. Department of Energy Contract no. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory.

1:39PM U3.00005 DFT Studies of Semiconductor and Scintillator Detection Materials, KOUSHIK BISWAS, Arkansas State University — Efficient radiation detection technology is dependent upon the development of new semiconductor and scintillator materials with advanced capabilities. First-principles based approaches can provide vital information about the structural, electrical, optical and defect properties that will help develop new materials. In addition to the predictive power of modern density functional methods, these techniques can be used to establish trends in properties that may lead to identifying new materials with optimum properties. We will discuss the properties of materials that are of current interest both in the field of scintillators and room temperature semiconductor detectors. In case of semiconductors, binary compounds such as TlBr, InI and CdTe and recently developed ternary chalcogenide Tl6Se4I will be discussed. Tl6Se4I mixes a halide (TII) with a chalcogenide (TII2Se5), which results in an intermediate band gap (1.86 eV) between that of TII (2.75 eV) and Tl2Se5 (0.6 eV). For scintillators, we will discuss the case of the elpasolite compounds whose rich chemical compositions should enable the fine-tuning of the band gap and band edges to achieve high light yield and fast scintillation response.
Generation a single auxiliary qubit regardless of the system size. Computation, but they require a significant overhead in the number of qubits. This prevents them from being useful for medium-scale systems used for quantum error correction. Full quantum error correction schemes are able to correct for arbitrary errors and enable universal quantum computation. Furthermore, we demonstrate that the same technique corrected by a quantum-feedback algorithm that is applied repeatedly. We encode a single logical qubit into three physical qubits and perform multiple rounds of quantum error correction with the aid of high-fidelity gate operations and a reset technique for the auxiliary qubits. Furthermore, we demonstrate that the same technique can be used to undo a quantum measurement. The conventional route to long-lived quantum coherence involves minimizing coupling to a dissipative bath. Paradoxically, it is possible to instead engineer specific couplings to a quantum environment that allow dissipation to actually preserve coherence. We will discuss our recent demonstration of quantum bath engineering for a superconducting qubit coupled to a microwave cavity. By tailoring the spectrum of microwave photon shot noise in the cavity, we create a dissipative environment that autonomously relaxes the qubit to an arbitrarily specified coherent superposition of the ground and excited states. In the presence of background thermal excitations, this mechanism increases the state purity and effectively cools the dressed atom state to a low temperature. We envision that future multi-qubit implementations could enable the preparation of entangled many-body states suitable for quantum simulation and computation.

This work was supported by the IARPA CSQ program.

Quantum measurement in action, MICHAEL HATRIDGE, Applied Physics, Yale University, A quantum system subject to the infinitely-strong measurement of textbook physics undergoes a discontinuous, random state collapse. However, in practice, measurements often involve a finite-strength, continuous process whose iteration leads to a projective evolution only asymptotically. Moreover, if the observation apparatus is fully efficient informationally, the measured system can remain at all times in a pure state. The stochastic evolution of this pure state is trackable from the measurement record. Thus, an initial superposition of states can be usefully transformed by a partial measurement rather than be entirely destroyed. This striking property has been demonstrated in superconducting qubit experiments in which readout is performed by a microwave signal sent through a cavity dispersively coupled to the qubit, and thereafter processed by an amplifier operating at the quantum limit. Such accurate monitoring of a qubit state is an essential prerequisite for measurement-based feedback control of quantum systems.

Work supported by: IARPA, ARO and NSF.

Quantum feedback in superconducting qubits: Towards creating and stabilizing entanglement in remote qubits, RAJAMANI VIJAYARAGHAVAN, Tata Institute of Fundamental Research, Mumbai, India, Recent advances in superconducting parametric amplifiers have enabled quantum limited measurements of superconducting qubits, ushering in a new era of measurement based control using quantum feedback. Quantum entanglement is a key aspect of the measurement process. Measurement creates a pointer state which is entangled with the system being measured. Typically, one analyzes the pointer state which in turn determines the state of the original system. I will discuss experiments where we entangle the state of a 3D transmon qubit with a coherent microwave field (the pointer) using the circuit QED architecture. The use of parametric amplifiers to analyze the microwave field enables us to actually observe this entanglement and the resulting strong correlations between the states of the pointer and the qubit. We reconstruct quantum trajectories of the qubit state as it evolves during measurement and show that the final state of the qubit is consistent with the trajectories. Further, we use quantum feedback to actively steer the state of the qubit and demonstrate Rabi oscillations which persist indefinitely. Finally, I will discuss how we can use the pointer states to generate entanglement between remote qubits and stabilize them using feedback. Applications to quantum computing and quantum error correction will also be discussed.

Cavity-assisted quantum bath engineering, KATER MURCH, QNL, UC Berkeley, In practice, quantum systems are never completely isolated, but instead interact with degrees of freedom in the surrounding environment, eventually leading to decoherence. Precision measurement techniques such as nuclear magnetic resonance and interferometry, as well as envisioned quantum schemes for computation, simulation, and data encryption, rely on the ability to prepare and preserve delicate quantum superpositions and entanglement. The conventional route to long-lived quantum coherence involves minimizing coupling to a dissipative bath. Paradoxically, it is possible to instead engineer specific couplings to a quantum environment that allow dissipation to actually preserve coherence. We will discuss our recent demonstration of quantum bath engineering for a superconducting qubit coupled to a microwave cavity. By tailoring the spectrum of microwave photon shot noise in the cavity, we create a dissipative environment that autonomously relaxes the qubit to an arbitrarily specified coherent superposition of the ground and excited states. In the presence of background thermal excitations, this mechanism increases the state purity and effectively cools the dressed atom state to a low temperature. We envision that future multi-qubit implementations could enable the preparation of entangled many-body states suitable for quantum simulation and computation.

This work was supported by the IARPA CSQ program.

Quantum feedback control in superconducting qubits: Towards creating and stabilizing entanglement in remote qubits, RAJAMANI VIJAYARAGHAVAN, Tata Institute of Fundamental Research, Mumbai, India, Recent advances in superconducting parametric amplifiers have enabled quantum limited measurements of superconducting qubits, ushering in a new era of measurement based control using quantum feedback. Quantum entanglement is a key aspect of the measurement process. Measurement creates a pointer state which is entangled with the system being measured. Typically, one analyzes the pointer state which in turn determines the state of the original system. I will discuss experiments where we entangle the state of a 3D transmon qubit with a coherent microwave field (the pointer) using the circuit QED architecture. The use of parametric amplifiers to analyze the microwave field enables us to actually observe this entanglement and the resulting strong correlations between the states of the pointer and the qubit. We reconstruct quantum trajectories of the qubit state as it evolves during measurement and show that the final state of the qubit is consistent with the trajectories. Further, we use quantum feedback to actively steer the state of the qubit and demonstrate Rabi oscillations which persist indefinitely [1]. Finally, I will discuss how we can use the pointer states to generate entanglement between remote qubits and stabilize them using feedback. Applications to quantum computing and quantum error correction will also be discussed.

1 Work supported by: IARPA, ARO and NSF.

Quantum feedback for preparing and stabilizing photon number states of a field stored in a cavity, MICHEL BRUNE, Laboratoire Kastler Brossel, Paris, The stabilization of complex classical systems requires feedback. A sensor performs measurements of the system’s state whose result is fed into a controller, which decides on an action bringing the system closer to a target state. Operating feedback for preparing and stabilizing against decoherence a quantum state is a promising tool for quantum control. It is however much more demanding than its classical counterpart, since a quantum measurement by the sensor changes the measured state. We present the first continuous operation of a closed feedback-loop for preparing and stabilizing photon number states of a microwave field stored in a high Q superconducting cavity. The field is probed by non-resonant Rydberg atoms performing a Quantum Non-Demolition photon counting. The feedback action consists either in the injection of a small coherent field pulse with a controlled amplitude and phase or in the emission and absorption of single photons with individual resonant atoms. The atomic measurement results are fed into a real-time controller, which performs an estimation of the field’s state before deciding on the actuator action bringing it closer to the target. We stabilize number states up to 7. We discuss perspectives for the stabilization of mesoscopic quantum superpositions.

Experimental quantum error correction with trapped ions, PHILIPP SCHINDLER, University of Innsbruck, The computational potential of a quantum information processor can only be utilized if errors occurring during a quantum computation can be controlled and corrected for. Quantum error correction protocols encode the quantum information of a single qubit in a larger register. Errors are then corrected by a quantum-feedback algorithm that is applied repeatedly. We encode a single logical qubit into three physical qubits and perform multiple rounds of error correction with the aid of high-fidelity gate operations and a reset technique for the auxiliary qubits. Furthermore, we demonstrate that the same technique can be used to undo a quantum measurement. Full quantum error correction schemes are able to correct for arbitrary errors and enable universal quantum computation, but they require a significant overhead in the number of qubits. This prevents them from being used for medium-scale systems used for quantum simulation. Therefore, we develop a quantum feedback scheme to reduce the dominant errors in an open-system quantum simulator. Our scheme requires only a single auxiliary qubit regardless of the system size.

This work was supported by: IARPA, ARO and NSF.
11:15AM U5.00001 Resonant inelastic transmission through a time-modulated region in graphene. LI CHANG, T. L. LIU, C. S. CHU, Department of Electrophysics, National Chiao Tung University — We investigate a number of resonant transmission processes through a time-modulated-potential region in graphene. Incident energies covering both low and high energy regimes are included, and the time-dependent transmission is treated within a tight-binding model. Three main results are obtained. Dip structures in the transmission are obtained when a band edge is involved. It can occur in the low energy regime, if the graphene is gapped, or in the high energy regime, when a graphene band edge is in the energy neighborhood. These dip structures cause significant deviation from Klein-type perfect transmission. Non-trivial Fabry–Pérot interference is observed when, staying upon a dip structure conditioned, the transmission exhibits an oscillation that has a longer than expected period in $L$, the width of the time-modulated region. Central band refocusing is found in the low energy regime, where the dominance in the transmission by the central-band will occur periodically with $L$. In all these results, we have demonstrated and analyzed detail intricate resonant interplays between sideband processes.

11:27AM U5.00002 Charge transport across tunable superlattice barriers in graphene. SUDIPTA DUBEY, AJAY BHAT, VIBHOR SINGH, PRITESH PARIKH, TANUJ PRAKASH, ABHILASH SEBASTIAN, PADMALEKHA K.G., Tata Institute of Fundamental Research, Mumbai, India, KRISHNENDU SENGUPTA, Indian Association for the Cultivation of Sciences, Kolkata, India, VIKRAM TRIPATHI, RAJDEEP SENARMA, MANDAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We create an artificial superlattice structure in graphene using an array of top gate and a bottom gate. A superlattice potential modifies the band structure of graphene, so that extra Dirac points appear in the dispersion periodically as a function of the superlattice barrier height. Tuning the amplitude of the barrier thus gives us control over number of Dirac points generated. We have performed measurements on this superlattice structure. Oscillations in resistance are observed when the charge carrier induced by top gate and back gate are of opposite sign. In this region, the number of oscillations increases with increasing gate voltage. Measurements as a function of temperature show that these oscillations persist even at 70 K. The behaviour of these oscillations in presence of magnetic field is also observed. At low magnetic field we see weak localisation behaviour. At high magnetic field, the superlattice is a small perturbation and quantum Hall effect of pristine graphene is restored.

11:39AM U5.00003 Graphene under spatially varying external potentials: Landau levels, magnetotransport, and topological modes. SI WU, MATTHEW KILLI, ARUN PARAMEKANTI, Department of Physics, University of Toronto — Superlattices (SLs) in monolayer and bilayer graphene, formed by spatially periodic potential variations, lead to a modified bandstructure with extra finite-energy and zero-energy Dirac fermions with tunable anisotropic velocities. We theoretically show that transport in a weak perpendicular (orbital) magnetic field allows one to not only probe the number of emergent Dirac points but also yields further information about their dispersion. or monolayer graphene, we find that a minimum magnetic field can lead to a strong reversal of the transport anisotropy imposed by the SL potential, an effect which arises due to the SL induced dispersion of the zero energy Landau levels. This effect may find useful applications in switching or other devices. For bilayer graphene, we discuss the structure of Landau level wave functions and local density of states in the presence of a uniform bias, as well as in the presence of a kink in the bias which leads to topologically bound ‘edge states’. We consider implications of these results for scanning tunneling spectroscopy measurements, valley filtering, and impurity induced breakdown of the quantum Hall effect in bilayer graphene.

11:51AM U5.00004 Confinement, transport gap, and valley polarization from a double barrier structure in graphene¹, DANIEL GUNLYCKE, CARTER WHITE, Naval Research Laboratory — Engineering a gap in graphene without degrading its exceptional transport properties is arguably the main obstacle preventing a breakthrough in graphene-based nanoelectronics. To create such a gap, a lot of effort has been devoted to making graphene nanoribbons. Unlike ordinary nanoribbons, we propose a structure formed between two thin parallel transport barriers that is penetrable by electrons in surrounding graphene states. The transport across this railroad track structure is governed by resonant tunneling through quasi-bound states within the confinement. The transport barriers, modeled by chemically decorated line defects, are highly reflective, causing the resonances to form continuous bands closely matching the band structure of a zigzag ribbon. Because boundary-localized states cannot carry any transport, the resonance bands must terminate at the dimensional crossover between extended and boundary-localized states. As the confined region contains no states near the Fermi level extending across the railroad track structure, electrons approaching it experience a transport gap $E_g = 2hv_F/W$, where $W$ is the separation between the barriers. In addition to offering confinement and a transport gap, the structure allows for nearly perfect valley polarization.

¹This work was supported by the Office of Naval Research, directly and through the Naval Research Laboratory.

12:03PM U5.00005 ABSTRACT WITHDRAWN —

12:15PM U5.00006 Transport Spectroscopy of gate controlled cavity in CVD bilayer graphene transistor. KYUNGHOON LEE, Department of Electrical Engineering and Computer Science, University of Michigan, YUN SUK EO, CAGLIYAN KURDAK, Randall Laboratory of Physics, University of Michigan, ZHAOHUI ZHONG, Department of Electrical Engineering and Computer Science, University of Michigan — Graphene nanostructure provides an ideal platform for understanding distinctive quantum transport properties such as Klein tunneling and suppression of backscattering due to its chiral nature. Quantum interference of phase coherent electron waves in single-layer graphene has attracted wide attention recently, while few experimental works examine the quantum transport of massive Dirac Fermion in bilayer graphene. To this end, we report the low temperature electrical transport spectroscopy of gated controlled cavity in CVD bilayer graphene transistor. Fabry–Pérot like conductance oscillation was observed in both monopolar and bipolar bilayer graphene structures defined by electrostatic gating. Transport comparison between single-layer graphene and bilayer graphene will also be discussed.

12:27PM U5.00007 Tunable superconductivity in decorated graphene¹, ZHENG HAN, ADRIEN ALLAIN, LAETITIA MARTY, NED.IMA BENDIAB, PIERRE TOULEMONDE, PIERRE STROBEL, JOHANN CORAUX, VINCENT BOUCHIAT, Neel Institute, CNRS-Grenoble, 38042 Grenoble, France — Graphene offers an exposed bidimensional gas of high mobility charge carriers with gate tunable density. Its chemical inertness offers an outstanding platform to explore exotic 2D superconductivity. Superconductivity can be induced in graphene by means of proximity effect [2]. Quantum interference of phase coherent electron waves in single-layer graphene has attracted wide attention recently, while few experimental works examine the quantum transport of massive Dirac Fermion in bilayer graphene. To this end, we report the low temperature electrical transport spectroscopy of gate controlled cavity in CVD bilayer graphene transistor. Fabry–Pérot like conductance oscillation was observed in both monopolar and bipolar bilayer graphene structures defined by electrostatic gating. Transport comparison between single-layer graphene and bilayer graphene will also be discussed.

¹Work supported by EU GRANT FP7-NMP GRENA.
12:39PM U5.00008 Electronic transport experiments on adatom-decorated graphene, E.A. HENRIKSEN, J.P. EISENSTEIN, California Institute of Technology — Single-layer graphene is expected to exhibit a wide range of novel behaviors when decorated with a disperse coating of various adatom species. Toward conducting experiments on these systems, we are developing a cryogenic ultra-high vacuum probe with the capability to explore the electronic transport of graphene and other materials that have been cleaned and annealed in situ, followed by coating via the controlled deposition of sub-monolayer coverages of a range of elements. We will report our progress on the fabrication of such thin layers, and on the characterization of surface-modified graphene devices. This work is supported by the DOE under grant No. DE-FG03-99ER45766 and the Gordon and Betty Moore Foundation.

12:51PM U5.00009 Quantum interference noise near the Dirac point in graphene\textsuperscript{1}, NINA MARKOVIC, ATIKUR RAHMAN, JANICE WYNN GUKEMA, Johns Hopkins University — We have studied low-frequency noise characteristics in single layer graphene, focusing specifically on the low-carrier density regime. We show that the $1/f$ noise at low temperatures is dominated by the time-dependent conductance fluctuations which occur due to quantum interference effects. Close to the Dirac point, the noise is reduced in magnetic field, but the relative noise reduction is larger than what might be expected based on the current theoretical understanding of quantum transport in graphene. The results reflect the inherent symmetry of the system and suggest the importance of additional degrees of freedom.

\textsuperscript{1}This work was supported in part by National Science Foundation under DMR-1106167. J.W.G. was supported in part by the M. Hildred Blewett Fellowship of the American Physical Society.

1:03PM U5.00010 Noise properties of graphene like systems\textsuperscript{1}, AVINASH RUSTAGI, C.J. STANTON, University of Florida — The unusual electronic properties of graphene and its potential for applications in nanoscale devices motivated us to study the noise properties of materials that have a graphene-like electronic dispersion. For high values of electric field, we find interesting behavior in the noise properties which appear due to the hot electron effects. We study the low-frequency noise based on the Boltzmann-Green function method within the relaxation time approximation considering an inelastic scattering term coming from phonon scattering and an elastic scattering term coming from impurity scattering. The steady-state distribution function is evaluated to calculate the average behavior of physical observables like current and energy. We find that as the field strength is increased, the noise decreases from the thermal noise value. We have also studied these properties for electronic dispersion with a gap parameter introduced in the Dirac spectrum. The inclusion of gap in the electronic dispersion causes initial heating of the electrons resulting in an increase in noise for intermediate values of field before it decreases at high fields.

\textsuperscript{1}Supported by NSF through grants OISE-0968405.

1:15PM U5.00011 Third harmonic generation in graphene, NARDEEP KUMAR, JATINDER KUMAR, CHRIS GERSTENKORN, Department of Physics and Astronomy, The University of Kansas, RUÍ WANG, Department of Physics and Astronomy, The University of Kansas; Laboratory for Photonics and Quantum Electronics, University of Iowa, HSIN-YING CHIU, Department of Physics and Astronomy, The University of Kansas, ARTURH SMIRL, Laboratory for Photonics and Quantum Electronics, University of Iowa, HUI ZHAO, Department of Physics and Astronomy, The University of Kansas — We report the measurement of optical third harmonic generation from single-layer graphene and few-layer graphite flakes produced by exfoliation. In the measurements, femtosecond near-infrared laser pulses were used to irradiate the samples. The emission observed scales with the cube of the intensity of the incident near-infrared pulse and with one third of the incident wavelength - both are clear evidences of third harmonic generation. We deduced an effective third-order susceptibility for single layer graphene to be on the order of $10^{-16} \, \text{m}^2/\text{V}^2$. For high values of electric field, we find interesting behavior in the noise properties which appear due to the hot electron effects. We study the low-frequency noise based on the Boltzmann-Green function method within the relaxation time approximation considering an inelastic scattering term coming from phonon scattering and an elastic scattering term coming from impurity scattering. The steady-state distribution function is evaluated to calculate the average behavior of physical observables like current and energy. We find that as the field strength is increased, the noise decreases from the thermal noise value. We have also studied these properties for electronic dispersion with a gap parameter introduced in the Dirac spectrum. The inclusion of gap in the electronic dispersion causes initial heating of the electrons resulting in an increase in noise for intermediate values of field before it decreases at high fields.

1:27PM U5.00012 Second Harmonic Generation in a Graphe Armchair Nanoribbon, GODFREY GUMBS, YONATAN ABRANYOS, Hunter College of CUNY — The second order nonlinear optical susceptibility $\chi^{(2)}$ for second harmonic generation is calculated for the 11H transition of a graded double quantum well (DQW) structure of undoped-GaAs/Al$_x$Ga$_{1-x}$As. These results are compared with the single quantum well (QW). Our results show that the values of $\chi^{(2)}$ have optimal magnitudes dependent on the width, depth and separation between the QWs in a DQW structure. When the electric field increases, the dipole moment increases due to the increasing separation between the electron and hole wave functions. On the other hand, the oscillator strength of the 11H transition is reduced as a result of the decrease in the overlap of the electron and hole envelope functions. These two competing factors give rise to optimal conditions for the enhancement of the second order nonlinear susceptibility $\chi^{(2)}$. It is demonstrated that $\chi^{(2)}$ for the DQW structure is more enhanced than for the biased single QW.

1:39PM U5.00013 Third-Harmonic Microscopy of Graphene\textsuperscript{1}, JERRY I. DADAP, SUNG-YOUNG HONG, NICHOLAS W. PETRONE, PO-CHUN YEH, JAMES C. HONE, RICHARD M. OSGOOD, JR, Columbia University, New York, NY — We report strong third-harmonic (TH) generation in monolayer graphene mounted on an amorphous silica substrate using a photon energy that is three-photon resonant with the exciton-shifted van Hove singularity at the M-point of graphene. Our polarization-dependent and azimuthal rotation measurements confirm the expected isotropic symmetry properties for the TH nonlinear optical process in graphene. Since this monolayer graphene TH signal exceeds that of bulk glass by more than two orders of magnitude, the signal contrast permits background-free scanning of graphene and provides structural information that is difficult to obtain via linear optical microscopy. We also discuss the dependence of TH signals on the number of graphene layers and compare the graphene signal strength with that from crystalline Au(111) sample.

\textsuperscript{1}We acknowledge support from AFOSR MURI Program #FA9550-09-1-0705.

1:51PM U5.00014 Tunable THz Metamaterial Coupled to Graphene, TSUNG-TA TANG, SUFEEI SHI, LONG JU, UC Berkeley, FENG WANG, UC Berkeley and Lawrence Berkeley National Laboratory — Metamaterial is a periodic sub-wavelength dielectric structure which can be tailored to have a strong resonance at particular frequencies. However, changing the electromagnetic response of metamaterial often involves changing the design. On the other hand, graphene is an atomic layer of carbon atoms arranged in honeycomb structure and its conductivity in THz regime is highly tunable by changing the Fermi energy of graphene. In our study, we couple graphene to a THz metamaterial device efficiently and demonstrate that the resonance of THz metamaterial can be changed over a wide range by controlling the conductivity of graphene. This graphene-THz metamaterial hybrid device can be used for future THz application such as THz modulator, which can be controlled electrostatically.
of electrical conductivity in the material. Oriented pyrolytic graphite (HOPG) samples were exposed to bromine vapor for times between 20 and 100 minutes. The reflectance was measured using FTIR.

Florida — Graphite intercalation compounds have a long and interesting history, with surprising thermal, electrical, and magnetic properties. In this study highly SAEIYI VARNOOSFADERANI, Physics department, University of Florida, Gainesville, Florida, SEFAATTIN TONGAY, Department of Material Science and.


IBr-GIC and use it to predict the device suitability of these intercalants. It is seen that adding a layer of these GIC’s to a single layer of graphene does not disturb spectroscopic measurements reveal


11:39AM U6.00003 Rb-intercalated bilayer graphene studied by high-resolution ARPES, JAMES KLEEMAN, Dept. of Physics, Tohoku University, KATSUUKI SUGAWARA, WPI-AIMR Tohoku University, TAKAFUMI SATO, Dept. of Physics, Tohoku University, TAKASHI TAKAHASHI, Dept. of Physics, Tohoku University; WPI-AIMR Tohoku University — To elucidate the electronic structure at the thinnest limit of the graphite intercalation compound (GIC) CsRb, we have performed high-resolution angle-resolved photoemission spectroscopy (ARPES) and low-energy electron diffraction (LEED) on Rb-intercalated graphene samples fabricated by in-situ evaporation of Rb atoms onto graphene grown epitaxially on SiC. Using LEED, the creation of an intercalated layer with in-plane geometry identical to bulk GICs was confirmed by the observation of a 2x2 spot pattern consistent with Rb intercalation. From ARPES measurement, we found that the Dirac point is at a binding energy of approximately 1 eV, compared to 0.4 eV in pristine epitaxial graphene on SiC [1]. The Fermi surface of this material was also measured. The critical differences between Cs,Rb, its sister compound Cs,K, and pristine bilayer graphene will be examined herein.


11:51AM U6.00004 First principles study of Stage-1 graphene intercalates, IBr and ICI, PRIYAMVADA JADAUN, LEONARD F. REGISTER, SANJAY K. BANERJEE, The University of Texas at Austin — In this study we examine, from a first-principles approach, the properties of 2 graphene intercalant systems namely, iodine monochloride (ICI-GIC) and iodine monobromide (IBr-GIC). These materials are being explored as possible interlayer dielectric candidates for 2D-to 2D-tunnel FETs (TFETs) and Bilayer pseudospin FETs (BiSFETs). To do so we employ density functional theory (DFT). Both these intercalants are stage-1 and acceptor type. We first put forth a structural description of these compounds that intercalate 2 successive layers of graphene, stacked AA type as obtained upon relaxation. Subsequently we describe the electronic structure of ICI-GIC and IBr-GIC and use it to predict the device suitability of these intercalants. It is seen that adding a layer of these GIC’s to a single layer of graphene does not disturb graphene electronic spectra except for opening a small gap and introducing doping. With the second graphene layer added, coupling between the graphene layers becomes evident through a small amount of band splitting.

[1] Texas Advanced Computing Center (TACC)

12:03PM U6.00005 Charge Density Waves on the Graphene Sheets of the Heavily-Doped Superconductor Graphitic Intercalate CaC$_6$, C.F. HIRJIBEHEDIN, K.C. RAHNEJAT, London Centre for Nanotechnology (LCN) and U. College London (UCL), UK, C.A. HOWARD, LCN, UCL, and Royal Holloway, U. of London, UK, N.E. SHUTTLEWORTH, S.R. SCHOFIELD, LCN and UCL, UK, K. IWAYA, Tohoku U., Japan, CH. TAKAHASHI, Switzerland, G. APPI, M. ELERBY, LCN and UCL, UK — The electronic properties of graphic materials can be readily tuned by adding charge carriers, and high levels of doping can even lead to superconductivity. We used scanning tunnelling microscopy to investigate the graphene-terminated surface of the superconducting material CaC$_6$ at temperatures well above T$_c$=11.5K [1]. We find two distinct surface types that show atomic resolution: one exhibits the expected structure of a graphene lattice superimposed on a hexagonal Ca superlattice while the other has stripes with a period three times that of the underlying Ca superlattice. A periodic distortion was found in the Ca atoms matching the periodicity of the electronic contrast on the graphene sheet, though no displacements of the carbon lattice were detected. Spectroscopic measurements reveal an energy gap in the electronic structure that can be directly associated with the stripe periodicity. This provides strong evidence that the stripes correspond to a charge density wave (CDW) in a graphene system that also superconducts at lower temperatures, offering an excellent test bed for studying the relationship between these two important phenomena. [1] K.C. Rahnejat et al., Nat. Commun. 2, 558 (2011).
12:15PM U6.00006 Phonon-mediated superconductivity in graphene by lithium deposition, GIANNI PROFETA, Università dell’Aquila, MATTEO CALANDRA, FRANCESCO MAURI, CNRS et Université P. et M. Curie — Graphene is the physical realization of many fundamental concepts and phenomena in solid-state physics. However, in the list of graphene’s many remarkable properties, superconductivity is notably absent. If it were possible to find a way to induce superconductivity, it could improve the performance and enable more efficient integration of a variety of promising device concepts. To this end, we explore, by first-principles DFT calculations, the possibility of inducing superconductivity in a graphene sheet by doping its surface with alkaline metal adatoms [1], in a manner analogous to which superconductivity is induced in graphite intercalated compounds (GICs). As for GICs, we find that the electrical characteristics of graphene are sensitive to the species of adatom used. However, unlike GICs, we find that lithium atoms should induce superconductivity in graphene at a higher temperature than calcium. [1] G. Profeta, M. Calandra, F. Mauri, Nature Physics 8, 131-134 (2012)

12:27PM U6.00007 Si on epitaxial graphene on SiC: intercalation and graphene-SiC transformation, FENG WANG, KRISTIN SHEPPERD, Georgia Institute of Technology, ALEXEI ZAKHAROV, MAX-lab, EDWARD CONRAD, Georgia Institute of Technology — The interface between epitaxial graphene and bulk SiC plays a dominant role in both the growth and transport properties of graphene on SiC. The differences in diffusion of Si through graphene on the two polar SiC surfaces is related to the different nucleation of Si diffusion channels on the two graphene-SiC interfaces. In this work we use LEEM, XPEEM and XPS to study how the excess Si at the graphene-vacuum interface reorders itself at high temperatures. We show that silicon deposited at room temperature onto multilayer graphene films grown on the SiC(0001) surface rapidly diffuses to the graphene-SiC interface when heated to temperatures above 1200 °C. The Si that does intercalate into the interface can be removed back out to the graphene-vacuum boundary by heating the sample to 1200 °C. Most of the Si evaporates at this temperature, however, a significant amount of Si reacts with the graphene at the vacuum interface and form a relative stable reconstructed (2×2) SiC structure. At significantly higher Si concentrations, graphene at the vacuum interface transforms to SiC.

1This work is supported by the NSF under grants DMR-0820382 and 1005880

12:39PM U6.00008 Silicon Layer Intercalation and Interface Properties between Graphene and Metal hosts, YELIANG WANG, JINHAI MAO, LEI MENG, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, JUNFENG HE COLLABORATION, SHIXUAN DU COLLABORATION, XINGJIANG ZHOU COLLABORATION, A. H. CASTRO NETO COLLABORATION — Graphene is being considered as a contender as the reference material with extraordinary properties for a post-CMOS technology. The availability of high quality and large scale single crystal graphene is fundamental for it to fulfill its promise in electronic applications. Graphene is usually grown on a metallic substrate from which it has to be transferred before it can be used. However, uncontrolled shear and strain, associated with the transfer and the presence of extended domains, lead to unavoidable tearing, rendering it useless for scalable production. We propose a way to overcome this bottleneck and produce high quality, free standing graphene by intercalating Si in graphene epitaxially grown on metals, like Ru(0001) & Ir(111). This Si/graphite architecture, produced by the silicon-layer intercalation approach (SIA), was characterized by STM/STS, Raman, and angle resolved photoelectron emission spectroscopy (ARPES) and proves the high structural and electronic qualities of the new composite. The SIA eliminates the need for the graphene transfer and also allows for an atomic control of the distance between the graphene and the metal. References: 1. Jinhai Mao, Yeliang Wang, H.-J. Gao, et al., Appl. Phys. Lett. 100, 093101 (2012) (Cover). 2. Lei Meng, Yeliang Wang, H.-J. Gao, et al., Appl. Phys. Lett. 100, 083101 (2012).

1Graphene Research Center, Singapore National University.

12:51PM U6.00009 Na induced changes in the electronic band structure of graphene grown on C-face SiC, CHARIYA VIROJANADARA, CHAO XIA, LEIF JOHANSSON, Department of Physics, Chemistry and Biology, Linköping University, SE-58183, Linköping, Sweden — Studies of the effects induced on the electronic band structure after Na deposition, and subsequent heating, on a C-face 2 MLs graphene sample will be presented. Na deposition shifts the Dirac point downwards from the Fermi level by about 0.5 eV due to electron doping. After heating at temperatures from around 120 to 300°C, the n-band appears considerably broadened. Collected Si 2p and Na 2p spectra then indicate Na intercalation in between the graphene layers and at the graphene SiC interface. The broadening is therefore interpreted to arise from the presence of two slightly shifted, but not clearly resolved, n-bands. Constant energy photoelectron distribution patterns, E(\{kx,ky\}), extracted from the clean 2MLs graphene C-face sample look very similar to earlier calculated distribution patterns for monolayer, but not Bernal stacked bi-layer, graphene. After Na deposition the patterns extracted at energies below the Dirac point appear very similar so the doping had no pronounced effect on the shape or intensity distribution. At energies above the Dirac point the extracted angular distribution patterns showed the flipped, “mirrored,” intensity distribution predicted for monolayer graphene at these energies. An additional weaker outer band is also discernable at energies above the Dirac point, which presumably is induced by the deposited Na.

1:03PM U6.00010 First-Principles Modeling of Low-Energy Electron Diffraction of Few Layer Graphene, JOHN MCCLAIN, University of New Hampshire, JIEBING SUN, Michigan State University, JAMES HANNON, IBM Thomas J Watson Research Center, KARSTEN POHL, JIAN-MING TANG, University of New Hampshire — We present calculations of the low-energy electron microscopy (LEEM) spectra of few layer graphene (FLG) systems using our newly developed theoretical approach based on density-functional theory (DFT). The traditional analysis using multiple scattering off muffin-tin potentials is replaced with a Bloch wave matching approach using self-consistent potentials via DFT to better describe the LEEM spectra, especially in the low energy range. Our calculated results for free-standing FLG exhibit oscillations in reflectivity for energies between 0 and 7 eV, in good agreement with the experimental LEEM spectra of FLG observed on various substrates. The number of oscillations is correlated to the number of graphene layers, a fact often used to determine the number of graphene layers in a sample region. We have calculated FLG on Ni(111)-(1x1) and find that the FLG features dominate those of the bare Ni(111) when two graphene layers are added, as seen in experiments. Our results show that the valleys in the LEEM spectra due to graphene appear only with more than one graphene layer, consistent with our results for free-standing FLG.

1We acknowledge funding support from NSF DMR-1006863.

1:15PM U6.00011 Theory of low-energy electron reflectivity from graphene, RANDALL FEENSTRA, NISHTHA SRIVASTAVA, MICHAEL WIDOM, Dept. Physics, Carnegie Mellon University, Pittsburgh, PA, IVAN VLASSIOUK, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN — We have developed a self-consistent description of low-energy electron reflectivity spectra, yielding results that compare well with experimental data for graphene on SiC and on Cu substrates (obtained by our group as well as by other groups [1]). Our approach utilizes wavefunctions for a thin multilayer graphene slab, computed with a first-principles method. By combining wavefunctions for positive and negative wavevectors, we form states with only outgoing character on one side of the slab, and hence deduce the electron reflectivity. For free-standing n-layer graphene, we obtain the reflectivity curves that show n-1 reflectivity minima over the energy range 0 - 10 eV. The minima are shown to arise from states with wavefunctions localized between the graphene layers (not on the layers, as previously suggested [1]). For graphene on a substrate, we match the states on one side of the graphene slab to bulk states of the substrate. For graphene on Cu(111) substrates, we find the same set of reflectivity minima as for free-standing graphene, together with an additional minimum whose location varies with the graphene-Cu separation. Hence, this separation can be deduced by comparing experimental and theoretical spectra. [1] H. Hibino et al., Phys. Rev. B 77, 075413 (2008)
1:27PM U6.00012 Bandgap opening in bilayer graphene via molecular doping1, DAVID CAREY, ALEXANDER SAMUELS, University of Surrey — We report the emergence of an electronic bandgap in bilayer graphene through the interaction with physisorbed molecules. The bandgap is found to scale linearly with induced carrier density though a slight asymmetry is found between n-type dopants where the bandgap varies as 47 meV/10^13 cm^-2 and p-type dopants where the bandgap varies as 38 meV/10^13 cm^-2. The n-type dopant molecules include tetraethylsilane (TFS), cobaltocene and decamethylcobaltocene (DMC) and p-type dopant molecules include NO2, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) and 3,6-difluoro-2,5,7,8-hexacyano-quinodimethane (F2-HCNQ). Ammonia is found to be weak amphoteric dopant on bilayer graphene, as it is on single layer graphene, where the charge transfer depends on the orientation of the N atom relative to the upper graphene layer. The bandgap opening is explained in terms of the asymmetric charge distributions on the upper graphene layer which is in contact with the molecules. The high binding energy found upon adsorption of some of these molecules results in an attractive way to a permanent bandgap and when combined with a variable external electric field can either close the gap or widen it still further.

1Support from the EPSRC is gratefully acknowledged

1:39PM U6.00013 Substrate Screening Effects in ab initio Many-body Green’s Function Calculations of Doped Graphene on SiC1, DEREK VIGIL-FOWLER, JOHANNES LISCHNER, STEVEN LOUIE, University of California, Berkeley and Lawrence Berkeley National Lab — Understanding many-electron interaction effects and the influence of the substrate in graphene-on-substrate systems is of great theoretical and practical interest. Thus far, both model Hamiltonian and ab initio GW calculations for the quasiparticle properties of such systems have employed crude models for the effect of the substrate, often approximating the complicated substrate dielectric matrix by a single constant. We develop a method in which the spatially-dependent dielectric matrix of the substrate (e.g., SiC) is incorporated into that of doped graphene to obtain an accurate total dielectric matrix. We present ab initio GW + cumulant expansion calculations, showing that both the cumulant expansion (to include higher-order electron correlations) and a proper account of the substrate screening are needed to achieve agreement with features seen in ARPES. We discuss how this methodology could be used in other systems.

1This work was supported by NSF Grant No. DMR10-1066184 and U.S. DOE Contract No. DE-AC02-05CH11231. Computational resources have been provided by the NERSC and NICs. D.V-F. acknowledges funding from the DOD’s NDSEG fellowship.

1:51PM U6.00014 Electronic Strengthening of Graphene by Charge Doping1, CHEN SI, Tsinghua University, University of Utah, ZHENG LIU, University of Utah, WENHUI DUAN, Tsinghua University, FENG LIU, University of Utah — Graphene is known as the strongest 2D material in nature, yet we show that moderate charge doping of either electrons or holes can further enhance its ideal strength by up to ~17%, based on first principles calculations. This unusual electronic enhancement, versus conventional structural enhancement, of material’s strength is achieved by an intriguing physical mechanism of charge doping counteracting on strain induced enhancement of Kohn anomaly, which leads to an overall stiffening of zone boundary K1 phonon mode whose softening under strain is responsible for graphene failure. Electrons and holes work in the same way due to the high electron-hole symmetry around the Dirac point of graphene, while over doping may weaken the graphene by softening other phonon modes. Our findings uncover another fascinating property of graphene with broad implications in graphene-based electromechanical devices.

1The work is supported by DOE-BES program. C.S. thanks Tsinghua exchange student fund for supporting her visit at U. of Utah. W. D. thanks support by the Ministry of Science and Technology of China

2:03PM U6.00015 Incremental Tuning of Graphene’s Fermi Level by Chemical Doping, KARA BERKE, University of Florida, SEFAATTIN TONGAY, University of California, Berkeley, ARTHUR HEBARD, University of Florida — We report a simple, scalable method for fine tuning the Fermi level of CVD-grown graphene, through controlled chemical doping by the addition of the polymer polyethylenimine (PEI) to the graphene surface. Graphene samples initially showed p-type behavior before doping. By dropcasting a low concentration solution of PEI in methanol onto graphene, the hole concentration was lowered. Repeated applications to the same sample shift the Fermi level of the graphene through the Dirac point, yielding an increasingly n-type sample. The graphene mobility increases with each application of PEI solution due to charge screening effects. Additionally, the magnetoresistance becomes increasingly linear near the Dirac point, consistent with the existence of charge puddles in neutral graphene.

Thursday, March 21, 2013 11:15AM - 2:15PM –
Session U9 DCMP: Three Dimensional Topological Insulators: Chalcogenides and New Materials 308 - Phillip King, Cornell University

11:15AM U9.00001 Spin Control of the topological surface states in 3D topological insulators using polarized light1, ANNA GURA, JEFF SECOR, MILAN BEGLIARBEKOV, LUKAS ZHAO, HAIMING DENG, LIA KRUSIN-ELBAUM, Physics Department, City College of New York — The topological surface states of 3D topological insulators (TIs) have been shown to interact non trivially with circularly polarized light. Here we report on the study of spin-polarized currents in several 2nd generation TIs, such as Sb2Te3, Sb2Se3, and Bi2Te3. In particular, to probe the robustness of the helical current surface states we will contrast the polarization dependence of the photocurrent in as grown crystals and crystals with controlled disorder introduced by magnetic and non-magnetic impurities. These result in the development of a gap in the energy spectrum of surface Dirac fermions (DFs), that is DFs acquire mass. The photo-response contrast between massless and massive Dirac fermions studied under electric field gating conditions will be presented.

1Supported in part by NSF-DMR-1122594

11:27AM U9.00002 Highly tunable electron transport in epitaxial topological insulator (Bi1−xSbx)2Te3 thin films, TONG GUAN, Institute of Physics, Chinese Academy of Sciences; Florida State University, XIAOYUE HE, KE-HUI WU, YONGQING LI, Institute of Physics, Chinese Academy of Sciences — Three dimensional topological insulators (TI) have potential applications in quantum computation and spintronics. These applications often require an insulating bulk and high tunability in chemical potential. Remarkable progresses have been made in synthesizing new TI material with more insulating bulk by alloying the binary compounds Bi2Te3, Sb2Te3, Bi2Se3 and Sb2Se3 in the past couple of years. Here we report the growth of single crystalline (Bi1−xSbx)2Te3 films on SrTiO3(111) substrates by molecular beam epitaxy. A full range of Sb-Bi compositions have been studied. Optimal Sb composition for minimum bulk conduction was found to be $x = 0.5 \pm 0.1$. For the samples (Bi0.5Sbx0.5)2Te3, the carrier density can be tuned from n-type to p-type with the help of a back-gate. Linear magnetoresistance has been observed at gate voltages close to the maximum in the longitudinal resistance of (Bi0.5Sbx0.5)2Te3 sample. These highly tunable (Bi1−xSbx)2Te3 thin films provide an excellent platform to explore the intrinsic transport properties of the three dimensional topological insulators.
11:39AM U9.00003 Iodine doping of p-type topological insulators 1. INNA KORZHOVSKA, LUKAS ZHAO, HAIMING DENG, CHEN ZHIYI, LIA KRUSIN-ELBAUM, City College of New York-CUNY — We report on the systematic iodine (I) doping of the ‘intrinsically’ p-type 2nd generation topological insulator (TI) $\text{Sb}_2\text{Te}_3$. Iodine will introduce additional holes into the system and thus pull the Fermi level $E_F$ ‘down’ from the Dirac point. Further, at a sufficient hole density, particle correlation effects are also expected to emerge. Iodine was incorporated into $\text{Sb}_2\text{Te}_3$ using two methods: (i) post-growth vapor exposure of crystals grown by the Vapor-Liquid-Solid (VLS) technique and (ii) in-situ doping of crystals grown in a modified Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the in-situ doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure in-situ Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the in-situ doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure in-situ Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the in-situ doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure in-situ Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the in-situ doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure in-situ Bridgman setup. The first method is self-limiting and only up to 2 at% iodine is entered, however the in-situ doping allowed us to increase iodine content up to 20%. Detailed XRD Rietveld refinement analysis of the doped crystals doping indicates that for the I-content greater than 10% the rhombohedral structure

1Supported in part by NSF-DMR-1122594

11:51AM U9.00004 Nuclear Magnetic Resonance Studies of Bulk States of Bi2Se3, D.M. NISSON, A.P. DIOGUARDI, P. KLAVINS, C.H. LIN, K. SHIRER, A. SHOCKLEY, J. CROCKER, N.J. CURRO, University of California, Davis, Department of Physics, N. J. CURRO NMR GROUP TEAM — We present $^{119}$Bi nuclear magnetic resonance (NMR) spectra and relaxation rate data on single crystals of Bi$_2$Se$_3$ measured under various conditions, whose carrier concentrations, resistivities, and Shubnikov-de Haas (SdH) frequencies have been measured. Our NMR data reveal properties of the bulk states, which are influenced by the presence of intrinsic carriers. We find that both the Knight shift and the electric field gradient of the Bi is correlated with carrier concentration, and atypically spectral profiles. Surprisingly, spin-lattice relaxation is not strongly temperature dependent.

12:03PM U9.00005 Origin of helical spin texture of topological phase transition family materials TIBI($\text{Se}_{1-x}\text{S}_x$)$_2$, JUSTIN WAUGH, YUE CAO, University of Colorado at Boulder, KOJI MIYAMOTO, TAICHI OKUDA, Hiroshima Synchrotron Radiation Center, CHETAN DHALIT, STEPHEN WILSON, Boston College, DANIEL DESSAU, University of Colorado at Boulder — The unique helical spin-polarized metallic states of topological insulators are believed to arise from an odd number of band inversions per unit cell. It is believed that the band inversion in the family of compounds TIBI($\text{Se}_{1-x}\text{S}_x$)$_2$ can be removed by replacing Se by S, removing the spin-polarized surface states. Using spin and angle-resolved photoemission spectroscopy we have shown that even on the gapped non-topological “trivial” state of the phase transition (x=0.7), Dirac-like helical spin polarization still exist, as well as small but finite gaps on the topological side of the phase transition (x=0.3). Additional spin helicity inversions are also present in the bulk bands of both samples. We consider various explanations for this effect, including a superposition of domains, massive Dirac states due to thin domains, and Rashba spin orbit splitting at the surfaces.

12:15PM U9.00006 Terahertz Quantum Hall Effect of Dirac Fermions in a Topological Insulator, A. PIMENOV, A. SHUVAEV, TU Vienna, Austria, G. ASTAKHOV, G. TKACHOV, CH. BRUENE, H. BUHMANN, L. W. MÖLKENKAMP, University of Wuerzburg, Germany — Using THz spectroscopy in external magnetic fields we investigate the low-temperature charge dynamics of strained HgTe, a three dimensional topological insulator. From the Faraday rotation angle and ellipticity a complete characterization of the charge carriers is obtained. In resonator experiments, we observe quantum Hall oscillations at THz frequencies. The 2D density estimated from the period of these oscillations agrees well with direct transport experiments on the topological surface state. The Dirac character of the surface state is proven by the observation of a half-integer plateau in the quantum Hall effect.

12:27PM U9.00007 Various Types of Dirac Cone Materials of Bi$_{1-x}$Sb$_x$ Thin Films, SHUANG TANG, MILDRED DRESSELHAUS, MIT — The band structure of bismuth antimony thin films varies as a function of stoichiometry, film thickness and growth orientation. Different types of Dirac cone materials can be constructed based on the bismuth antimony thin films system, including single-Dirac-cone, bi-Dirac-cone and tri-Dirac-cone materials, and also including exact-Dirac-cone and quasi-Dirac-cone materials. The degree of anisotropy of a Dirac cone can be controlled, which range from ~ 2 to ~ 14. Interesting transport phenomena are expected in different Dirac cone materials, which may be optimized for different purposes of applications, e.g. thermoelectrics, electronics etc.

12:39PM U9.00008 Dirac fermions, Fermi surface and magnetotransport in bulk crystals of layered SrZnSb$_2$, KEFENG WANG, LIMIN WANG, Brookhaven National Laboratory, DAVID GRAF, National High Magnetic Field Laboratory, Florida State University, CEDOMIR PETROVIC, Brookhaven National Laboratory — We report evidence for anisotropic Dirac-like pockets and the large magnetoresistance in the quasi-two-dimensional Sb rectangular layers of bulk SrZnSb$_2$ crystals. Due to the two-fold symmetry of the Sb layers, there are three different Dirac-like pockets as revealed by the calculated Fermi surface. Angular dependent in-plane magnetoresistance and oscillation frequencies indicate the quasi-two-dimensional character of the pockets. This is different from the identical Dirac-cone-like points in the Bi square net of SrMnBi$_2$. The large linear magnetoresistance and magnetothermopower were observed in crystals. The magnetoresistance behavior can be described very well by combining the semiclassical cyclotron contribution and the quantum limit magnetoresistance. Magnetic field also enhances the thermopower. Our results can be well understood by the magnetotransport of Dirac states in the bulk band structure. Work at BNL supported by Office of Basic Energy Sciences, US DOE, under contract No. DE-AC02-98BC (K. W. L. W and C. P.). Work at the National High Magnetic Field Laboratory is supported by the DOE NNSA DE-FG52-10NA29659, by the NSF Cooperative Agreement No.DMR-0654118, and by the state of Florida (D. G.)

12:51PM U9.00009 $\beta$-Ag$_3$Te: A topological insulator with strong anisotropy 1, LAN WANG, AZAT SULAEV, PENG REN, BIN XIA, QINGHUA LING, TING YU, CAIYU QIU, School of Physical and Mathematical Science, Nanyang Technological University, Singapore, SHUHONG-YUAN ZHANG, MING-YONG HAN, Institute of Material Research and Engineering, Singapore, ZHIPENG LI, WEI GUANG ZHU, School of Electrical and Electronic Engineering, Singapore, Nanyang Technological University, Singapore, QINGYU WU, YUAN PING FENG, LEI SHEN, Department of Physics, National University of Singapore, Singapore, SHUH-QING SHEN, Department of Physics, The University of Hong Kong, Hong Kong, China — We present evidence of topological surface states in $\beta$-Ag$_3$Te through first-principles calculations, periodic quantum interference effect and ambipolar electric field effect in single crystalline nanoribbon. Our first-principles calculations show that $\beta$-Ag$_3$Te is a topological insulator with a gapless Dirac cone with strong anisotropy. To experimentally probe the topological surface state, we synthesized high quality single crystalline $\beta$-Ag$_3$Te nanoribbon and performed electron transport measurements. The coexistence of pronounced Aharonov-Bohm oscillations and weak Al'tshuler-Aronov-Spivak oscillations clearly demonstrates coherent electron transport around the perimeter of $\beta$-Ag$_3$Te nanoribbon and therefore the existence of topological surface states, which is further supported by the ambipolar electric field effect for devices fabricated by $\beta$-Ag$_3$Te nanoribbons. The experimentally confirmed topological surface states and the theoretically predicted isotropic Dirac cone of $\beta$-Ag$_3$Te suggest that the material may be a promising material for fundamental study and future spintronic devices.

1RCA-08-018 (Singapore), MOE2010-T2-2-059 (Singapore), HKU705150P (Hong Kong), NTU-SUG M4080513
1:03PM U9.00010 Topological Surface State Observed in Superconducting (Ir1-xPtx)Te2, TIAN QIAN, HU MIAO, GANG XU, XI DAI, ZHONG FANG, AIFA FANG, NANLIN WANG, HONG DING, Institute of Physics, Chinese Academy of Sciences — Topologically non-trivial surface state is the hallmark of 3D topological insulators and topological superconductors, where spin-orbit coupling (SOC) plays an essential role. By Ir site doping of 5% Pt, the huge SOC material IrTe2 becomes a superconductor with maximal Tc = 3K. Our angle resolved photoemission spectroscopy (ARPES) study combined with LDA analysis demonstrate the surface states of (Ir1-xPtx)Te2 is topologically non-trivial.

1:15PM U9.00011 Transport properties of crystalline topological insulator Pb1-xSnxSe, TIAN LIANG, Dept. Phys. Princeton University, New Jersey 08544, QUINN GIBSON, Dept. Chem. Princeton University, New Jersey 08544, JUN XIONG, M.A. HIRSCHBERGER, Dept. Phys. Princeton University, New Jersey 08544, R.J. CAVA, Dept. Chem. Princeton University, New Jersey 08544, N.P. ONG, Dept. Phys. Princeton University, New Jersey 08544 — The narrow-band gap semiconductors Pb1-xSnxSe and Pb1-xSnxTe have received considerable attention recently following the prediction [1] that they are examples of a topological crystalline insulator with surface states characterized by a mirror Chern number. Several ARPES groups have reported evidence for the topological surface states [2,3]. We have investigated the transport properties of crystals of Pb1-xSnxSe. For Sn content x bracketing 0.23, we observe strong quantum oscillations from bulk carriers (either n or p type) with concentrations near 2×10^18 cm^-3 and mobilities ~ 3,000 cm^2/Vs. The results of experiments to tune the chemical potential into the gap using chemical doping and liquid gating will be reported.


1Supported by Army Research Office (ARO W911NF-11-1-0379) and NSF-MRSEC Grant DMR 0819860.

1:27PM U9.00012 NMR Studies of the Candidate Topological Superconductor Sn1−xInxTe: Spin-Triplet Superconductivity Robust against Magnetic Impurities, X.R. LU, L. MA, J. DAI, P. WANG, B. NORMAND, W. YU, Department of Physics, Renmin University of China, Beijing, China, R.D. ZHONG, J. SCHNEELOCH, Z.J. XU, G.D. GU, Condensed Matter Physics and Materials Science, Brookhaven National Laboratory, NY 11973, USA — In-doped SnTe is a low-carrier-density semiconductor with strong spin-orbit coupling, and has been proposed to be a topological superconductor. We report nuclear magnetic resonance (NMR) studies of both 119Sn and 125Te nuclei, performed on single crystals of Sn1−xInxTe, where Tx = 1.8 K for x = 0.1. Under an applied field of 0.33 T, the spin-lattice relaxation rate 1/T1 drops rapidly below 1.2 K, indicating bulk superconductivity. We observe absolutely no change in the Knight shift with temperature when T < Tx, which in NMR is normally an indicator of spin-triplet superconductivity. We find no coherence peak below Tx in 119T1, suggesting an unconventional order parameter but also the possible role of impurities. In the normal state we find that 1/119T1 and 1/125T1 have Fermi-liquid behavior at high fields, but at low fields show a large Curie-Weiss-type enhancement indicative of magnetic impurity effects. Thus the fact that Tx in our samples is insensitive to the sample purity suggests that superconductivity in Sn1−xInxTe is robust against magnetic impurities, in contrast to the situation in conventional superconductors.

1:39PM U9.00013 Electronic Structure Study on a 3D Dirac Semimetal Candidate, Y.L. CHEN, Oxford University, Z.K. LIU, Stanford University, B. ZHOU, S.K. MO, Laurence Berkeley National Lab, D. PRABHAKARAN, Oxford University, Z.J. WANG, Z. FANG, X. DAI, Institute of Physics, Chinese Academy of Sciences, Z.X. SHEN, Stanford University, Z. HUSSAIN, Laurence Berkeley National Lab — A family of 3D Dirac semimetals candidates (A3Bi, A=alkali metal, B=As, Sb, or Bi) have recently been predicted to exist at the phase transition between a topological and a normal insulator when inversion symmetry is preserved. In such a semimetal, the condensation and valence bands touch only at Dirac points around which the dispersion is linear in all directions, leading to distinct physical properties, such as giant diamagnetism and linear quantum magneto-resistance. We used angle resolved photoemission spectroscopy (ARPES) to study a 3D Dirac semimetal candidate, Na3Bi and revealed interesting electronic structures. We will discuss our observation, its possible topological origin and the connection to recent theory investigation.

1:51PM U9.00014 Competing Orders in the Surface State of Topological Kondo Insulators, JEFFREY BOTIMER, DAE-JEONG KIM, SEAN THOMAS, ZACHARY FISK, JING XIA, University of California, Irvine — The recent discovery of topological (band) insulators (TI) reveals a conceptually new family of quantum materials with novel properties. The bulk energy gap closes at the surface, leading to a gap-less metallic topological surface state. Recently several Kondo insulators have been theoretically proposed in this category, dubbed “Topological Kondo Insulators” (TKI). In a TKI, the topological order arises from strong electron correlation and will display new physics. For example, various broken symmetry orders are expected to compete with the topological order. In this talk we will present electrical transport evidence for a high mobility conducting surface state, as well as magneto-optic evidence for broken time reversal symmetry at the surface of several TKI materials. These results suggest that the surface state of the TKI are not only topological but also magnetic, thus providing a convenient system to study topological magneto-electric effects where magnetization can be induced by pure electric field.

2:03PM U9.00015 Transport Signature of Floquet Majorana Fermions, ARJIT KUNDU, BARAK SERAD-JEH, Indiana University, Bloomington — It has been recently predicted that a periodically-driven superconducting quantum wire can support unpaired Floquet Majorana fermions (FMFs), steady-state equal mixtures of electrons and holes bound to the ends of the wire. We further study this proposition and elucidate the range of parameters and drives that give rise to FMFs. We also look for possible transport signatures of FMFs within a non-equilibrium Green’s function approach. We analyze the conduction process for different driving schemes and compare the behavior with that of the static system. We comment on possible experimental setups to observe and exploit FMFs in quantum information processing.

References:

1Supported by College of Arts and Sciences, Indiana University, Bloomington.

Thursday, March 21, 2013 11:15AM - 2:15PM –
Session U13 DCMP: Topological Insulators: Bi2Se3 and Bi2Te2Se 315 - Gregory Jenkins, University of Maryland
11:15AM U13.00001 Topological dangling bonds with large spin splitting and enhanced spin polarization on the surfaces of Bi$_2$Se$_3$. HSIN LIN, Northeastern University, TANMOY DAS, Los Alamos National Laboratory, YOSHINORI OKADA, Boston College, MIKE C. BOYER, W. DOUG WISE, MICHELLE TOMASIK, BO ZHEN, ERIC W. HUDSON, Massachusetts Institute of Technology, WENWEN ZHOU, VIDYA MADHAVAN, Boston College, CHUNG-YUAN REN, National Kaoshiung Normal University, Taiwan, HIROSHI IKUTA, Nagoya University, Japan, ARUN BANSIL, Northeastern University — We investigate the topological surface state properties at various surface cleaves in the topological insulator Bi$_2$Se$_3$, via first principles calculations and scanning tunneling microscopy/spectroscopy (STM/STS). While the typical surface termination occurs between two quintuple layers, we report the existence of a surface termination within a single quintuple layer where dangling bonds form with giant spin splitting owing to strong spin-orbit coupling. Unlike Rashba split states in a 2D electron gas, these states are constrained by the band topology of the host insulator with topological properties similar to the typical topological surface state, and thereby offer an alternative candidate for spintronics usage. We name these new states “topological dangling-bond states.” The degree of the spin polarization of these states is greatly enhanced. Since dangling bonds are more chemically reactive, the observed topological dangling-bond states provide a new avenue for manipulating band dispersions and spin-textures by adsorbed atoms or molecules. Work supported by DOE.

11:27AM U13.00002 ABSTRACT WITHDRAWN —

11:39AM U13.00003 Transient Surface Photoemission Involving Nonlinear Surface Sheet Polarization Developed on the Doped Bi$_2$Se$_3$ Topological Insulator$^1$. YUKIAKI ISHIDA, HIROAKI KANTO, WALID MALAEB, SHUNTO WATANABE, ISSP, Univ. Tokyo, CHUANGTIAN CHEN, TIPC, CAS, AKIKO KIKKAWA, YASUJIRO TAGUCHI$^2$, YOSHINORI TOKURA$^3$, CERG, RIKEN ASI, SHIK SHIN$^4$, ISSP, Univ. Tokyo — Time- and angle-resolved photoemission spectroscopy is performed on the doped Bi$_2$Se$_3$ topological insulator. We observe unusual variation in the efficiency of photoemission from femto-to-picosecond non-equilibrium particularly when two-dimensional electron gas (2DEG) states are developed on surface, while the surface confinement potential is virtually unchanged. The results indicate that a surface sheet polarization, which is induced nonlinearly by both the photon field and inversion-symmetry-breaking field, grows in magnitude as the 2DEG states become pronounced and opens a so-called surface photoemission channel, $div\mathbf{A}$, that can be varied transiently. Matrix element effects investigated by linearly-polarized angle-resolved photoemission also supports the presence of $div\mathbf{A}$. The asymmetric charge distribution developed around vacuum-surface interface is considered as a key to understand and control Rashba splitting of the 2DEG states.

$^1$This research is partially supported by KAKENHI(23740256) and by the JSPS through its "FIRST Program"
$^2$also at CMRG, RIKEN ASI
$^3$also at CMRG, RIKEN ASI and Dept. Appl. Phys., Univ. Tokyo
$^4$also at CREST, JST

11:51AM U13.00004 High mobility topological insulator Bi$_2$Se$_3$ exfoliated devices with hexagonal Boron Nitride dielectrics. HADAR STEINBERG, VALLA FATEMI, LUCAS ORONA, JAVIER SANCHEZ-YAMAGISHI, MIT, KENJI WATANABE, TOSHIE TSUGA, University of Tokyo, National institute of Materials Science, JAXA, PARIS CREON, SHIN-ICHI SAKAMOTO, AIST, NISSHIN, OKADA, Boston College, MIKE C. BOYER, W. DOUG WISE, MICHELLE TOMASIK, BO ZHEN, ERIC W. HUDSON, Massachusetts Institute of Technology, WENWEN ZHOU, VIDYA MADHAVAN, Boston College, CHUNG-YUAN REN, National Kaoshiung Normal University, Taiwan, HIROSHI IKUTA, Nagoya University, Japan, ARUN BANSIL, Northeastern University — Recently, 3D topological insulators, featuring spin helical topological surface states (SS), have attracted strong attention in condensed matter physics. Although the SS have been directly revealed and intensively studied by surface sensitive measurements, such as ARPES and STM, transport measurements remain challenging due to coexistence of the surface and bulk conduction channels and the sensitivity of sample surfaces to ambient exposure. We have grown high quality Bi$_2$Se$_3$ crystals by Bridgman method. Resistance showed an insulating behavior followed by saturation at low temperature, indicating surface conduction. Through magnetotransport measurements, we demonstrated high mobility SS on freshly cleaved crystals. The transport signatures of surface Dirac fermions were uncovered from 2D SdH oscillations and non-linear Hall effect. We have also compared transport properties of the samples before and after exposure to air. A giant cusp in magnetoresistance at zero B field was observed after exposure. Our studies may help understand the interplay between the surface and the bulk conduction channels and the degradation of SS due to environmental exposure. We will also present some experimental results of gate tuning and thermoelectric measurements on Bi$_2$Se$_3$.

The transport properties of the samples before and after exposure to air. A giant cusp in magnetoresistance at zero B field was observed after exposure. Our studies may help understand the interplay between the surface and the bulk conduction channels and the degradation of SS due to environmental exposure. We will also present some experimental results of gate tuning and thermoelectric measurements on Bi$_2$Se$_3$.

$^1$Supported by NSF-MRSEC (DMR 0819860), Army Research Office (ARO W911NF-11-1-0379) and DARPA under SPAWAR program (Grant N66001-11-1-4110).

12:03PM U13.00005 Magneto-transport study of magnetically-doped Bi$_2$Se$_3$. JOSEPH HAGMANN, JONATHON LEINER, DAVID HOWE, University of Notre Dame, YONGSEONG CHOY, Argonne National Laboratory, ABDEL AL-ASMADI, The Hashemite University, CERG, RIKEN ASI, HELIN CAO, IRENEUSZ MIOTKOWSKI, JIFA TIAN, Department of Physics, Purdue University, YONG CHEN, Department of Physics, School of Electrical and Computer Engineering, Purdue University — Recently, 3D topological insulators, featuring spin helical topological surface states (SS), have attracted strong attention in condensed matter physics. Although the SS have been directly revealed and intensively studied by surface sensitive measurements, such as ARPES and STM, transport measurements remain challenging due to coexistence of the surface and bulk conduction channels and the sensitivity of sample surfaces to ambient exposure. We have grown high quality Bi$_2$Te$_2$Se$_3$ crystals by Bridgman method. Resistance showed an insulating behavior followed by saturation at low temperature, indicating surface conduction. Through magnetotransport measurements, we demonstrated high mobility SS on freshly cleaved crystals. The transport signatures of surface Dirac fermions were uncovered from 2D SdH oscillations and non-linear Hall effect. We have also compared transport properties of the samples before and after exposure to air. A giant cusp in magnetoresistance at zero B field was observed after exposure. Our studies may help understand the interplay between the surface and the bulk conduction channels and the degradation of SS due to environmental exposure. We will also present some experimental results of gate tuning and thermoelectric measurements on Bi$_2$Te$_2$Se$_3$.

$^1$We acknowledge support from DARPA MESO program (Grant N66001-11-1-4107).
12:39PM U13.00008 ABSTRACT WITHDRAWN

12:51PM U13.00009 Promising topological surface states with persistent high spin polarization across Dirac point in Bi\textsubscript{2}Te\textsubscript{2}Se and Bi\textsubscript{2}Te\textsubscript{3}Se\textsubscript{2}. KOJI MIYAMOTO, AKIO KIMURA, TAICHI OKUDA, HIROKAZU MIYAHARA, HIROFUMI NAMATAME, MASAKI TANIGUCHI, Hiroshima University, SERGEY EREMEEV, Tomsk State University, EGVUENI CHULKOV, Donostia International Physics Center, OLEG TERESHCHENKO, Novosibirsk State University — Topological insulators (TIs) have attracted a great deal of attention as key materials for spintronics technology. Among the established TIs, Bi\textsubscript{2}X\textsubscript{3} (X=Se, Te) has been mostly studied because of their relatively large energy gap and the simplest topological surface state (TSS) with helical spin texture. However, an absence of the topological natures of TSS below Dirac point (E\textsubscript{D}) has been shown by spin- and angle-resolved photoemission spectroscopy (SARPES) and scanning tunneling spectroscopy under perpendicular magnetic field. It could be a disadvantage for extending its spintronic applications. Recently, one of the ternary tetradymite compounds, Bi\textsubscript{2}Te\textsubscript{2}Se was shown to be a TI by the SARPES measurement. Importantly, a highly bulk resistive feature in this compound has successfully led to the observation of its surface-derived quantum oscillations in the magnetotransport experiment. We have unambiguously clarified the spin feature of TSS in Bi\textsubscript{2}Te\textsubscript{2}Se and Bi\textsubscript{2}Te\textsubscript{3}Se\textsubscript{2} for the first time by our novel SARPES. The markedly high spin polarization of topological surface states has been found to be 77% and is persistent in the wide energy range across E\textsubscript{D} in those compounds. The finding promises to extend the variety of spintronic applications.

1:03PM U13.00010 Low frequency noise in exfoliated Bi\textsubscript{1.5}Sb\textsubscript{1.5}Te\textsubscript{1.7}Se\textsubscript{1.3} field effect devices. MITALI BANERJEE, SEMONTI BHATTACHARYYA, HARIRHAN N, SUJA ELIZABETH, ARINDAM GHOSH, Department of Physics, Indian Institute of Science, Bangalore 560012, DEPARTMENT OF PHYSICS, INDIAN INSTITUTE OF SCIENCE, BANGALORE 560012 TEAM — Topological insulators are a new class of materials which have as emerged as the new paradigm to study the exotic topological phases of matter. Electron transport is studied for field effect devices of Bi\textsubscript{1.5}Sb\textsubscript{1.5}Te\textsubscript{1.7}Se\textsubscript{1.3} thin films, mechanically exfoliated on Si/SiO\textsubscript{2} substrates. The resistivity initially decreases with decreasing temperature indicating metallic-like behavior. However the resistivity shows an upturn below 13K which can be associated with the weak localization effect. The resistivity as a function of gate voltage shows hysteresis at low carrier densities and is independent of different sweep rates of the gate voltages. In addition to resistivity measurements, we have investigated low frequency noise or “1/F” noise as a function of temperature and gate voltage. The magnitude of 1/f noise increases at lower temperatures and with decreasing carrier densities. At lower carrier densities just like resistivity, noise is also saturated indicating long range disorder in the systems due to selenium vacancies. [1] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010) [2] E. Rossi, J. H. Bardarson, M. S. Fuhrer, and S. Das Sarma, Phys. Rev. Lett. 109, 096801 (2012)

1:15PM U13.00011 Scanning tunneling microscopy of topological insulator Bi\textsubscript{2}Te\textsubscript{2}Se, YINGSHUANG FU, TETSUHO HANAGURI, RIKEN Advanced Science Institute, SHUHEI YAMAMOTO, KYUSHIRO IGARASHI, Tokyo Institute of Technology, HIDENORI TAKAGI, RIKEN Advanced Science Institute, University of Tokyo, TAKAO SASAGAWA, Tokyo Institute of Technology — Using scanning tunneling microscopy, we study a prototypical topological insulator Bi\textsubscript{2}Te\textsubscript{2}Se having suppressed bulk carrier density. Landau level states of its topological surface state remarkably exhibit hysteresis behavior, which shift in energy controllably with the limits of ramping bias, forming hysteresis loops thereafter. The observed hysteresis behavior is attributed to the interplay between a tip-induced gating effect and an impurity-generated random charging effect. This provides a new avenue to controlling the topological surface state.

1:27PM U13.00012 Characterization of surface conducting states in Bi\textsubscript{1.5}Sb\textsubscript{0.5}Te\textsubscript{1.7}Se\textsubscript{1.3} topological insulator single crystals, JANGHEE LEE, JOONBUM PARK, JAE-HYEONG LEE, JUN SUNG KIM, HU-JONG LEE, Department of Physics, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea — Topologically protected surface state (TSS) of a topological insulator (TI) can be described in terms of a spin-resolved Dirac band with helical-spin texture. In general, however, as-grown TIs are doped so that the surface conduction can be dominated by the bulk conduction. In this study, we minimized the bulk conduction using high-quality Bi\textsubscript{1.5}Sb\textsubscript{0.5}Te\textsubscript{1.7}Se\textsubscript{1.3} TI single crystals, with the Fermi level lying in the bulk gap without gating. We confirmed that the weak anti-localization (WAL) effect and universal conductance fluctuations in our samples arose from the top and bottom surfaces. By back-gate tuning the WAL characteristics, we identified the TSS conducting characteristics and the coupling between the TSS and the topologically trivial two-dimensional electron gas (2DEG) states that emerged due to the band bending near the surface. The intrinsic small resistivity, which is consistent with the back-gate-voltage dependence of the longitudinal resistance of the TSS. This study provides a highly coherent picture of the surface transport properties of TIs by successfully differentiating the transport of the TSS from those of the bulk conducting state and the topologically trivial 2DEG states.

1:39PM U13.00013 Two Dimensional universal conductance fluctuations in topological insulator Bi\textsubscript{2}Te\textsubscript{2}Se microribbons$, FENGQI SONG, ZHAOGUO LI, BAIGENG WANG, GUANGHOU WANG, Nanjing University — The universal conductance fluctuations (UCFs), one of the most important manifestations of mesoscopic electronic interference, have not yet been demonstrated for the two-dimensional surface state of topological insulators (TIs) to date. Even if one delicately suppresses the bulk conductance of TI crystals, the fluctuation of the bulk conductance still keeps competitive and difficult to be separated from the desired UCFs of the surface carriers. Here we report on the experimental evidence of the UCFs of the two-dimensional surface state in the bulk insulating Bi\textsubscript{2}Te\textsubscript{2}Se nanoribbons. The solely-B\textsubscript{1}l-dependent UCF is achieved and its temperature dependence is investigated. The surface transport is further revealed by weak antilocalizations. Such quantum interference unexpectedly survives through the limited dephasing length of the bulk carriers in the ternary TI crystals. Based on the temperature-dependent scaling behavior, the electron-phonon interaction is addressed as a secondary source of the surface state dephasing. (Scientific Reports, 2, 595 (2012))

3We thank the National Key Projects for Basic Research of China (Grant numbers: 2013CB922103, 2010CB923400, 2011CB922103), the National Natural Science Foundation of China (Grant numbers: 11023002, 11134005, 60825402, 61176088, 11075076),

1:51PM U13.00014 Surface state transport suppression in topological insulators$, ANJAN A. REJINDERS, Y. TIAN, G. POHL, I.D. KIVLICHAN, S.Y. FRANK ZHAO, Y-J. KIM, University of Toronto, S. JIA, R.J. CAVA, Princeton University, D.C. KWOK, N. LEE, S.W. CHEONG, Rutgers University, KENNETH S. BURCH, University of Toronto — An unresolved question in experimental research on topological insulators (TI) is the suppression mechanism of a TI’s surface state transport. While room temperature ARPES studies reveal clear evidence of surface states, their observation in transport measurements is limited to low temperatures. A better understanding of this suppression is of fundamental interest, and crucial for pushing the boundary of device applications towards room-temperature operation. In this talk, we report the temperature dependent optical properties of the topological insulator Bi\textsubscript{2}Te\textsubscript{2}Se (BTS), obtained by infrared spectroscopy and ellipsometry, probing surface and bulk states simultaneously. We see clear evidence of coherent surface state transport at low temperature and find that electron-phonon coupling causes the gradual suppression of surface state transport as temperature rises to 43K. In the bulk, electron-phonon coupling enables the emergence of an indirect band gap transition, which peaks at 43K, and is limited by thermal ionization of the bulk valence band above 43K. For comparison with other resistive TIs, we also discuss the optical properties of BiSb\textsubscript{2}Se\textsubscript{3}.

1Financially supported by NSERC CRSNG, Ontario Research Fund, Canadian Foundation for Innovation, Prins Bernhard Cultuurfonds, NSF
**Thursday, March 21, 2013 11:15AM - 2:15PM**
Session U19 DCMP: Metal-Insulator Transitions II 321 - Rongwei Hu, University of Maryland

**11:15AM U19.00001 MBE synthesis and characterization of charge ordered La$_{1/3}$Sr$_{2/3}$FeO$_3$ thin films**

REBECCA SICHEL-TISSOT, ROBERT DEVLIN, Drexel University, PHILIP RYAN, JONG-WOO KIM, Argonne National Laboratory, ALEX DAGG, University of California, Riverside, STEVEN MAY, Drexel University — La$_{1/3}$Sr$_{2/3}$FeO$_3$ (LSFO) is a transition metal oxide which exhibits strongly correlated electronic behavior. When cooled below 180-190K, an electronic phase transition occurs during which the resistivity abruptly increases. LSFO was deposited on (001) SrTiO$_3$ substrates using molecular beam epitaxy (MBE). The transition temperature $T^* = 183$ K was measured from a sharp increase in the resistivity and confirmed by the appearance of x-ray reflections with wavevectors of $q = n/3$[111]. Oxygen loss from the film over a period of 8 months was observed to have significant effects on the structural and electronic properties, but was shown to be reversible by annealing in oxygen. This work is supported by the Office of Naval Research under grant number N00014-11-1-0664. Work at the Advanced Photon Source is supported by the U.S. Department of Energy (DOE), Office of Basic Energy Sciences under contract DE-AC02-06CH11357.

**2:03PM U19.00005 High-Temperature Andreev Tunneling in the Surface States of a Topological Insulator**

PARISA ZAREAPOUR, ALEX HAYAT, SHU YANG FRANK ZHAO, MICHAEL KRESCHCHUK, ACHINT JAIN, Department of Physics and Institute for Optical Sciences, University of Toronto, ZHJUN XU, ALINA YANC, C.D. GU, CMP&MS Department, Brookhaven National Laboratory, SHUANG JIA, ROBERT CAVA, Department of Chemistry, Princeton University, KENNETH BURCH, Department of Physics and Institute for Optical Sciences, University of Toronto — Topological insulators (TIs) are materials with high spin-orbit coupling that possess conductive helical surface states. In order to study the exotic properties of the TI surface states, it is unfavorable to work with Tls that have a low bulk conductivity and exhibit insulating behavior. Bi2Te2Se has been confirmed to have a high bulk resistivity, and it still shows Shubnikov-de Haas oscillations originating from the two-dimensional surface states. We report the observation of coherent Andreev tunneling into the surface states of Bi2Te2Se in high-temperature superconductor (Bi2Sr2CaCu2O8+δ)/Bi2Te2Se junctions fabricated by mechanical bonding method. The differential conductance measurements will be presented in various temperatures and magnetic fields. The characterization of the zero-bias conductance peak observed, suggests that we are tunneling into the surface states of the TI rather than the bulk states.

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**12:03PM U19.00005 Doping induced metallization of a narrow gap insulator FeGa$_3$**

MONIKA GAMZA, Brookhaven National Laboratory, AKSHAT PURI, Stony Brook University, JAN TOMCZAK, Rutgers University, JIM QUINN, Stony Brook University, MEIGAN ARONSON, Stony Brook University and Brookhaven National Laboratory — Narrow gap semiconductors attract great interest owing to an unusual metallization process which remains poorly understood despite decades of extensive research [1]. Here, we report on the effects of hole doping on properties of a nonmagnetic semiconductor FeGa$_3$ with a band gap of 0.4 eV [2]. By means of electrical resistivity, magnetization and specific heat measurements performed on single crystals grown from gallium flux we have found that a substitution of Mn for Fe in Fe$_{1-x}$Mn$_x$Ga$_3$ (0.005$<x<0.03$) yields an insulating state at high temperatures with residual magnetic moments. With lowering temperature, resistivity deviates from an activation-type behavior and nearly saturates at T$<$100 K. Finally, it drops by as much as two orders of magnitude at temperature of 6 K, indicating a metal-insulator transition. Magnetization measurements did not show magnetic order associated with the transition. When an external magnetic field is applied, the metal-insulator transition moves to lower temperatures and eventually the resistivity returns to the insulating-type behavior in fields higher then 5 Tesla.

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12:15PM U19.00006 Role of long range Coulomb interaction near the disorder driven metal-insulator transition in Ga$_{1-x}$Mn$_x$As, S. MAHMOUDIAN, Florida State University, E. MIRANDA, Univ. of Campinas, V. DOBROSAVLJEVIC, Florida State University — Surprising signatures of interaction effects on disorder-driven localization in Ga$_{1-x}$Mn$_x$As, where visualizing the electronic wave function near the metal-insulator transition revealed a pronounced suppression of the local tunneling density of states (LDOS) and enhanced localization only near the Fermi energy. These features highlight the limitation of the non-interacting picture, and point to the crucial importance of the long-range Coulomb interaction. Here, we implement a theoretical approach based on the recently developed Typical-Medium Theory, the conceptually simplest approach to interaction-localization. We show that the presence of long-range Coulomb interaction leads to the simultaneous opening of a soft pseudogap in both the typical (geometrically averaged) and the average (algebraically averaged) LDOS, as the transition is approached. This result is consistent with the experimentally observed features of the STM spectra, suggesting new experiments that should be performed to fully characterize the quantum critical behavior at the metal-insulator transition.


12:27PM U19.00007 Fitting of Diverging Thermoelectric Power in a Strongly Interacting 2D Electron System of Si-MOSFETs, HYUN-TAK KIM, ETRI in Korea — The diverging-effective mass (DEM) in a metallic system is evidence of strong correlation between fermions in strongly correlated systems. The identification of the DEM still remains to be revealed. The effective mass, $m^* = m_0/(1-\rho^2)$ [1] where $\rho$ is band filling helps clarify the diverging thermoelectric power, $S$, measured in inhomogeneous Si-MOSFET systems [2]. As a carrier density $n_x$ decreases, $S$ increases rapidly. This is regarded as the metal-insulator transition (MIT) near $n_x \approx 79 \times 10^{-14}$ cm$^{-2}$, where $n_x$ is about 0.02% to $n_x \approx 3.4 \times 10^{-14}$ cm$^{-2}$ in Si. This can be solved in assuming that $\rho = n_0/n_x$ increases as $n_x$ decreases. $n_0$ is an excited(doped) carrier density in the semiconductor induced by gate and can also be regarded as a metallic carrier density, that is, $n_c \equiv n_0$ is a metallic, $n_x$ is given as $n_0 = n_x = n_x - n_{0 \text{semicon}}$, where $n_{0 \text{semicon}}$ is a carrier density in a nonmetallic phase. The carrier density measured by Hall effect is the sum of carriers both induced by gate field and generated by MIT. Moreover, a large metallic phase is not possible due to the constant density of states in the field-effect structure after a metallic phase is formed. Thus, increasing $n_x$ indicates increasing $n_{0 \text{semicon}}$; this corresponds to an over-doping to increase inhomogeneity. It’s fitting is given from $S = (\alpha/m^* T/3e)/(1/E_F) = (8\pi T/3h)\left(\alpha m^* e^2/n_x\right) = 0.123.6$ are used. The data $S$ [2] are closely fitted by $m^* [1]$ Physica C 341-348(2000)259. [2] Phys. Rev. Lett. 109 (2012) 096405.

12:39PM U19.00008 Metal-insulator and glass transitions in a 2D electron system in Si MOSFETs with a screened Coulomb interaction$^1$, PING V. LIN, DRAGANA POPOVIČ, Natl. High Magnetic Field Lab., Florida State Univ. — We present a study of conductivity $\sigma$ of a 2D electron system (2DES) in Si MOSFETs with the oxide thickness $d_{ox} = 7$ nm. In the low density regime of interest, the average electron-electron (e-e) separation is larger than $d_{ox}$, so that the e-e interaction is screened by the metallic gate. The carrier density $n_x$ was changed at a high temperature $T \approx 20$ K. The 2DES was then cooled to a desired $T$ with a fixed $n_x$ and $\sigma$ was measured as a function of time $t$. At the lowest $n_x$, in the insulating regime, transport occurs via variable-range hopping. Near the critical density $n_{c}$ on the metallic side of the metal-insulator transition (MIT), the time-averaged $\langle \sigma(t) \rangle$ follows a power-law behavior, giving a reliable extrapolation of $\langle \sigma(n_x, T = 0) \rangle$. The critical exponents are discussed and compared to the case of MIT with long-range Coulomb interactions. The statistical analysis of the fluctuations in $\sigma(t)$ provides evidence for the glassy freezing of electrons for $n_x < n_{c}$ ($n_{c} < n_{c}$) as $T \rightarrow 0$, similar to the results on samples with long-range interactions. The data suggest that interacting droplet models, rather than hierarchical pictures of glassy dynamics, might be more appropriate.

$^1$Supported by NSF DMR-0905843, NHMFL via NSF DMR-0654118, and the State of Florida.

12:51PM U19.00009 Valence Band Character of NiS$_2$-$\text{Se}_x$ using 3p-3d Resonant ARPES, GARAM HAN, YEONGKWAN KIM, YOONYOUNG KOH, BEOMYOUNG KIM, DONGJOON SONG, JUNGJIN SEO, WONSHIK KYUNG, Institute of Physics and Applied Physics, Yonsei university, Korea, KYUNGDONG LEE, Department of Physics, Inha university, Korea, CHANGYOUNG KIM, Institute of Physics and Applied Physics, Yonsei university, Korea — Understanding the strong correlated system is one of the most challenging tasks in condensed matter physics. Especially, the metal insulator transition (MIT) has been one of the major topics recent few decades. NiS$_2$-$\text{Se}_x$ is known as one of famous material which has MIT. The cubic pyrite NiS$_2$ is a charge-transfer (CT) insulator. NiS$_2$ attracts particular interest as it easily forms a solid solution with NiSe$_2$ (NiS$_{1-x}$Se$_x$) which, while being isoelectronic and isostructural to NiS$_2$, is nevertheless a good metal. MIT, induced by Se alloying, is observed at low temperature (T) for $x=0.45$. Perucchi and his collaborators revealed closed relation between MIT and band width through comparison of infrared spectroscopy result and LDA calculation. However, it was only an indirect observation, and is inconsistent with recent proposal that NiS$_{1-x}$Se$_x$ is a CT insulator but an insulator due to the bonding-antibonding splitting in the S - S (Se – Se) dimers. To reveal the true mechanism in the MIT in NiS$_{1-x}$Se$_x$, resonant photoemission experiment is essential. According to competing theories (CT insulator and insulator due to bonding-antibonding splitting), it is expected that the character of the main band that is responsible for the MIT should be different. Therefore, we performed 3p->3d resonant ARPES for various Se doping ($x=0.43$; insulator, $x=0.5$, 0.7, 2.0; metal) and observed a significant change between on- and off-resonances near the MIT. Our experimental result supports that the origin of MIT in NiS$_{1-x}$Se$_x$ is the CT theory rather than the dimer theory.

1:03PM U19.00010 Low temperature conductance spectra of STO at the nanoscale, ALIREZA MOTTAGHIZADEH, QIAN YU, ALEXANDRE ZIMMERS, HERVE AUBIN, Laboratoire de Physique et d’Etudes des Matériaux (LPEM), UMR 8213, ESPCI ParisTech-CNRS-UPMC, 10 Rue Vauquelin, 75005 Paris, France — The electronic properties of transition metal oxide materials depend on the electronic carrier density, which can be tuned with the oxygen stoichiometry. In binary MO$_x$ or ternary perovskite oxide. For this work, metallic electrodes, separated by distances about 100 – 300 nm, are deposited on the surface of a STO crystal and ions migration procedures and current characteristics measurements are done at low temperature, T ~ 260 mK. Upon applying large voltage up to 30 V, oxygen vacancies migration is identified as the apparition of resistance switching events in current-voltage characteristics. Detailed measurements of the junction show that the switching event led to the formation of a nanosized region of highly doped STO, located within the electrodes where the current-voltage characteristics show the presence of the doped-in-gap states. This work was supported by the French ANR grants 10-BLAN-0409-01 and 09-BLAN-0388-01.
1:15PM U19.00011 Crystalline and Magnetic Anisotropy of the 3d Transition-Metal Oxides, ANDREAS SCHRON, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany, CLAUDIA RÖDL, Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France, FRIEDHELM BECHSTEDT, Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — The 3d transition-metal oxides (TMOs) are subject of debate since many decades due to their extraordinary properties, such as the formation of an antiferromagnetic ordering AFM2 below their Néel temperature. Many studies, both experimental and theoretical, focus only on MnO and NiO, where the crystalline anisotropy is solely driven by exchange striction along the unique symmetry axis in the [111] direction and where the magnetic anisotropy is explained in terms of magnetic dipole interactions. In the other TMOs, FeO and CoO, however, orbital magnetization and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy. We present density-functional-theory (DFT) studies including an on-site interaction \( U \) of the crystalline and magnetic anisotropy of the electronic systems with non-collinear spins. The influence of the (semi-)local description of exchange and correlation (XC) by means of the local density approximation (LDA) and generalized gradient approximation (GGA) on the orbital moments in FeO and CoO and the implications on the aforementioned properties is investigated. We discuss the quenching of the orbital magnetization due to the gradient corrections.

1:27PM U19.00012 Spatially resolved dynamic susceptibilities of disordered two dimensional Hubbard model, NANDINI TRIVEDI, OINAM NGANBA MEETEI, The Ohio State University — We predict the existence of an emergent metallic phase in the disordered two dimensional Hubbard model [1] that has recently been confirmed by experiments on 1T-TaS\(_2\) intercalated with Cu. The metallic state has a finite dc conductivity but unusual dynamical properties. We present here a comprehensive analysis of the spatially resolved spin susceptibility, screened charge density, and optical conductivity of the disordered Hubbard model. We develop a new method in which the exact eigenstates from inhomogeneous mean-field theory are used to calculate dynamical susceptibilities within the random phase approximation. By combining the non-perturbative effects of self-consistent mean-field theory with analytical perturbative methods, this approach gives insights about fluctuations near the quantum phase transitions. We make several predictions which can be directly tested in spatially resolved experiments.


1:39PM U19.00013 Dual fermion approach for disordered interacting fermion systems, SHUXIANG YANG, Louisiana State University, PATRICK HAASE, University of Goettingen, HANNA TERLETSKA, Louisiana State University, Brookhaven National Laboratory, ZIYANG MENG, JUANA MORENO, MARK JARRELL, Louisiana State University, THOMAS PRUSCHKE, University of Goettingen — Understanding the combined effect of electron-electron interaction and disorder is one of the crucial questions in condensed matter physics. There is an obvious need of theoretical tools which allow to treat both these effects on equal footing. To study the intricate interplay of these effects, we generalize our recently proposed dual fermion approach to both electron-electron interaction and disorder. Since the constraint imposed on the dual-space Feynman diagrams in the disordered case does not apply to those generated due to interactions, it is essential to treat elastic scattering processes due to the disorder separately from the inelastic scattering processes due to the pure interaction and mixed contributions, I will discuss the resulting diagrammatic formalism and an algorithm for its implementation. The possible applications for the Anderson Falicov-Kimball and the Anderson-Hubbard models are also discussed.

1:51PM U19.00014 Dual fermion method for disordered electronic systems, HANNA TERLETSKA, Brookhaven National Laboratory, SHUXIANG YANG, ZI YANG MENG, JUANA MORENO, MARK JARRELL, Louisiana State University — While the coherent potential approximation (CPA) is the most commonly used theoretical method to study disordered systems, it by construction misses non-local correlations and Anderson localization. We have recently extended the dual fermion approach [1] to disordered non-interacting systems using the replica method, which allows one to include such non-local physics. Our method utilizes an exact transform to the dual variables, and includes inter-site scattering via diagrammatic perturbation theory in dual fermion space, with the CPA being a zeroth-order approximation. Analyzing one-particle quantities we demonstrate good agreement with the CPA and we discuss the resulting diagrammatic formalism and an algorithm for its implementation. The possible applications for the Anderson-Falicov-Kimball and the Anderson-Hubbard models are also discussed.


2:03PM U19.00015 Metal-Insulator Transitions in Crystalline Phase Change Materials, WEI ZHANG, RWTH Aachen, Germany, ALEXANDER THIESS, Forschungszentrum Jülich, Germany, PETER ZALDEN, RWTH Aachen University, Germany, RUDOLF ZELLER, PETER DEDEŘÍCHS, Forschungszentrum Jülich, Germany, JEAN-YVES RATY, University of Liege, Belgium, MATTHIAS WUTTIG, RWTH Aachen University and JARA, Germany, STEFAN BLUGEL, Forschungszentrum Jülich and JARA, Germany, RICCARDO MAZZARELLO, RWTH Aachen University and JARA, Germany — Phase-change materials are capable of undergoing fast and reversible transitions between amorphous and crystalline phase upon heating and have been exploited in data storage applications based on the strong optical/electrical contrast between the two phases. Recently, compelling evidence for an insulator-metal transition (MIT) solely due to disorder has been observed in the crystalline PCM Ge\(_2\)Sb\(_2\)Te\(_5\) (GST) and similar compounds: upon annealing at temperatures \( T \) below 548K, the system exhibits insulating behavior due to Anderson localization; at higher \( T \), it shows metallic behavior. In contrast to the MITs observed in other systems such as P-doped Si, in GST correlation effects do not play a role and the MIT occurs at fixed stoichiometry. In this work, we present a Density Functional Theory study of this effect. We consider a set of very large models of GST containing one to several thousand atoms and different degree of disorder. We identify the microscopic mechanism that localizes the electron wavefunctions near the Fermi energy in the insulating phase: these states are localized inside regions having large vacancy consequent dissolution of these vacancy clusters. These results could help to develop new device based on multiple resistance states.

Thursday, March 21, 2013 11:15AM - 2:15PM — Session U22 DCMP: Optical Properties of Nanowires

324 - Joe Tischler, Naval Research Laboratory
Numerical results are applied to GaAs and CdSe rods. The dissociation at the threshold field. The field dependence of the effects are also investigated as a function of the rod length and the radius of the nano rod. The quantum confinement can increase the fundamental gap in InN nanowires as high as near-ultraviolet energies. We thereby accurately predict the electronic band gaps, effective masses, and band dispersions of these nanostructured materials. We further solve the Bethe-Salpeter equation to predict the optical absorption spectra of InN nanowires as a function of cross-sectional dimension and geometry. We demonstrate that the support of the Australian Research Council is kindly acknowledged.

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12:03PM U22.00005 Stark Effect of Excitons in a Quantum Nano-rod with Parabolic Confinement

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11:51AM U22.00004 Electronic and optical properties of InN nanowires from first principles

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11:27AM U22.00002 Time Resolved Photoluminescence Studies of ZnO and Zn$_2$SnO$_4$ Nanowires for Solar Cells Applications

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11:15AM U22.00001 Exciton Dynamics in Hexagonal InP Nanowires

11:15AM U22.00001 Exciton Dynamics in Hexagonal InP Nanowires

1 This work was supported by DOE/BES under Contract No.DE-AC04-94AL85000.
12:15PM U22.00006 Observation of quantum dots in GaAs/AlGaAs core-multishell nanowire quantum well tubes¹. TENG SHI, HOWARD JACKSON, LEIGH SMITH, University of Cincinnati, JAN YARRISON-RICE, Miami University, CHANGLIN ZHENG, PETER MILLER, JOANNE ETHERIDGE, Monash University, BRYAN WONG, Sandia National Laboratories, QIANG GAO, HARK TAN, CHENNUPATI JAGADISH, Australian National University — We use photocurrent spectroscopy to study the electronic structure of GaAs/Al_{0.5}Ga_{0.5}As core-multishell nanowires (NW) which define 4 nm GaAs quantum well tubes (QWTs) embedded inside AlGaAs barriers wrapped around a central 50 nm GaAs core. HAADF-STEM images of NW cross-sections show a GaAs layer wrapped around the hexagonal facets with some tapering. Numerical calculations of this structure show the ground states are localized at the corners of the hexagonal QWT. Because of the strong quantum confinement, localized states can easily be formed through width or alloy concentration fluctuations. By using a hemispherical solid immersion lens, we are able directly observe such localized quantum dots (QDs) and map the emission of QDs with a spatial resolution of 600 nm in a single NW. Excitation and emission light polarized parallel and perpendicular to the NW long axis show multiple QDs along the NW long axis with ~100 micro-eV emission lines. PLE measurements on single dots reveal excited state transitions between confined light or heavy holes to electrons at or above the AlGaAs conduction band barrier.

¹We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, DOE and the ARC.

12:27PM U22.00007 Photocurrent Spectroscopy of ZB and WZ InP Nanowire Ohmic devices. K. PEMA Surisi, S. PERERA, H.E. JACKSON, L.M. SMITH, University of Cincinnati, OH, J.M. YARRISON-RICE, Miami University, Oxford, OH, S. MAIMAN, Q. GAO, H.H. TAN, C. JAGADISH, Australian National University, Canberra, Australia — We use photocurrent spectroscopy to study InP nanowire Ohmic devices having either zincblende (ZB) or wurtzite (WZ) crystal structures at 10K. Photolithography is used to fabricate Ohmic Ti/Al contact pads separated by 5 μm. Using a tunable Ti-Sapphire laser, photocurrent is measured as a function of bias voltage and excitation energy. At low temperatures (10 K), the ZB device shows strong evidence for excitonic resonance peaks at 1.425eV and 1.539eV relevant to the degenerate heavy and light holes band and the split-off band. The WZ device shows three excitonic peaks at 1.504eV, 1.530eV, and 1.655eV corresponding to the A, B and C valence band energies, respectively. These energies coincide with recent photoluminescence excitation measurements. In some WZ InP nanowire devices, the A, B and C peaks have been observed at 20-30meV higher energies compared with those above, suggesting a possible quantum confinement in the nanowires. The polarization dependence of photocurrent spectra measured from 275nm ZB nanowire and 20nm WZ nanowire shows very good agreement with theoretical absorption of light by nanowires as a function of diameter and photon energy. We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

12:39PM U22.00008 Photocurrent spectroscopy of GaAs/GaP hetero-structured nanowires. P. KUMAR, H.E. JACKSON, L.M. SMITH, University of Cincinnati, OH, USA, J. YARRISON-RICE, Miami University, Oxford, OH, USA, J.H. KANG, Q. GAO, H.H. TAN, C. JAGADISH, The Australian National University, Canberra, ACT 0200, Australia — We study the photocurrent from photoexcited charge carriers in GaAs/GaP axial and radial hetero-structured nanowires (NWs). These NWs are grown using Metal-Organic Chemical Vapor Deposition (MOCVD) in [111]B direction with Au nano-particles as catalysts. As grown axial GaAs/GaP NWs are sonicated in methanol and dispersed on SiO/SiO insulating substrate. Photocurrent images are taken using a Ti-Sapphire laser (775nm-890nm) and a broadly tunable (550-1060 nm) pulsed excitation from a coherent super continuum light source. Spatial imaging of photocurrent at different wavelengths distinguishes the GaP and GaAs regions in these NWs. Peak photocurrent is observed around GaP region for light wavelengths > 458nm whereas peak photocurrent is shift towards GaAs region for light wavelength < 800nm. Photocurrent measurements in GaAs/GaP strained core-shell NWs are in progress.

¹We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

12:51PM U22.00009 Photocurrent spectroscopy of single ZB GaAs and GaAs/AlGaAs core-shell nanowires. BEKELE BADADA, LEIGH SMITH, HOWARD JACKSON, Department of Physics, University of Cincinnati, Ohio 45220-0011, USA, JAN YARRISON-RICE, Department of Physics, Miami University, Oxford, Ohio 45056, USA, TIM BURGESS, CHENNUPATI JAGADISH, Department of Electronic and Materials Engineering, Australian National University, Canberra, ACT, 0200, Australia — We investigate the band structure of single ZB GaAs nanowires and GaAs/Al_{0.5}Ga_{0.5}As core shell nanowires using photocurrent spectroscopy at room and low temperatures. The single nanowire devices were fabricated photolithographically to define Ti (20nm)/Al (300nm) metal contacts on either end of the nanowire. Photocurrent measurements were performed using CW excitation from a tunable CW Ti-Sapphire laser (775nm-890nm) and a broadly tunable (550-960 nm) pulsed excitation from a coherent super continuum photon crystal fiber. At room temperature we observe an Urbach tail near the absorption edge at 1.42 eV for both GaAs and GaAs/Al_{0.5}Ga_{0.5}As core-shell nanowires. In the core shell structure, we also observe the exponential tail from the Al_{0.5}Ga_{0.5}As superimposed on the GaAs absorption in the core. The 2eV onset is consistent with 50%. At low temperature, 10K, similar measurements were performed and a peak is observed near the band edge ~ 1.50-1.51 eV for both bare and core-shell structure for GaAs reflecting the contribution of excitons to the photocurrent.

¹We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

1:03PM U22.00010 Strain-induced piezoelectric field effects on the optical properties of ZnO nanowires. WENHAO GUO, SHUIGANG XU, NING WANG, M.M.T. LOY, SHENGWANG DU, Hong Kong University of Science and Technology — In our work, we report the evidence of piezoelectric effects which modifies the spatial distribution of the photo-generated carriers in bent ZnO nanowires. This piezoelectric effect, together with strain-induced changes of the energy band structure, results in redshift of free excitation photo-luminescence emission in strained ZnO nanowires. The net redshift is only dependent on the strain, independent on the diameter of the nanowire unless the depth of depletion layer is comparable to the size of nanowire. The experimental results obtained by the near-field scanning microscopy agree well with our numerical simulation.

³The work was supported by the Hong Kong Research Grants Council under Project Nos. CityU5/CRF/08, 604009, 603408, and HKUST11/CRF/11G (or HKU5/CRF/11G).

1:15PM U22.00011 Tip-enhanced Raman scattering of an InGaN/GaN quantum well on a single GaN nanorod. EMANUELE POLIANI, MARKUS WAGNER, AXEL HOFFMANN, JANINA MAULTZSCH, Technische Universität Berlin, 10623 Berlin, Germany, JUAN SEBASTIAN REPARAZ, Catalan Institute of Nanotechnology, 08193 Bellaterra, Spain, MARTIN MANDL, WERNER BERGBAUER, MARTIN STRASBURG, Osram Opto Semiconductors GmbH, 93055 Regensburg, Germany — Vertical GaN nanorods with double In0.2Ga0.8N/GaN quantum well were studied by tip-enhanced Raman spectroscopy (TERS). Exploiting the spatial resolution below the diffraction limit, we were able to perform a Raman map of the nanorod top part with 35 nm spatial resolution. Undetectable in the far field, enhanced phonons belonging to InGaN, InN rich regions and GaN were detected and analyzed as Raman shift map. These enhanced spatially resolved phonons revealed an Indium cluster region nucleated at the end of a planar dislocation in the GaN core. The dislocation continues inside the cluster area as an interface between zincblende and wurtzite modification. A narrow localized strain zone was found close to the interface on the zinc blende side surrounding material. On the wurtzite side instead, the Raman map of the GaN surface optical phonon revealed a more extended charge depletion region.
1:27PM U22.00012 Raman Spectroscopy on GaAs/GaP Nanowire Axial Heterostructures1

YUDA WANG, MOHAMMAD MONTAZARI, LEIGH SMITH, HOWARD JACKSON, University of Cincinnati, JAN YARRISON-RICE, Miami University, QIANG GAO, JUNG-HYUN KANG, CHENNIJU JAGADISH, Australian National University — We use Raman scattering to study the spatially-resolved strain and stress in Zinc Blende GaAs/GaP axial heterostructure nanowires at room temperature. The nanowires are grown by Metal-Organic Chemical Vapor Deposition in the [111] direction with Au nanoparticle catalysts. After initial growth of a 6 µm-long GaP wire, a short GaAs segment is grown. Since Raman scattering reflects the phonon energies that are in turn related to the stress, we control the polarization of the incident and scattered light to acquire and resolve the TO1 (Transverse Optical) and TO2 phonon modes of both GaAs and GaP. High spatial resolution Raman scans along the nanowires show that the GaAs/GaP interface is clearly identifiable. Within the GaP section of the wire, GaP TO modes are observed at lower energies compared to bulk GaP since it is under tension, while GaP shell TO modes are at higher energies than bulk GaAs since it is under compression. A strain gradient exists across the interface so the GaP phonon energies shift to lower and GaAs phonon shift to higher energies as one approaches the interface.

1We acknowledge the NSF through DMR-1105362, 1105121 and ECCS-1100489, and the ARC.

1:39PM U22.00013 Anisotropic surface plasma resonance in self-assembled ErSb quantum nanostructures of tunable shape and orientation, DANIEL OUELLETTE, Physics Department, University of California, Santa Barbara, HONG LU, Materials Department, University of California, Santa Barbara, SASCHA PREU, Chair of Applied Physics, Univ. of Erlangen-Nuremberg, Germany, JUSTIN WATTS, BEN ZAKS, MARK SHERWIN, Physics Department and Institute for Terahertz Science and Technology, University of California, Santa Barbara, ARTHUR GOSSARD, Materials Department, University of California, Santa Barbara — Incorporation of erbium during MBE growth of GaSb leads to various self-assembled, semi-metallic ErSb nanostructures. At the lowest concentration, spheres of diameter 4-5 nm are observed. By contrast, at 7-10% Er, ~5 nm diameter nanowires self-align along the <001> growth direction, and at 15-20%, the nanowires align in the growth plane along the <T10> direction. Light polarized along the wires is strongly attenuated over a broad range from THz to near-IR. By contrast, light polarized perpendicular to the wires experiences minimal attenuation apart from a very strong surface plasma resonance at 0.46 eV. Surprisingly, the resonant frequency of the nanospheres is slightly higher than that of the wires, despite the smaller depolarization factor. Motivated by this observation and estimates of the confinement energy, we construct an effective medium theory for the nanostructures which includes a single characteristic intersubband transition. This model provides an excellent description of the IR reflectance and transmission over the whole range of Er concentration, in contrast to a model which excludes the effect of quantum confinement.

1:51PM U22.00014 Continuous frequency multiplication in a strongly driven modulated nanowire1, KATHLEEN HAMILTON, ALEXEY KOVALEV, AMRIT DE, LEONID PRYADKO, University of California, Riverside — High-order harmonic generation in a bulk solid driven by a few-cycle pulsed infrared laser has recently been observed [1]. We consider the possibility of observing an analogous effect using a continuously driven, single-band one-dimensional metal. In the absence of phonon scattering, the quantum efficiency of frequency tripling for such a system can be as high as ~93%. Combining the Floquet quasi-energy spectrum with the Keldysh Green's function technique, we derive the quantum transmission equation for strongly and rapidly driven electrons in the presence of weak scattering by phonons. The power absorbed from the driving field is continuously dissipated by phonon modes, leading to a quasi-equilibrium in the electron distribution. We assume terahertz frequency range, and use the Kronig-Penny model with varying effective mass to establish fundamental limits and modulation periodicity of an InAs/InP nanostructure. Driving such nanostructures could lead to efficient third and higher-harmonic generation. [1] S. Ghimire et al., Nature Physics 7, 138-141 (2011).

2:03PM U22.00015 Generation of core-shell structures and segregation of dopants in Si/SiO2 nanowires, SUNGYUN KIM, JI-SANG PARK, K.J. CHANG, Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 305-701, Republic of Korea — Oxidized Si nanowires (SiNWs) are usually synthesized by subsequent thermal annealing of as-grown SiNWs. It has been observed that B diffusivity is enhanced during thermal annealing in SiNWs, similar to the phenomena called transient enhanced diffusion or oxidation enhanced diffusion in planar Si/SiO2 interfaces. However, previous theoretical studies have been focused on hydrogen or hydroxyl terminated SiNWs. In this work, we generate realistic atomic models for oxidized SiNWs in which crystalline Si core is sheathed by amorphous SiO2 by using a combined approach of classical molecular dynamics simulations with first-principles density functional calculations. For realistic core-shell structures, we investigate the stability and segregation behavior of B and P dopants. A single substitutional B is more stable in the Si core, with a very small energy variation with the radial position of B. On the other hand, B dopants easily segregate to the oxide shell with the aid of Si self-interstitials generated during thermal oxidation. In contrast to B dopants, P dopants prefer to reside in the Si core even in the presence of Si self-interstitials but tend to aggregate in the Si region near the interface, forming nearest-neighbor donor pairs which are electrically inactive.

This research was supported in part by the U.S. Army Research Office under Grant No. W911NF-11-1-0027, and by the NSF under Grant No. 1018953.


11:15AM U30.00001 Criticality in dynamic arrest: Correspondence between glasses and traffic1, DANIEL MIEDEMA, ASTRID DE WIJN, BERNARD NIENHUIS, PETER SCHALL, University of Amsterdam — Dynamic arrest is a general phenomenon across a wide range of dynamic systems including glasses, traffic flow, and dynamics in cells, but the universality of dynamic arrest phenomena remains unclear. We connect the emergence of traffic jams in traffic flow to the dynamic slow down in glasses. A direct correspondence is established by identifying a simple traffic model as a kinetically constrained model. In kinetically constrained models, the formation of glass becomes a (singular) phase transition in the zero temperature limit. Similarly, using the Nagel-Schreckenberg model to simulate traffic flow, we show that the emergence of jammed traffic acquires the signature of a sharp transition in the deterministic limit, corresponding to overcautious driving. We identify a true dynamical critical point marking the onset of coexistence between free flowing and jammed traffic, and demonstrate its analogy to the kinetically constrained glass models.

11:27AM U30.00002 Glass-like dynamics of a struttural colloidal crystal in a disordered potential landscape1, KEVIN APTOWICZ, West Chester University of Pennsylvania, TIM STILL, MATTHEW GRATELA, YE XU, ARJUN YODH, University of Pennsylvania — Disordered solids exhibit a boson peak at low frequencies, where many more modes appear than is expected for sound modes behavior. The origin of the boson peak remains unclear, although two explanations have risen to the forefront: (i) the boson peak is composed of quasi-localized modes arising from peculiarities of the interatomic forces in amorphous materials and (ii) the boson peak is the amorphous equivalent of the Van Hove singularity in crystalline systems. We experimentally explore these two possible explanations by studying a quasi-two-dimensional colloidal structural crystal residing in a disordered potential landscape. The potential landscape is generated by non-uniform heating of the sample. Thermostropic effects lead to a heterogeneous force distribution that is tunable with temperature. With this experimental geometry, we explore the evolution of the density of vibrational states as a function of the strength of the disorder potential landscape.

1This work is funded by DMR-1206231 (K.B.A.), PENN-MRSEC DMR11-20901 (A.G.Y.), NASA NNX08AOOG (A.G.Y.), and DMR12-05463 (A.G.Y.).
11:39 AM U30.00003 Correlations Between Structure, Vibrational Modes and Collective Motion in Dense Attractive 2D Colloidal Packings

Kumar A, Higdon J.J.L, Physics and Astronomy, KEVIN APTOWICZ, West Chester University, Department of Physics and Astronomy — In this work, we investigate the microscopic dynamics of quasi-2D dense attractive colloidal systems. We confine bidisperse polystyrene spheres between glass coverslips in a suspension of water and 2.6-lutidine; as we increase the temperature of the sample into a critical regime, lutidine wets the colloids, creating a strong attractive interaction (>4kT). We specifically study suspensions in the “dense gel” regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of both lower-volume-fraction gel states and higher-volume-fraction glassy states. Despite similarities in local structure, we find several consistent differences in the dynamic and vibrational properties of these two extreme systems. Specifically, we observe a drastic change of the presence of low-frequency modes between the two states. These modes appear to be coupled to collective motion of large groups of particles. By investigating the correlation between these collective motions and local packing structures, we gain further insight into the origins of dynamic heterogeneity in disordered systems.

1This work is supported by funding from NSF grant DMR12-05463 and PENN MRSEC grant DMR11-20901.

11:51 AM U30.00004 Resolving structural modifications of colloidal glasses by combining x-ray scattering and rheology

WAGNER, ERIC M. FURST, University of Delaware — Nonspherical colloidal particles exhibit a variety of equilibrium structures, including colloidal crystals. A central question concerns the relation between the structure and mechanical properties of glasses, but structural changes remain difficult to resolve. We use a novel combination of rheology and x-ray scattering to resolve structural changes in colloidal glasses and link them directly to their mechanical behavior. By combining stress and structure factor measurements, we resolve shear induced changes in the nearest neighbor configuration as a function of applied stress, allowing us to elucidate the structural origin of the genuine shear banding transition of glasses. Our results reveal a coupling between structural parameters and the applied shear that underlies the instability: the non-monotonic behavior of the flow curve is directly mirrored in simple structural measures such as the position, the width, and the height of the nearest neighbor peak of the structure factor. Besides small changes in the nearest neighbor distances, our results underscore the importance of anisotropy in the structure of out of-equilibrium systems, in agreement with structure analysis of jammed and unjammed granular packings.

12:03 PM U30.00005 Free energy transition of sheared colloidal glasses

ZHAO, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Science, JOINT LABORATORY OF POLYMER SCIENCE & MATERIALS, ICCAS — Poly(N-isopropylacrylamide) microgel is adsorbable to the polystyrene microsphere surface. The saturated adsorption concentration of microgel (\(\Phi_{MG}\)) is in a linear relationship with the given concentration of microsphere (\(\Phi_{MG}\)). We specifically study suspensions in the “dense gel” regime, i.e., at a volume fraction high enough that the attractive particles form a spanning cluster, yet just low enough that there exists some structural heterogeneity larger than the individual particle size. We track the particle locations via bright-field video microscopy and analyze the dynamics of both lower-volume-fraction gel states and higher-volume-fraction glassy states. Despite similarities in local structure, we find several consistent differences in the dynamic and vibrational properties of these two extreme systems. Specifically, we observe a drastic change of the presence of low-frequency modes between the two states. These modes appear to be coupled to collective motion of large groups of particles. By investigating the correlation between these collective motions and local packing structures, we gain further insight into the origins of dynamic heterogeneity in disordered systems.

This work is supported by the National Science Foundation (Grant No. CBET-0930549).

12:15 PM U30.00006 Phonon Dispersion and Elastic Properties of Two-Dimensional Soft Particle Colloidal Crystals and Glasses

ZANGAR, DANIEL BONN, PETER SCHALL, University of Amsterdam — Glasses have liquid-like structure, but solid-like properties. An important question concerns the relation between the macroscopic flow behavior and the microscopic structure. However, for atomic glasses, microscopic configurations are prohibitively difficult to visualize due to the small molecular length scales. Here, we use a colloidal glass to directly visualize and analyze particle configurations of quiescent and sheared colloidal glasses. We determine the free volumes of the particles, and relate this free volume distribution directly to the free energy of the glass. This allows us to obtain novel insight into the relation between rigidity/flow and changes in the amorphous structure. We identify a clear change in the free energy at the transition from homogeneous to inhomogenous flow.

12:27 PM U30.00007 Aggregation, Gelation and Glass Transition in Mixed Suspension of Polystyrene Microsphere and Poly(N-isopropyl-acrylamide) Microgel

GUANGCUI YUAN, CHUANZHANG ZHAO, CHARLES C. HAN, Institute of Chemistry, Chinese Academy of Science, JOINT LABORATORY OF POLYMER SCIENCE & MATERIALS, ICCAS TEAM — Poly(N-isopropylacylamide) microgel is adsorbable to the polystyrene microsphere surface. The saturated adsorption concentration of microgel (\(\Phi_{MG}\)) is in a linear relationship with the given concentration of microsphere (\(\Phi_{MG}\)). Depending on the concentration of microgel (\(\Phi_{MG}\)) added into the suspension microspheres, the microgel can induce bridging (\(\Phi_{MG} < \Phi_{MG}^*\)) and depletion (\(\Phi_{MG} > \Phi_{MG}^*\)) effect. With combination of various \(\Phi_{MG}\) and \(\Phi_{MG}^*\) different structures including stable solution, bridging and depletion cluster, bridging and depletion gel, attractive glass and repulsive glass, were obtained. The transitions between these states were investigated by rheology and microscopy. Two-step yielding behavior was observed in attractive glass, which was contributed from bridging bonds of microgels and caging effect of dense microspheres.

1This work is supported by the National Basic Research Program of China (973 Program, 2012CB821503).

12:39 PM U30.00008 Dynamics of concentrated dicolloid particles

MARK M. PANCZYK, NORMAN J. WAGNER, ERIC M. FURST, University of Delaware — Nonspherical colloidal particles exhibit a variety of equilibrium structures, including colloidal crystals. However, with increasing concentration, particle dynamics in these suspensions slow, and the creation of equilibrium close-packed structures may be ultimately inhibited by the presence of a glass transition. For dicolloid particles, dimer particles with asymmetric or symmetric lobes, suspension dynamics have been studied using Stokesian dynamics simulations [1] and mode-coupling theory [2], and the glass transitions have been determined using rheology [3]. In this study, the dynamics of polystyrene dicoloids in water are measured by diffuse wave spectroscopy (DWS) at particle concentrations between 1 and 60 volume percent. Relaxation times of the dicolloid particle suspensions are determined as a function of particle concentration and shape. Strong particle localization occurs at the highest concentrations. The localization lengths measured by DWS are compared to their mode coupling theory predictions.


1This work is supported by the National Science Foundation (Grant No. CBET-0930549).
12:51PM U30.00009 On the Absence of Red Structural Color in Colloidal Glasses. SOFIA MAGIKIRI-ADOU, Department of Physics, Harvard University, Cambridge, MA, USA, JIN-GYU PARK, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA, YOUNG-SEOK KIM, Korea Electronics Technology Institute, S.Korea, GI-RA YI, Department of Polymer Science and Engineering, Sungkyunkwan University, Suwon, Gyunggi 440-746, S.Korea, VINOTHAN N. MANOHARAN, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, USA — When a colloidal glass is illuminated, the short-ranged spatial correlations between neighboring particles can give rise to constructive interference for a particular wavelength. Unlike the structural colors arising from Bragg diffraction in colloidal crystals, the colors of these colloidal glasses are independent of angle due to the disordered, isotropic microstructure. We therefore call them “photonic glasses.” A similar coloration mechanism is found in the feathers of certain birds. However, there are few examples of red photonic glasses either in nature or in colloidal systems. Using scattering theory, we show that the absence of red photonic glasses can be explained by the wavelength-dependence of the single-particle scattering cross-section, which can override the interference conditions set by the structure. We propose ways to overcome this obstacle, and we report on experimental methods to make non-iridescent, structural red color.

1:03PM U30.00010 Structure/dynamics coupling in suspensions of microgel particles on their approach to the glass. A. FERNANDEZ-NIEVES, J. CLARA-RAHOLA, Georgia Tech, P.N. SEGRE, Oxford College, A.B. SOUTH, L.A. LYON, Georgia Tech — We measure the structure factor, \(S(q)\), and the q-dependent diffusion coefficient, \(D(q)\), of dense suspensions of pNIPAm microgel particles. We do this at different temperatures, and hence different swelling degrees, at constant generalized volume fraction, and find dramatic changes in behavior. While for certain temperatures, \(1/D(q)\) follows the behavior of \(S(q)\), at other temperatures the behavior of these two quantities completely decouples. Interestingly, this behavior correlates with fragility: Structure/dynamics decoupling is observed for suspensions resembling strong glass formation.

1:15PM U30.00011 Evolution of dynamical facilitation approaching the glass transition. RAPHAEL CANDELER, LIP - UPMC, ASAPH WIDMER-COOPER, School of Chemistry, University of Sydney, DAVID REICHMAN, Columbia University, GIULIO BIROLI, IPHT - CEA, OLIVIER DAUCHOT, EC2M - ESPCI — We investigate the relaxation dynamics of simulated dense bidimensional supercooled liquids composed of softly interacting particles. We show that the long time scale dynamical heterogeneities result from the aggregation of several elementary relaxation events, themselves formed by collective leaps. By varying the temperature, we show that for low temperatures there is a growing excess of probability to find cage jumps that are close both in space and time, and that the network of spatio-temporal facilitation evolves towards a collection of clearly defined large events. We discuss these observations and specifically the relative importance of facilitation when approaching the glass transition.

1:27PM U30.00012 Aging in dense colloids through the growth and breakup of strongly correlated clusters1. S.KANDA VIVEK, STEFAN BOETTCHER, Physics Dept., Emory University, PAOLO SIBANI, University of Southern Denmark — Colloidal systems exhibit glassy behaviour under the right physical conditions that can be observed through mean square displacements in experiments. Our phenomenological model of aging in colloids is based on the growth and breakup of strongly correlated clusters, which introduces dynamical heterogeneity in the limit of large particle number. Different colloidal density regimes correspond to different probabilities. The mean square displacements measured in this system for a low density colloid shows a linear increase in time and shows a linear increase in log-time for high densities, which matches experimental data. The cluster breakup rate was measured to be uniform in time for low densities and \(\propto 1/t\) in the aging regime, which provides a clock for the slowing down of the dynamics. Measurements of the four-point susceptibility \(\chi_4\) show a peak indicating the response to a growing lengthscale that satisfies a scaling relation with sample age, \(t_w\). For larger \(t_w\), \(\chi_4\) peaks higher, and decays more slowly with time, which we hypothesize is due to the dominance of relatively stable large clusters.

1Supported through NSF-DMR grant #1207431.

1:39PM U30.00013 Pinning Susceptibility at the Jamming Transition1. AMY GRAVES, ELLIOT PADGETT, Swarthmore College, CARL GOODRICH, ANDREA LIU, University of Pennsylvania — Jamming in the presence of fixed or pinned obstacles, representing quenched disorder, is a situation of both practical and theoretical interest. We study the jamming of soft, bidisperse discs in which a subset of discs are pinned while the remaining particles equilibrate around them at a given volume fraction. The obstacles provide a supporting structure for the jammed configuration which not only lowers the jamming threshold, \(\phi_j\), but affects the coordination number and other parameters of interest as the critical point is approached. In the limit of low obstacle density, one can calculate a pinning susceptibility \(\chi_p\), analogous to the magnetic susceptibility, with obstacle density playing the role of the magnetic field. The pinning susceptibility is thus expected to diverge in the thermodynamic limit as \(\chi_p \propto |\phi - \phi_j|^{-\gamma_p}\). Finite-size scaling calculations allow us to confirm this and calculate the critical exponent, \(\gamma_p\).

1Acknowledgement is made to the Donors of the Petroleum Research Fund administered by the American Chemical Society, Swarthmore College’s Eugene M. Lang Faculty Fellowship, NSF grant DMR-1062638 and DOE grant DE-FG02-05ER46199.

1:51PM U30.00014 Probing the depinning transition: contrasting lattice and continuum models. YAN-JIUN CHEN, LASSP, Cornell University, STEFANO ZAPPERI, IENI-CNR, Milano,Italy, and ISI in Torino, Italy. JAMES P. SETHNA, LASSP, Cornell University — Models of depinning are used to study a wide variety of disordered systems where there are interfaces with jerky motion, including magnetic domain wall motion, fluid imbibition, and superconductor vortex lines. Analytic results from field theories are written in continuous time and space coordinates; but efficient algorithms are often done with cellular automata (CA). The equivalence of CA rules with the continuum models were justified by the appearance of a cusp in the disorder correlator after a finite-number of RG steps, especially for avalanche behavior that involve many degrees of freedom. However, in between this abrupt behavior, there exist slower dynamics where the avalanche almost stops, involving fewer degrees of freedom, and these regions may alter the scaling, as seen in recent studies of plastic deformation in crystals and crackling noise in glasses. Also, in our simulations, we find that discretization may introduce unwanted effects or relevant perturbations, such as a broken rotational symmetry. We compare and contrast results of the spatial and temporal structure of depinning from lattice and continuum simulations, and also provide complete functional forms to describe crossovers between different model classes.

2:03PM U30.00015 Dynamical Instabilities of a Brownian Particle in Weak Adhesion. DEEPAK KUMAR, SHANKAR GHOSH, SHOBO BHATTACHARYA, Tata Institute of Fundamental Research, DEPARTMENT OF CONDENSED MATTER PHYSICS AND MATERIALS SCIENCE TEAM — Dynamical processes involved in weak adhesion are explored through Brownian colloidal silica particle detaching from, and reattaching to, a glass substrate immersed in a fluid in the presence of an externally applied force. Micro-rheology, video-microscopy and Nyquist noise measurements reveal both stochastic and deterministic dynamics of the process. When analyzed in terms of the viscoelastic response of the stress coupling medium between the objects, the unsticking instability shows remarkable similarities with yielding and fracture-mechanics of macro-scale solids. The restricting dynamics demonstrates stochastic instabilities through a spatio-temporally punctuated descent of the particle down an energy landscape with a hierarchy of metastable minima.
11:15AM U36.00001 Fermiology and Superconductivity of LaNiGa$_2$\textsuperscript{1} — DAVID J. SINGH, Oak Ridge National Laboratory — LaNiGa$_2$ has been identified as a possible centrosymmetric triplet superconductor based on observations of time reversal symmetry breaking in $\mu$SR experiments. Here we report calculations of the Fermiology and related properties. In spite of the seemingly layered crystal structure, the Fermi surface has several large sheets and is only moderately anisotropic, so that the material is best described as a three dimensional metal. These include sections that are open in the in-plane direction as well as a section that approaches the zone center. The density of states is high and primarily derived from Ga $p$ states, which hybridize with Ni $d$ states. Comparing with experimental specific heat data, we infer a superconducting $\lambda \leq 0.55$, which implies that this is a weak to intermediate coupling material. Ni occurs in a nominal $d^{10}$ configuration in this material, which places the compound far from magnetism. The implication is that this is most likely a standard electron phonon mediated s-wave superconductor.

\textsuperscript{1}Work supported by DOE, BES, Materials Sciences and Engineering Division.

11:27AM U36.00002 Electron-phonon coupling in potassium-doped superconducting picene — MICHELE CASULA, MATTEO CALANDRA, FRANCESCO MAURI, CNRS and Université P. et M. Curie — We explore the properties of electron-phonon couplings in K$_n$Picene, in the framework of density functional theory (DFT). By exploiting the maximally localized Wannier function formalism, we identify the contribution of the intra- and intermolecular phonon vibrations and the role of local and non-local electronic states in determining the electron-phonon coupling. Despite the molecular nature of the crystal, we find that the purely molecular contributions account for only 20% of the total electron-phonon interaction $\lambda$. In particular, the Holstein-like contribution to $\lambda$ are four times smaller than those computed for an isolated neutral molecule, as they are strongly screened by the metallic bands of the doped crystal. The major contribution (80%) to $\lambda$ in K$_n$Picene comes from non-local couplings due to phonon modulated hopings. We show that the crystal geometry together with the molecular picene structure leads to a strong 1D spatial anisotropy of the non-local couplings. Finally, we propose a lattice model of the electron-phonon couplings in K$_n$Picene that gives 90% of the $\lambda$ obtained in first principles calculations [1].


11:39AM U36.00003 First-principles study of cobalt pnictide SrCo$_2$N$_2$\textsuperscript{3} — ANDREW O’HARA, ALEXANDER DEMKOV, The University of Texas at Austin — With the recent discovery of high temperature superconductivity in BaFe$_2$As$_2$, there has been renewed interest in other members of the AT$_2$X$_2$ family (A = alkaline earth element or lanthanide, T = transition metal, X = an element of groups IIIB-VIB) and in particle isovalent members of the 122 family. In this work, we describe a hypothetical cobalt pnictide, SrCo$_2$N$_2$, using density functional theory (DFT) in the local density approximation (LDA) with a Hubbard U correction. In this work, we determine both the lattice and chemical stability of SrCo$_2$N$_2$ as well as explore how the substitutions affect the electronic and magnetic properties in comparison to BaFe$_2$As$_2$ and 122 rare-earth cobalt phosphides.

11:51AM U36.00004 Dynamical Jahn-Teller effect in Cs$_3$C$_{60}$ superconductors — LIVIU CHIBOTARU, NAOYA IWAHARA, None — The Cs$_3$C$_{60}$ shows a superconducting critical temperature of 38K which is one of the highest among phonon-mediated superconductors. Recent infrared spectroscopy data of insulating Cs$_3$C$_{60}$ apparently support the presence of Jahn-Teller dynamics in this fulleride [1]. To check this possibility, we have performed the DFT calculations of vibronic constants and multiplet splitting parameters, and have calculated from the first principles the spectrum of low-lying vibronic states on C$_{60}^+$ sites by diagonalizing the full vibronic Hamiltonian in a large vibrational basis. The splitting of the $t_{1u}^1$ shell into degenerate multiplets and their vibronic mixing has been fully taken into account, as well as the effect of the environment on the local vibrations. The results show that in the insulating phase an unhindered dynamical Jahn-Teller effect takes place at each C$_{60}^+$ site. Using Gutzwiller approach in combination with LDA band structure, we demonstrate that the Jahn-Teller instability also persists in the metallic phase for a wide range of values of intrastate repulsion energy ($U$).


12:03PM U36.00005 Repulsive interaction helps superconductivity in fullerides — SATOSHI YAMAZAKI, YOSHIO KURAMOTO, Tohoku University — Alkali metal (A) doped fullerenes (A$_x$C$_{60}$) show not only superconductivity (SC) with high transition temperature Tc up to about 40K, but also antiferromagnetism (AF) with $T_N \approx 25K$. In this work, we propose a lattice model of the electron-phonon couplings in K$_x$C$_{60}$ superconductors, which hybridizes with Ni $d$ states. Comparing with experimental specific heat data, we infer a superconducting $\lambda \leq 0.55$, which implies that this is a weak to intermediate coupling material. Ni occurs in a nominal $d^{10}$ configuration in this material, which places the compound far from magnetism. The implication is that this is most likely a standard electron phonon mediated s-wave superconductor.

12:15PM U36.00006 Phonon Vibrations and Superconductivity of a Bi-based Superconductor — JOOSEOP LEE, University of Virginia, MATTHEW STONE, Oak Ridge National Laboratory, TANER YILDIRM, NIST Center for Neutron Research, ASHIFA HUSSIN, GEORGE EKEDAL, Oak Ridge National Laboratory, YOSHIKAZU MIZUGUCHI, Tokyo Metropolitan University, SEUNGHUN LEE, University of Virginia, UNIVERSITY OF VIRGINIA TEAM, OAK RIDGE NATIONAL LABORATORY TEAM, NIST CENTER FOR NEUTRON RESEARCH TEAM, TOKYO METROPOLITAN TEAM — Elastic and Inelastic neutron scattering experiments have been carried out on polycrystalline samples of the newly discovered layered superconductor LaO$_{0.5}$F$_{0.5}$BiS$_2$, and its nonsuperconducting parent compound LaOBiS$_2$ to determine their crystal structures and lattice vibrational modes. The Bragg peaks from the superconducting sample shows large broadening in width in the powder diffraction pattern. For the lattice vibrations, significant difference was observed upon $F$ doping. Using the density functional perturbation theory, we identified all phonon modes, and showed the major change in the phonon spectrum comes mainly from the change in the Oxygen mode. Even though strong electron phonon coupling constant was estimated, no significant difference in the phonon spectrum from BiS$_2$ superconducting layer was found above and below Tc.

12:27PM U36.00007 Intercalant dependent superconducting graphite compounds studies on alkali metal intercalated graphite compounds\textsuperscript{1} — WONSHIK KYUNG, YEONGKWAN KIM, GARAM HAN, CHOONSHIK LEEM, CHUL KIM, Yonsei University, Korea, YEONGWOOK KIM, JUNSUNG KIM, Postech, Korea, CHANGYOUNG KIM, Yonsei University, Korea, YONSEI UNIVERSITY TEAM, POSTECH COLLABORATION — We present electronic structure studies on various alkali-metal intercalated graphite compounds (GIC) using angle-resolved photoemission spectroscopy (ARPES). There are two competing theories on where the superconductivity occurs in this material; intercalant metal or charge doped graphene layer. To elucidate this issue, we measured electron doping amount of each alkali-metal intercalated GICs. In addition, there are some mysterious problems that can’t be explained with current theories.

\textsuperscript{1}Superconducting graphite intercalation compounds studies with ARPES
12:39PM U36.00008 Strong Variations of Density of States and Anomalous Isotope Effect in Low and High Tc Superconductors, GUANG-LIN ZHAO, Southern University and A&M College — In this work, first-principles density functional theory (DFT) calculations of electronic structures are integrated into the fundamental formalism of many-body physics for superconductivity in Zr, Nb, Sn, and YBa2Cu3O7. It is shown that the electronic structures of the transition metals and compounds such as Zr, Nb, Sn, and YBa2Cu3O7 are very complex. The electronic densities of states around their Fermi levels possess sharp variations that have a large contribution to the anomalous isotope effect in these superconductors. The work was funded in part by NSF LASIGMA Project (Award No. EPS-1003897, NSF2010-15-RII-SUB), AFOSR (FA9550-09-1-0367), and NSF project CBET-0754821.

12:51PM U36.00009 Charge density wave transport in heterogeneously doped NbSe3 single crystals by masked ion (B+, Li+) implantation, KALYAN SASMAL, ASANGA WIJESINGHE, DHARSHANA WIJESUNDERA, Department of Physics and TCSUH, University of Houston, Houston, TX 77204, USA, ZHONGJIA TANG, ARNOLD GULOY, Department of Chemistry and TCSUH, University of Houston, Houston, TX 77204, USA, WEI-KAN CHU, JOHN H. MILLER, Department of Physics and TCSUH, University of Houston, Houston, TX 77204, USA, ION BEAM LAB DEPARTMENT OF PHYSICS.UH COLLABORATION, DEPARTMENT OF CHEMISTRY. UH COLLABORATION — Charge-density wave is competing electron spectrum instability of superconductivity (SC). CDW transport vs. SC with boundary between CDWs and SC are well known examples of correlated transport of macroscopic numbers of electrons.CDW superconductors include layered dichalcogenides, NbSe3. On selective area medium energy ion (B+, Li+) implantation was used to create irradiated/unmodified/irradiated CDW heterostructures with well-defined interfaces on single NbSe3 crystal. The effects of impurities go beyond simply increasing CDW pinning (J.P.McCarten et.al J.Phys.IV France 9,1999). The dV/dI vs. bias at several temperatures, and zero-bias resistance vs. temperature, where two voltage contacts straddle the interface (near the boundary between B+/Li+/im implanted and unimplanted regions) are well studied. Injected charge B+/Li+ is a non-isoelectronic impurity. The results of ongoing investigations of similar studies of boron- and lithium-doped NbSe3 will be discussed.

1:03PM U36.00010 A Time-Domain Susceptibility Model for a BCS Superconductor in FDTD Calculations1, G.L. CARR, XIAOXIANG XI, Photon Sciences, Brookhaven National Laboratory. - COLLABORATION — We have developed a simple time-domain electric susceptibility model for a BCS type superconductor, valid for the spectral range spanning the optical energy gap frequency \(\hbar\omega >> \Delta\) and \(\hbar\omega < \Delta\). The model has been derived for the thin film of NbN on a substrate, and compare with both conventional frequency domain calculations as well as actual experimental results.

1:15PM U36.00011 Influence of the interplay between de Gennes boundary conditions and cubicity of Ginzburg-Landau equation on the properties of superconductors1, OLEG OLENSKI, King Abdullah Institute for Nanotechnology, King Saud University — Solutions of the Ginzburg-Landau (GL) equation for the film subjected to the de Gennes boundary conditions (BCs) with extrapolation length \(\lambda\) are analyzed with emphasis on the interaction between \(\lambda\) and the coefficient \(\beta\) of the cubic GL term and its influence on the temperature \(T\) of the strip. Very substantial role is played also by the carrier density \(n\). Physical interpretation is based on the \(n\)-dependent effective potential \(V_{eff}(r)\) created by the nonlinear term and its influence on the lowest eigenvalue of the corresponding Schrödinger equation. For the large cubicities, the temperature \(T\) becomes \(\lambda\) independent linearly decreasing function of the growing \(\beta\) since in this limit the BCs can not alter very strong \(V_{eff}\). The temperature increase produced in the linear GL regime by the negative de Gennes distance is wiped out by the growing cubicity. In this case, the decreasing \(T\) passes through its bulk value \(T_c\) at the unique density \(n^{(1)}\) only, and the corresponding \(\Delta_{T=T_c}\) is an analytical function of \(\beta\). For the large cubicities, the concentration \(n^{(1)}\) transforms into the density of the bulk sample. Other analytical asymptotics are analyzed too.

1:27PM U36.00012 Numerical study of the magnetic and pair binding properties in aromatic hydrocarbon superconductors, ZHONGBING HUANG, Department of Physics, Hubei University, CHAO ZHANG, HAIQING LIN, Beijing Computational Science Research Center — We performed a systematic numerical study of the magnetic and pair binding properties in recently discovered aromatic hydrocarbon superconductors, by using exact diagonalization and quantum Monte Carlo methods. The \(\pi\)-electrons on the carbon atoms of a single molecule are modelled by the one-orbital Hubbard model, which takes into account the energy difference between carbon atoms with and without hydrogen bonds. Our results show that the spin polarized ground state is realized for charged molecules in the physical parameter region. This provides a reasonable explanation of local spins observed in experiments. In alkali-metal-doped picene and phenanthrene, the pairing binding energy is always negative for different electron doping densities, suggesting that electron correlation has no contribution to the formation of Cooper pairs. However, a positive pair binding energy for the charged dibenzopentacene molecule with one or three added electrons indicates that electron correlation may produce an effective attraction between electrons.

iiiSupported by the U.S. Dep’t. of Energy under contract DE-AC02-98CH10886 at Brookhaven Nat’l Lab

This work was supported in part by NPST Program by King Saud University Project No. 11-BIO1947-02.

1:27PM U36.00012 Numerical study of the magnetic and pair binding properties in aromatic hydrocarbon superconductors1, ZHONGBING HUANG, Department of Physics, Hubei University, CHAO ZHANG, HAIQING LIN, Beijing Computational Science Research Center — We performed a systematic numerical study of the magnetic and pair binding properties in recently discovered aromatic hydrocarbon superconductors, by using exact diagonalization and quantum Monte Carlo methods. The \(\pi\)-electrons on the carbon atoms of a single molecule are modelled by the one-orbital Hubbard model, which takes into account the energy difference between carbon atoms with and without hydrogen bonds. Our results show that the spin polarized ground state is realized for charged molecules in the physical parameter region. This provides a reasonable explanation of local spins observed in experiments. In alkali-metal-doped picene and phenanthrene, the pairing binding energy is always negative for different electron doping densities, suggesting that electron correlation has no contribution to the formation of Cooper pairs. However, a positive pair binding energy for the charged dibenzopentacene molecule with one or three added electrons indicates that electron correlation may produce an effective attraction between electrons.

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This work was supported by NSFC under Grants Nos. 11174072 and 91221103.

Thursday, March 21, 2013 11:15AM - 2:03PM

11:15AM U39.00001 Statistical Mechanics of Nanoscale Metallic Materials Based on Thermodynamic Availability, ROBERT CAMMARATA, Johns Hopkins University — When characterizing the equilibrium behavior of small metallic systems, capillary effects can strongly influence the thermal behavior and need to be taken into account in a complete thermodynamic analysis. Although a variety of approaches have been offered to incorporate these effects, they sometimes invoke certain intensive thermodynamic quantities (e.g., chemical potentials) that are not well-defined when dealing with a physically and/or chemically inhomogeneous interfacial region. It has been proposed that many of these difficulties can be resolved by employing the thermodynamic availability function rather than the conventional free energy potentials [R.C. Cammarata, Phil Mag. 88, 927 (2008); R.C. Cammarata, Sol. State Phys. 61, 1 (2009)]. When applied to statistical mechanical calculations, capillary effects on nanoscale system behavior can be obtained in a natural and rigorous way. This procedure will be briefly reviewed and then applied to nanoscale metallic fluid and solid systems. Important issues contrasting the thermodynamic differences between fluid and solid surfaces and how they need to be included in order to obtain physically meaningful results will be discussed. Applications to gas adsorption and nucleation will be presented.
11:27AM U39.00002 Grain Rotation and Growth in Nanocrystalline Silver and Silver/Copper Alloys, MICHAEL CHANDROSS, SHENGFENG CHENG, Sandia National Laboratories — Grain rotation and growth play important roles in nanotribology and the plastic deformation of nanocrystalline metals and alloys. It is difficult, however, to study these processes with full atomistic detail experimentally. We used molecular dynamics simulations to investigate the grain rotation, coalescence, and growth in pure silver and silver/copper alloys after imposing various modes of deformation, including stretch, compression, and shear. Our results show that the degree of grain rotation and growth in pure silver depends on the state of stress in the sample and is most significant under shear deformation, where very large grains are observed after substantial shear. However, in silver/copper alloys, almost no grain rotation was found even under strong shear. The presence of atoms with different lattice constants in alloys stabilizes the grain boundaries and makes grain coalescence less energetically favorable. The implications of these results on nanotribology of pure metals and alloys are discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

11:39AM U39.00003 Temperature-driven Phase Transformation in Y₃Co: Neutron Scattering and DFT Studies, A. PODLESNYAK, G. EHLERS, H. CAO, M. MATSUDA, Neutron Sciences Directorate, ORNL, Oak Ridge, TN 37831, USA. M. FRONTZEK, O. ZAHARKO, Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232, Switzerland, V.A. KAZANTSEV, A.F. GUBKIN, N.V. BARANOV, Institute for Metal Physics RAS, 620041 Ekaterinburg, Russia — The effects of a crystal structure deformation due to subtle atomic displacements have attracted much attention because they can result in colossal changes of the electronic and magnetic properties of solids. The R₃Co binary intermetallic systems exhibit a number of complicated phenomena, including field-induced magnetic phase transitions (R=Er, Ho, Tb), giant magnetoresistance (R=Dy), a substantial magnetocaloric effect (R=Gd) and superconductivity (R=La). Contrary to previous studies that defined the ground state crystal structure of the entire R₃Co series as orthorhombic Pnma, we find that Y₃Co undergoes a structural phase transition upon cooling around Tc 160K. Density functional theory calculations reveal a dynamical instability of the Pnma structure of Y₃Co. Employing inelastic neutron scattering measurements we find a strong damping of the [00l] acoustic phonon mode below the critical temperature Tc. We suggest that some other members of the R₃Co series (or even all of them) have ground state crystal structure symmetry lower than reported Pnma. This raises a question about the true magnetic structures and hence the influence of magnetic properties of the entire R₃Co series.

11:51AM U39.00004 Optical Absorption Spectrum of Gold from First Principles, JAMAL MUSTAFA, University of California at Berkeley, Lawrence Berkeley National Lab, EMMANOUIL KIOUKAKIS, University of Michigan, STEVEN LOUIE, University of California at Berkeley, Lawrence Berkeley National Lab — Phonon-assisted optical absorption is an important optical process in metals for photons in the visible part of the spectrum. Developments in first-principles computational methods have enabled the calculation of phonon-mediated optical absorption spectra of materials. The use of Maximally Localized Wannier Functions enables the interpolation of the GW quasiparticle band structure, along with the optical and electron-phonon coupling matrix elements, to very fine meshes in the Brillouin zone, which are needed for the calculation of the phonon-assisted absorption coefficient. We present calculations on gold that include the quasiparticle band structure and lifetimes, phonon dispersion, Wannier functions, and the phonon-assisted absorption spectrum. Since indirect absorption is a second-order process, the lifetime of the virtual intermediate state is of central importance. The results are compared to experimentally determined optical constants.

12:03PM U39.00005 Less than perfect C_{2v} symmetry: loss of mirror plane symmetry in angle-resolved photoemission, THOMAS SCOTT, University of Nebraska, Lincoln, KEISUKE FUKUTANI, Department of Physics, University of Nebraska, Lincoln, 68588, USA. HIROKAZU HAYASHI, Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan. TULA PAUDEL, Department of Physics, University of Nebraska, Lincoln, 68588, USA. EIKE SCHWIER, Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima 739-0046, Japan. TAIKI HORIKE, YORITO NAGATA, Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan. JIAN JIANG, HIDEAKI IWASAWA, KENYA SHIMADA, Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima 739-0046, Japan. EVGENY TSYMBAL, Department of Physics, University of Nebraska, Lincoln, 68588, USA. YAROSLAV LOSOVYJ, Department of Chemistry, Indiana University, E.Kirkwood Ave Bloomington, IN 47405, PETER DOWBEN, Department of Physics, University of Nebraska, Lincoln, 68588, USA. — The effects of lack of in-plane C_{2v} invariance of the crystal on the angle-resolved photoemission spectra are investigated for Mo(112). The results indicate that, for Mo(112), the absence of C_{2v} symmetry gives rise to noticeable asymmetry in the ARPES band mapping along the <1 1 1>-direction. The apparent differences in the experimental band structure in +k versus -k wave vectors can be understood quantitatively in terms of the symmetries in the electronic bulk band structure, photoelectron diffraction as well as the initial state contribution to the photoemission matrix elements.

12:15PM U39.00006 Prediction of dislocation junction strength in hexagonal close-packed crystals, CHI-CHIN WU, PETER CHUNG, Army Research Laboratory, COMPUTATIONAL MATERIALS SCIENCE RESEARCH TEAM — Determination of dislocation junction strengths in hcp crystals is important in order to understand and control the fundamental mechanisms in plastic deformation in new lightweight metals and structures. The many factors that may be involved, such as combinations of available slip systems, native material properties, and local morphology due to growth conditions, make systematic investigations via combinational experimental approaches challenging. Utilizing discrete dislocation (DD) simulations, we determine yield surfaces comprised by loci of critical configurations in an angle-resolved photoemission measurements on Mo(112). The results indicate that, for Mo(112), the absence of C_{2v} symmetry gives rise to noticeable asymmetry in the ARPES band mapping along the <1 1 1>-direction. The apparent differences in the experimental band structure in +k versus -k wave vectors can be understood quantitatively in terms of the symmetries in the electronic bulk band structure, photoelectron diffraction as well as the initial state contribution to the photoemission matrix elements.

12:27PM U39.00007 Phonon Engineering in Metals from First Principles, NICHOLAS LANZILLO, J. THOMAS, E.B. WATSON, M. WASHINGTON, SAROJ K. NAYAK, Rensselaer Polytechnic Institute — The electron-phonon interaction in metallic systems controls the electronic transport properties, including both electrical and thermal resistivity. The effect of compressive strain on the electron-phonon interaction in metals is investigated using first-principles density functional theory, and we propose various ways to “engineer” this interaction for various technological applications. In particular, we show that by applying compressive strain on the FCC crystals of Al, Cu, Ag and Au, the net electron-phonon scattering rate decreases and likewise the electrical resistivity decreases with increasing pressure. This trend is corroborated by experimental measurements of the resistance of a 0.5 mm diameter high-purity Al wire pressurized up to 2 GPa in a solid-media pressure apparatus at room temperature. The rate of the decrease in electrical resistivity as a function of pressure as determined by experiment is matched by the rate predicted by theory. Our simulations show that Al nanowires have the same response to strain as the bulk crystal; the net electron-phonon scattering can be reduced through compressive strain. Modifying the electron-phonon interaction in metallic structures shows great promise for future nano-electronic devices.
Density-functional study of U-TRU-Zr and U-TRU-Mo alloys. ALEXANDER LANDA, PER SODERLIND, PATRICE TURCHI, Lawrence Livermore National Laboratory — The U-Zr and U-Mo alloys proved to be very promising fuels for liquid metal fast breeder reactors. The optimal composition of these alloys is determined from the condition that the fuel could remain stable in the bcc phase ($\gamma$-U) in the temperature range of stability of $\alpha$-U phase. In other words, both Zr and Mo play a role of "$\gamma$-stabilizers" helping to keep U in the metastable bcc phase upon cooling. In the present study we perform KKR-ASA-CPA and EMTO-CPA calculations of the ground state properties of $\gamma$-U-Zr and $\gamma$-U-Mo alloys and compare their heats of formation with CALPHAD assessments. Though the U-Zr and U-Mo alloys can be used as nuclear fuels, a fast rector operation on a closed fuel cycle will, due to the nuclear reactions, contain significant amount of TRU elements (Np, Pu, and Am). Above mentioned density-functional theory techniques are extended to study ground-state properties of the bcc-based X-Zr and X-Mo ($X = Np, Pu, Am$) solid solutions. We discuss how the heat of formation correlates with the charge transfer between the alloy components, and how magnetism influences the deviation from Vegard’s law for the equilibrium formation correlates with the charge transfer between the alloy components, and how magnetism influences the deviation from Vegard’s law for the equilibrium.

Thermal properties of UO$_2$ single crystal. K. GOFRYK, S. DU, A.D. ANDERSSON, C.R. STANEK, R. SCHULZE, D. SAFARIK, B. MIHAILA, J.C. LASHLEY, J.L. SMITH, Los Alamos National Laboratory — For decades UO$_2$ has been the most widely studied actinide oxide because of its technological importance as fuel material for nuclear reactors. Therefore there is a large interest in understanding its thermal, transport and thermodynamic properties. We present recent experimental results for the thermal conductivity and thermal expansion of high quality UO$_2$ single crystal, obtained for different crystallographic directions, and compare with results of molecular dynamics simulations. We will discuss the implications of this study.

Imaging electronic hot spots in the spectral function of the actinide UCoGa$_5$. MATTHIAS J. GRAF, TANMOY DAS, TOMASZ DURAKIEWICZ, JIAN-XIN ZHU, JOHN J. JOYCE, JOHN L. SARRAO, Los Alamos National Laboratory — We performed self-consistent GW-like calculations within the intermediate Coulomb-U coupling regime to investigate dynamic correlation effects in the intermetallic actinide UCoGa$_5$. This material is often used to contrast anomalous behavior in other U-115 and Pu-115 compounds, because it is presumed to be a conventional Fermi liquid that resembles a "vegetable." First-principles electronic structure calculations were used as input, combined with the spin-fluctuation exchange approximation, to compute self-consistently the many-body self-energy responsible for dynamic correlation effects. We validated the approach by angle-resolved photoemission spectroscopy (ARPES). The occurrence of electronic hot spots in the spectral function, accompanied by kinks and abrupt breaks in the slope of the quasiparticle dispersion were detected both at low (130 meV) and high (1 eV) binding energies below the Fermi energy. In conclusion, we found that dynamic correlation anomalies are adequately described by coupling between itinerant fermions and spin fluctuations arising from the particle-hole continuum of the spin-orbit-split 5f states of uranium.

Probing the f-state configuration of $\alpha$-U and URu$_2$Si$_2$ with RXES. SCOTT MEDLING, CORWIN H. BOOTH, Lawrence Berkeley National Lab, RYAN BAUMBACH, ERIC D. BAUER, Los Alamos National Lab — We directly probed the electronic configuration of several uranium compounds using Resonant X-ray Emission Spectroscopy (RXES). Previous investigations by several groups into the magnetic properties of uranium compounds (such as URu$_2$Si$_2$) suggested that some are multiconfigurational. RXES is particularly useful for probing the configurations because measuring the energies of both the incident and scattered photons reveals information about both the empty and occupied electronic states. We collected data for several uranium samples ($\alpha$-U, UO$_2$, and URu$_2$Si$_2$) which indicate that in some of these compounds the uranium is multiconfigurational, with a mixture of $f^1$, $f^2$, and $f^3$ occupancies. The degree of intermediate valence that this implies will be related to electronic and magnetic properties of the compound.

Towards a Density Functional Theory Exchange-Correlation Functional able to describe localization/delocalization. We performed self-consistent GW-like calculations within the intermediate Coulomb-U coupling regime to investigate dynamic correlation effects in the intermetallic actinide UCoGa$_5$. This material is often used to contrast anomalous behavior in other U-115 and Pu-115 compounds, because it is presumed to be a conventional Fermi liquid that resembles a "vegetable." First-principles electronic structure calculations were used as input, combined with the spin-fluctuation exchange approximation, to compute self-consistently the many-body self-energy responsible for dynamic correlation effects. We validated the approach by angle-resolved photoemission spectroscopy (ARPES). The occurrence of electronic hot spots in the spectral function, accompanied by kinks and abrupt breaks in the slope of the quasiparticle dispersion were detected both at low (130 meV) and high (1 eV) binding energies below the Fermi energy. In conclusion, we found that dynamic correlation anomalies are adequately described by coupling between itinerant fermions and spin fluctuations arising from the particle-hole continuum of the spin-orbit-split 5f states of uranium.

Actinide electronic structure based on the Dirac equation and density functional theory. JOHN M. WILLS, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, ANN E. MATTSSON, Sandia National Laboratories, Albuquerque, NM 87185, USA — Density functional theory (DFT) provides a formally predictive basis for predicting the structural properties of actinides. Although available approximations to the exchange/correlation functional provide accurate predictions for many materials, they fail qualitatively and sometimes quantitatively when applied to actinides. Major contributors to this deficiency are an inadequate treatment of confinement physics and an incomplete treatment of relativity in the underlying equations. The development of a functional correctly incorporating confinement physics with a proper treatment of relativity would provide definitive, internally consistent predictions of actinide properties. To enable the development of such a functional and quantify the predictions of currently available functionals, we have developed an efficient first-principles electronic structure method based on the Dirac equation. Results are compared with current methods, and the implications for relativistic density functionals discussed. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s National Nuclear Security Administration under contract DE-AC04-94AL85000.

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Towards a Density Functional Theory Exchange-Correlation Functional able to describe localization/delocalization
2:30PM W1.00001 Achieving higher $T_C$ superconductivity in dense cuprates, iron selenides, and hydrocarbons

et al., XIAO-JIA CHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — Pressure plays an essential role in inducing or tuning superconductivity as well as shedding insight on the mechanism of superconductivity. There are many rich phase diagrams in unconventional superconductors under pressure. Finding ways to control the quantum coherence properties to have a higher critical temperature $T_C$ than the material has remains a challenge. Here we will talk about our recent experimental efforts in achieving higher temperature superconductivity in cuprates, iron selenides, and hydrocarbons. We will show how to enhance remarkably $T_C$ through the pressure tuning of competing electronic order in multilayer cuprates [1] and how to have superconductivity in two distinct regimes in iron selenides [2,3]. We will present a discovery of an enhancement of $T_C$ at more than doubled ambient value in a highly compressed aromatic hydrocarbon [4]. Our results have important implications for designing and engineering superconductors with much higher $T_C$s at ambient conditions.


1This work is supported by the U.S. DOE under Grant No. DE-SC0001057.

3:06PM W1.00002 Elemental superconductivity at high pressure

et al., KYOKUGEN, Osaka University — Most of superconducting materials show a negative pressure effect in the superconducting critical temperature, $T_C$, however, some of simple elements show the positive effect. It has been already revealed that not a few elements that are not the superconductor at ambient pressure became superconductive under combination of low temperature and high pressure. Not only for searching higher $T_C$, but also for understanding the fundamental mechanism of “superconductivity” systematically, we have worked on pressure effect as well as pressure-induced superconductivity especially in simple elements. Here we report two characteristic results of the high-pressure phenomena including superconductivity in calcium (Ca) and lithium (Li). The $T_C$ of Ca increases with pressure and reaches 29 K in the highest $T_C$ in elements, at very high pressure above 200 GPa. The lightest metal element of Li exhibits relatively high $T_C$ at high pressure, however suddenly becomes semiconductor at 80 GPa. Recently we discovered the reentrance of the superconductivity in Li at around 120 GPa.

1This research is supported by JSPS through its NEXT Program (GR068).

3:42PM W1.00003 NMR Studies of Novel Electronic Phases in Low Dimensional Molecular Solids at High Pressure and Low Temperature

et al., UCLA Physics and Astronomy — Molecular superconductors are known for anisotropic electronic band structure, correlations, and a sensitivity to mechanical or chemical pressure which acts to control the relative strength of the respective kinetic and potential energies. Modest pressures, of order 1 GPa are commonly used to continuously tune from a Mott insulating ground state to a superconducting state, and NMR has been particularly successful in identifying the orders involved, and the nature of the excitations in the various phases encountered. The family of quasi-two dimensional systems $\text{Cu}(\text{NCS})_2$ [1] includes a line of first order phase transitions separating the Mott and superconducting phases, with the superconducting state exhibiting signatures for line nodes associated with an order parameter sign-change over the Fermi surface. The pressure/temperature phase diagram of the quasi-one dimensional materials (TMTSF)$_2X$, $X=PF_6$, ClO$_4$,... includes more phases, as a consequence of effective 4/5-filling and a substantial density wave susceptibility. The SC ground state is singlet, and there is evidence for a sign-change of the order parameter over the Fermi surface. The high-conductivity normal state exhibits properties associated with two-dimensional spin fluctuations, with signatures in the relaxation rate, as well as transport that are reminiscent of behaviors observed in other correlated superconductors.

1Supported by the NSF under grant no. DMR-1105531

4:18PM W1.00004 Pressure effects in cuprate and iron-based superconductors studied by muon spin rotation

et al., STUART BROWN, UCLA Physics and Astronomy — Molecular superconductors are known for anisotropic electronic band structure, correlations, and a sensitivity to mechanical or chemical pressure which acts to control the relative strength of the respective kinetic and potential energies. Modest pressures, of order 1 GPa are commonly used to continuously tune from a Mott insulating ground state to a superconducting state, and NMR has been particularly successful in identifying the orders involved, and the nature of the excitations in the various phases encountered. The family of quasi-two dimensional systems $\text{Cu}(\text{NCS})_2$ [1] includes a line of first order phase transitions separating the Mott and superconducting phases, with the superconducting state exhibiting signatures for line nodes associated with an order parameter sign-change over the Fermi surface. The pressure/temperature phase diagram of the quasi-one dimensional materials (TMTSF)$_2X$, $X=PF_6$, ClO$_4$,... includes more phases, as a consequence of effective 4/5-filling and a substantial density wave susceptibility. The SC ground state is singlet, and there is evidence for a sign-change of the order parameter over the Fermi surface. The high-conductivity normal state exhibits properties associated with two-dimensional spin fluctuations, with signatures in the relaxation rate, as well as transport that are reminiscent of behaviors observed in other correlated superconductors.

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1Supported by the NSF under grant no. DMR-1105531

1This work is supported in part by the NCCR MaNEP Switzerland

112133
4:54PM W1.00005 Pressure tuning of magnetic fluctuation and superconductivity in CeCoIn$_5$\textsuperscript{1}.

CARMEN ALMASAN, Kent State University — One of the greatest challenges to Landau’s Fermi liquid theory – the standard theory of metals - is presented by complex materials with strong electronic correlations. The non-Fermi liquid transport and thermodynamic properties of these materials are often explained by the presence of strong quantum critical fluctuations associated with a quantum phase transition that happens at a quantum critical point (QCP). The heavy-fermion material CeCoIn$_5$ is a prototypical system for which its pronounced non-Fermi liquid behavior in the normal state and unconventional superconductivity are thought to arise from the proximity of this system to a QCP [1-5]. Previous experiments address the physics of this QCP by extrapolating results obtained in the normal state, i.e., there were no direct probes of antiferromagnetism and quantum criticality in the superconducting state. This motivated us to study the transport in the mixed state, thus revealing the physics of antiferromagnetism and quantum criticality of the underlying normal state [6]. In this talk I will present the results obtained in these studies by measuring the vortex core dissipation under applied hydrostatic pressure ($P$). The vortex core resistivity increases sharply with decreasing magnetic field ($H$) and temperature ($T$) due to quasiparticle scattering on critical antiferromagnetic fluctuations. This behavior is greatly suppressed with increasing $P$. Using our experimental results, we obtained an explicit equation for the antiferromagnetic boundary inside the superconducting dome and constructed an $H-T-P$ phase diagram. This work provides direct evidence for a quantum critical line inside the superconducting phase and reveals the close relationship between quantum criticality, antiferromagnetism, and superconductivity.

In collaboration with T. Hu, H. Xiao, T. A. Sayles, M. Dzero, and M. B. Maple.

\textsuperscript{1}Research supported by NSF DMR 1006606.

Thursday, March 21, 2013 2:30PM - 5:30PM –
Session W2 DCMP: Invited Session: Theory of Interacting Topological Insulators Ballroom II - Shou-Cheng Zhang, Stanford University

2:30PM W2.00001 Simplified topological invariants for interacting insulators and superconductors\textsuperscript{1}, ZHONG WANG, Tsinghua University — Topological invariants are precise mathematical tools characterizing the topological properties of topological insulators and superconductors. While many simple and powerful topological invariants for noninteracting insulators and superconductors have been well established, the topological invariants for interacting systems are much less investigated, despite of their great importance in studies of topological states in interacting systems. In this talk I will report some recent progress in the search of topological invariants for interacting systems. I will show that topological invariants defined in terms of zero frequency Green’s function are precise and convenient tools for interacting topological insulators and superconductors. They have much simpler forms compared to earlier interacting topological invariants, and have the potential to facilitate discoveries of new topological insulators with strong electron-electron interaction.

\textsuperscript{1}We acknowledge the support by Tsinghua University Initiative Scientific Research Program (No. 20121087986).

3:06PM W2.00002 Interaction effects on 3D topological insulators and semi-metals\textsuperscript{1}, WILLIAM WITCZAK-KREMPA, Perimeter Institute — We discuss the effects of interactions on 3D Z2 topological insulators and related phases such as axion insulators, Weyl semi-metals and topological Mott insulators. Our analysis is motivated by the pyrochlore iridates but is of general scope. We begin by studying the effects of interactions on topological phases adiabatically connected to non-interacting Hamiltonians using both regular and dynamical mean field theories. Both the bulk and boundary topological signatures are analyzed. We then move to stronger interactions where a Mott transition from a topological insulator to a fractionalized topological Mott insulator can occur. We discuss the effects of gauge fluctuations on the transition and the resulting spin liquid.

\textsuperscript{1}Supported by NSERC, FQRNT, the Walter Sunner Foundation, the University of Toronto and Perimeter Institute.

3:42PM W2.00003 Topological Insulator Materials with Strong Interaction\textsuperscript{1}, HAIJUN ZHANG, Department of Physics, Stanford University — All kinds of topological insulator materials have recently been discovered in two-and three-dimensional systems with strong spin-orbit coupling (SOC) hosting helical gapless edge or surface states consisting of odd number of Dirac fermion states inside the bulk band gap. Most of these discovered topological insulators have negligible interaction. Here we theoretically predict a new class of topological insulators with strong interaction. The typical examples are PuTe$_2$ and AmN, with a simple rocksalt structure, which lie on the boundary between metals and insulators. We show that the interaction can effectively enhance SOC and drives a quantum phase transition to the topological insulator phase with a single Dirac cone on the surface (001). In addition, this kind of compounds has fully or partly filled $f$ states, which could exhibit all kinds of magnetic phases, potentially leads to the discovery of intrinsic quantum anomalous Hall effect (QAHE) and topological magnetic insulators with dynamic axion field.

\textsuperscript{1}I acknowledge the support of the Army Research Office (No.W911NF-09-1-0508).

4:18PM W2.00004 Interacting topological phases and quantum anomalies, SHINSEI RYU, University of Illinois at Urbana-Champaign — Since the quantum Hall effect, the notion of topological phases of matter has been extended to those that are well-defined (or “protected”) in the presence of a certain set of symmetries, and that exist in dimensions higher than two. In the (fractional) quantum Hall effects (and in “chiral” topological phases in general), Laughlin’s thought experiment provides a key insight into their topological characterization: it shows a close connection between topological phases and quantum anomalies. Compared to genuine topological phases, symmetry protected topological phases are more fragile and less entangled states of matter, and hence for their characterization we need to sharpen our understanding on how topological properties of the systems manifest themselves in the form of a quantum anomaly. By taking various kinds of symmetry protected topological phases as an example, I will demonstrate that quantum anomalies serve as a useful tool to diagnose (and even define) topological properties of the systems. I will also discuss quantum anomalies play an essential role when developing descriptions of these topological phases in terms bulk and boundary (effective) theories.
Thursday, March 21, 2013 2:30PM - 5:30PM —

Session W5 DCMP: Focus Session: Graphene: Transport and Optical Phenomena: Nanostructures

2:30PM W5.00001 Large Scale Mesoscopic Transport in Nanostructured Graphene

HAIJING ZHANG, JIANMING LU, WU SHI, ZHE WANG, TING ZHANG, MINGYUAN SUN, YUAN ZHENG, QIHONG CHEN, NING WANG, Hong Kong University of Science and Technology, JUHN-JONG LIN, National Chiao Tung University, PING SHENG, Hong Kong University of Science and Technology — We report the observation of strong 2D Anderson localization at the charge neutrality point (CNP) in nanostructured antidot graphene samples. A localization length of 2 micron is obtained through sample size scaling up to 10 micron. Localization length is seen to increase with applied magnetic field, in accurate agreement with the theoretical prediction of Ono [Prog. Theor. Phys. Suppl. 84, 138 (1985)]. Our observation is made possible by the very large dephasing length of 10 micron, owing to the opening of a Coulomb quasiparticle, observable below 25 K, that suppresses the inelastic electron-electron scatterings. Such a large dephasing length is further substantiated by the observation of a crossover from the mesoscopic transport (with exponential size scaling) to diffusive transport (with size independence) at 10 micron. Large scale mesoscopic transport may provide promising future to graphene nanoelectronic device applications.

2:42PM W5.00002 Ballistic transport in nanometer-scale suspended graphene

V. TAYARI, A.C. MCREA, S. YIGEN, J. PORTER, J.O. ISLAND, A. R. CHAMPAGNE, Department of Physics, Concordia University, Montreal, Canada — We study electron transport in suspended ultra-short graphene transistors. We fabricate narrow bowtie gold junctions on exfoliated graphene, and use oxygen plasma to etch away the graphene crystal except under the gold junctions. We then use a wet etch to remove the SiO₂ under the junctions and suspend the devices. Finally, we use a feedback-control electromigration procedure to break the gold junctions and expose sections of graphene which are ~100 nm wide, and as short as ~10 nm. Using low-temperature electron transport, we observe Fabry-Perot oscillations in the conductivity as a function of charge density, as expected for ballistic transport. The conductivity is asymmetric for electron and hole gate-doping, signaling charge doping from the gold contacts and the formation of p-n junctions. At temperatures below ~1 Kelvin, a very strong hysteresis is observed in the gate-dependence of conductivity. We study these devices as a function of charge density, temperature, magnetic field and aspect ratio.

2:54PM W5.00003 The Effects of the Mean-Field Interaction on the Anderson Localization of Graphene Nanoribbons

JACK BALDWIN, Y. HANCOCK, Department of Physics, University of York, UK — A generalized tight-binding (TB) model which includes a mean-field Hubbard-\(U\) and up to 3rd nearest-neighbor hopping terms, is applied to edge-disordered zigzag graphene nanoribbons in order to study spin-transport within the Landauer-Büttiker formalism. Edge-disorder is modeled by random perturbation of the on-site energy in the range \(-E...E\) on all edge atoms, and the resulting Anderson localization lengths determined. We compared the Anderson localization lengths and spin-transport features obtained from the generalized model, an extended TB model (non-interacting) and the simplified TB model (1st nearest neighbor hopping only). Within the range \(\pm E = 0.5\ eV\) the Anderson localization length for a single spin was found to decrease by 86.4% with the introduction of the Hubbard-\(U\) in the generalized model compared to the non-interacting models, whereas the opposite spin remained unchanged across all model types. For the range \(\pm E = 2.0\ eV\) the Anderson localization length for both spin types decreased by 71.4% and 76.2% in the generalized model when compared to the extended TB model, and 76.5% and 80.4% when compared to the simplified TB model.

3:06PM W5.00004 Graphene-based spaser

OLEG BERMAN, ROMAN KEZERASHVILI, New York City College of Technology, the City University of New York, YURILO LOZOVUK, Institute of Spectroscopy — We propose graphene-based surface plasmon amplification by stimulated emission of radiation (spaser) formed in the graphene nanoribbon located near a semiconductor quantum dot (QD). The population inversion of the two electron levels of the QD can be achieved by applying external electric current or laser pumping. If the frequency of the dipole plasmon resonance in a graphene nanoribbon comes in the resonance with the transition frequency for the QD, it is possible to excite plasmons and generate the coherent surface plasmon states in the graphene nanoribbon. Therefore, the oscillating dipole in the QD excites coherent surface plasmons in the graphene nanoribbon. By solving the system of equations for the number of coherent localized plasmons in a graphene-based spaser the optimal design, optimal width of graphene nanoribbon and optimal regime for the graphene-based spaser are found. The minimal size and minimal threshold pumping intensity for the graphene-based spaser is obtained. The advantage of using graphene for the spaser is discussed.

3:18PM W5.00005 ABSTRACT WITHDRAWN —

3:30PM W5.00006 Shearing graphene and its transmission properties

ANDRES CONCHA², School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA, SHENGFENG CHENG, Sandia National Laboratories, Albuquerque, New Mexico 87185, USA, L. MAHADEVAN¹, School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA — Graphene being the thinnest possible membrane is prone to deformations under slight external forcing or even under thermal fluctuations. Here, we take advantage of this proneness to deformations to manipulate transport properties of graphene ribbons. We do so by using the spontaneous pattern produced when a wide ribbon is subject to shear. The deformation of the ribbon produces pseudo-magnetic fields as well as scalar potentials, resulting in the modification of transmission properties without the need of an external gate potential. Our proposal is a concrete realization of a quantum device that takes full advantage of an elastic instability that spans from the nano to macro-scales.

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²School of Engineering and Sciences, Adolfo Ibañez University. Diagonal las torres 2640, Peñalolen, Santiago, Chile
³Department of Physics, Harvard University, Cambridge, MA 02138, USA
change not only in graphene, but also in general mesoscopic systems in the localized regime. Different strategies to examine the crossover behavior of conductance between Q1D and 2D systems, we find that a transition from 2D to Q1D is attainable by system, we consider hydrogenated graphene systems which have attracted much attention due to the observation of a metal-insulator transition. Adopting two conductance distribution function. Although the distribution functions show distinctive behavior depending on the dimension of system, previous studies have been mainly focused on one, two, and three dimensional systems individually. Here, we investigate the dimensional transition from two-dimensional (2D) graphene to quasi-one-dimensional (Q1D) graphene nanoribbons and discuss the effect of the dimensional crossover on the conductance fluctuation. As a model system, we consider hydrogenated graphene systems which have attracted much attention due to the observation of a metal-insulator transition. Adopting two different strategies to examine the crossover behavior of conductance between Q1D and 2D systems, we find that a transition from 2D to Q1D is attainable by reducing the sample width, while it is not possible by increasing the length of the 2D system. Our results provide fundamental insights into the dimensionality change not only in graphene, but also in general mesoscopic systems in the localized regime.
adaptation of the Monte Carlo algorithm described in [Phys. Rev. Lett. 104, 157201 (2010)], we compute the topological entanglement entropy (TEE) at the Rokhsar-Kivelson (RK)-like ground state wavefunctions. Using the construction proposed by Kitaev and Preskill [Phys. Rev. Lett. 96, 110404 (2006)] and an $1$-demonstrate the universality of TEE over a wide range of parameter values within a topologically ordered phase approaching a quantum phase transition. For $n$, BRYAN CLARK, Station Q, ANDREI BERNEVIG, Princeton University — The structure of the original band, as well as the details of the periodic perturbation. We also generalize this one-to-two band splitting case to one-to-many splitting, breaking lattice translation symmetry that results in a doubled unit cell, the subbands have a set of Chern numbers whose sum has to be the same as the origin Florida State University, KUN YANG, National High Magnetic Field Laboratory, Florida State University — When a Chern band is split into two subbands by a period potential, the subbands carry Z2 topological quantum numbers. We argue that this provides a way to tune the properties of topological systems. We turn in to trivial insulators or insulators with a higher Chern number. We discuss signatures of such states in the context of non-adiabatic Thouless pumping. We show that and under proper drive conditions they can be formed into resonant states in the band continuum and both low energy approximations and numerical evaluation of the Green’s functions indicate that the amplitude of the wave function decays as a power law with exponents depending on sublattice, direction, and the impurity species. We revisit the VRH theory in view of this result and find that considering only the overlap and energy difference of the impurity states, the conductivity obeys a power law of the temperature with an exponent related to the localization of the wave function. Other factors that were ignored in the original VRH are included due to the weaker temperature dependence, which contribute an additional exponent. We show that this relationship is in agreement with available experimental results.

Gate-tuned two-channel Kondo screening in Graphene: Universal scaling of the nonlinear conductance$^1$, CHUNG-HOU CHUNG, Department of Electrophysics, National Chiao-Tung University and Physics Division, National Center for Theoretical Sciences, HsinChu, Taiwan, R.O.C., TSUNG-HAN LEE, KENNETH YI-JIEH ZHANG, Department of Electrophysics, National Chiao-Tung University, HsinChu, Taiwan, R.O.C. STEFAN KIRCHNER, Max-Plank-Institut fuer Physik komplexer Systeme and Max-Planck-Institut fuer chemische Physik Stoffe, Dresden, Germany — We study the nonlinear conductance through magnetic adatoms on Graphene. In particular, we address the finite-temperature crossover from a quantum critical to the two-channel Kondo regime expected to occur in doped Graphene. Based on the non-crossing approximation, We calculate both the linear and nonlinear conductance within the two-lead single-impurity Anderson model where the conduction electron density of states vanishes in a power-law fashion $\sim \left| \omega - \mu \right|^r$ with $r = 1$ near the Fermi energy, appropriately for Graphene. For given gate voltage, we study the universal crossover from a 2-channel Kondo (2CK) phase to a un-screened local moment (LM) phase. We extract universal scaling functions governing charge transport through the adatom and discuss our results in the context of a recent scanning tunneling spectroscopy (STM) experiment on Co-doped Graphene.

We acknowledge the support from the NSC grants No.98-2112-M-009-010-MY3, No.101-2628- M-009-001-MY3, the MOE-ATU program, the CTS of NCTU, the NCTS of Taiwan, R.O.C. (C.H.C.), and DFG research unit 960 under “Quantum Phase Transitions”.

2:42PM W8.00002 Band Splitting by Period Potential and Resultant Topological Quantum Numbers, LIANG SUN, Department of Modern Physics, University of Science and Technology of China and National High Magnetic Field Laboratory, Florida State University, KUN YANG, National High Magnetic Field Laboratory, Florida State University — When a Chern band is split into two subbands by breaking lattice translation symmetry that results in a doubled unit cell, the subbands have a set of Chern numbers whose sum has to be the same as the original band. This, however, does not uniquely determine the Chern numbers of individual subbands. We show how the subbands Chern numbers are related to the structure of the original band, as well as the details of the periodic perturbation. We also generalize this one-to-two band splitting case to one-to-many splitting, as well as the case with time-reversal symmetry, where the Chern number is zero but the bands can carry Z2 topological quantum numbers.

4:2PM W8.00003 Using topological entanglement entropy to identify low energy effective field theories of fractional Chern Insulators, BRYAN CLARK, Station Q, ANDREI BERNEVIG, Princeton University — The physics of quantum interacting many-body systems allow for a wide variety of phases, whose properties are governed by low energy field theories. In this talk, we write down prototypical parton Chern insulating wave-functions with Chern numbers 1, 2, 3, and 5 and determine their corresponding low energy effective field theory by computing their topological entanglement entropy. We also discuss non-universal aspects of the entanglement entropy including the effect of changing the mass on the corner terms and the slope of the area law.

5:06PM W5.00014 Impurity state and variable range hopping conduction in graphene, SANG-ZI LIANG, JORGE O. SOFO, Department of Physics, the Pennsylvania State University — The variable range hopping (VRH) theory is widely accepted as explaining the temperature dependence of the conductivity of doped semiconductors. However, as formulated for exponentially localized impurity states, it does not necessarily applies in the case of graphene with covalently attached impurities. We analyze the localization of impurity states in graphene using the nearest neighbor tight-binding model of an adatom-graphene system with Green’s function perturbation methods. The impurity states in graphene are characterized as resonant states in the band continuum and both low energy approximations and numerical evaluation of the Green’s functions indicate that the amplitude of the wave function decays as a power law with exponents depending on sublattice, direction, and the impurity species. We revisit the VRH theory in view of this result and find that considering only the overlap and energy difference of the impurity states, the conductivity obeys a power law of the temperature with an exponent related to the localization of the wave function. Other factors that were ignored in the original VRH are included due to the weaker temperature dependence, which contribute an additional exponent. We show that this relationship is in agreement with available experimental results.

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2:30PM W8.00001 Modifying properties of Chern insulators by time dependent perturbations, BENJAMIN M. FREGOSO, VICTOR GALITSKI, Joint Quantum Institute and Condensed Matter Theory Center, University of Maryland — We study the quantum dynamics of topological Chern insulators in the presence a time dependent perturbation. We show that and under proper drive conditions they can be turned in to trivial insulators or insulators with a higher Chern number. We discuss signatures of such states in the context of non-adiabatic Thouless pumping. We argue that this provides a way to tune the properties of topological systems.

funding provided by PFC

2:54PM W8.00003 Using topological entanglement entropy to identify low energy effective field theories of fractional Chern Insulators, BRYAN CLARK, Station Q, ANDREI BERNEVIG, Princeton University — The physics of quantum interacting many-body systems allow for a wide variety of phases, whose properties are governed by low energy field theories. In this talk, we write down prototypical parton Chern insulating wave-functions with Chern numbers 1, 2, 3, and 5 and determine their corresponding low energy effective field theory by computing their topological entanglement entropy. We also discuss non-universal aspects of the entanglement entropy including the effect of changing the mass on the corner terms and the slope of the area law.

3:06PM W8.00004 Adiabatic continuity between Hofstadter and Chern insulator states, YINHAI WU, JAINENDRA JAIN, Penn State University, KAI SUN, U of Maryland and U of Michigan — We show that the topologically nontrivial bands of Chern insulators are adiabatic cousins of the Landau bands of Hofstadter lattices. We demonstrate adiabatic connection also between several familiar fractional quantum Hall states on Hofstadter lattices and the fractional Chern insulator states in partially filled Chern bands, which implies that they are in fact different manifestations of the same phase. This adiabatic path provides a way of generating many more fractional Chern insulator states and helps clarify that nonuniversality in the distribution of the Berry curvature is responsible for weakening or altogether destroying fractional topological states.

3:18PM W8.00005 Entanglement Entropy at Generalized RK Points of Quantum Dimer Models, ALEXANDER SELEM, University of California, Berkeley, CHRISTOPHER HERDMAN, University of Vermont, K. BIRGITTA WHALEY, University of California, Berkeley — We study the $n = 2$ Rényi entanglement entropy of the triangular quantum dimer model via Monte Carlo sampling of Rokhsar-Kivelson(RK)-like ground state wavefunctions. Using the construction proposed by Kitaev and Preskill [Phys. Rev. Lett. 96, 110404 (2006)] and an adaptation of the Monte Carlo algorithm described in [Phys. Rev. Lett. 104, 157201 (2010)], we compute the topological entanglement entropy (TEE) at the RK point $\gamma = (1.001 \pm 0.003)$ in 2 confirming earlier results. Additionally, we compute the TEE of the ground state of a generalized RK-like Hamiltonian and demonstrate the universality of TEE over a wide range of parameter values within a topologically ordered phase approaching a quantum phase transition. For systems sizes that are not negligible numerically, we find that the quantization of TEE depends sensitively on correlations. We characterize corner contributions to the entanglement entropy and show that these are well described by shifts proportional to the number and types of corners in the bipartition.

This work was supported by NSF grant number PH4-0803249.
3:30 PM W8.00006 Thermal Instability of Edge States in a 1D Topological Insulator¹. OSCAR VIVUELA, ANGEL RIVAS, MIGUEL ANGEL MARTIN-DELGADO, Universidad Complutense de Madrid — The stability of topological phases of matter, also known as topological orders, against thermal noise has provided several surprising results in the context of topological codes used in topological quantum information. However, very little is known about the behavior of a topological insulator (TI) subjected to the disturbing thermal effect of its surrounding environment. This is of great relevance if we want to address key questions such as the robustness of TIs to thermal noise, existence of thermalization processes, use of TIs as platforms for quantum computation, etc. In this work, we have studied the dynamical thermal effects on the protected edge states of a TI when it is considered as an open quantum system in interaction with a noisy environment at a certain temperature T. Let us recall that stable edge states are a defining signature of topological insulators. Outstandingly, we find that the usual protection of edge states against quantum perturbations and randomness is lost in the case of thermal effects, despite the fermion-boson interaction with the thermal environment respects chiral symmetry, which is the symmetry responsible for the protection (robustness) of the edge states in this TI. We are able to compute decay rates for practical implementations. PRB (2012)

3:42 PM W8.00007 Torsional Response, bulk-boundary correspondence, and Viscosity in Topological Insulators, TAYLOR HUGHES, ROBERT LEIGH, ONKAR PARRIKAR, University of Illinois at Urbana-Champaign — We discuss the relationship between torsion and visco-elastic response of 2D time-reversal breaking topological insulators. We connect the bulk topological response to a new anomalies in the momentum current of the chiral edge theory that we have determined. We also discuss the implications for spectral flow and the emergence of a chiral-gravity type response theory.

3:54 PM W8.00008 Effect of static charge fluctuations on the conduction along the edge of two-dimensional topological insulator¹. JUKKA VAYRYNEN, MOSHE GOLDSTEIN, LEONID GLAZMAN, Yale University — Static charge disorder may create electron puddles in the bulk of a material which nominally is in the insulating state. A single puddle – quantum dot – coupled to the helical edge of a two-dimensional topological insulator enhances the electron backscattering within the edge. The backscattering rate increases with the electron dwell time in the dot. While remaining inelastic, the backscattering off a dot may be far more effective than the proposed earlier inelastic processes involving a local scatterer with no internal structure. We find the temperature dependence of the dot-induced correction to the universal conductance of the edge. In addition to the single-dot effect, we calculate the classical temperature-independent conductance correction caused by a weakly conducting bulk. We use our theory to assess the effect of static charge fluctuations in a heterostructure on the edge electron transport in a two-dimensional topological insulator.

¹The work at Yale University is supported by NSF DMR Grant No. 1206612 and the Simons Foundation.

4:06 PM W8.00009 Backscattering Between Helical Edge States via Dynamic Nuclear Polarization, ADRIAN DEL MAESTRO, University of Vermont, TIMO HYART, BERND ROSENOW, Institute for Theoretical Physics, University of Leipzig — We describe how the non-equilibrium spin polarization of one dimensional helical edge states at the boundary of a two dimensional topological insulator can dynamically induce a polarization of nuclei via the hyperfine interaction. When combined with a spatially inhomogeneous Rashba coupling, the resulting steady state polarization of the nuclei produces backscattering between the topologically protected edge states leading to a reduction in the conductance which persists to zero temperature. We study these effects in both short and long edges, uncovering deviations from Ohmic transport at finite temperature and a current noise spectrum which may hold the fingerprints for experimental verification of the backscattering mechanism.

4:18 PM W8.00010 Symmetries in the entanglement spectrum and topological phases protected by spatial discrete symmetries, PO-YAO CHANG, SHINSEI RYU, University of Illinois at Urbana-Champaign — We study topological phases protected by spatial (non-local) symmetries using the entanglement spectrum. Exploiting the structure of the entanglement Hamiltonian that can be formulated as the supersymmetric quantum mechanics, we study how a spatial symmetry constrains the entanglement spectrum when the bipartitioning is consistent with the spatial symmetry. Specific examples we took a look at include a reflection symmetric topological insulator composed of two Chern insulators with opposite chiralities in one and two spacial dimensions. For both topological insulators, the edge states in the physical energy spectrum can be gapped while the entangling boundary remains gapless.

4:30 PM W8.00011 Interfacial Protection of Topological Surface States in Ultrathin Sb Films, GUANG BIAN, Department of Physics, University of Illinois at Urbana-Champaign, XIAOXIONG WANG, College of Science, Nanjing University of Science and Technology, YANG LIU, THOMAS MILLER, TAI-CHANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign — Spin-polarized gapless surface states in topological insulators form chiral Dirac cones. When such materials are reduced to thin films, the Dirac states on the two faces of the film can overlap and couple by quantum tunneling, resulting in a thickness-dependent insulating gap at the Dirac point. Calculations for a freestanding Sb film with a thickness of four atomic bilayers yield a gap of 36 meV, yet angle-resolved photoemission measurements of a film grown on Si(111) reveal no gap formation. The surprisingly robust Dirac cone is explained by calculations in terms of interfacial interaction. Our work suggests that quantum tunneling, an intrinsic property dependent on the film thickness, and substrate bonding, an extrinsic factor amenable to interfacial engineering, can be effectively manipulated to achieve desired electronic and spintronic properties of topological thin films.

4:42 PM W8.00012 ABSTRACT WITHDRAWN

4:54 PM W8.00013 Controlling topological insulating phases by tuning the coupling strength of Dirac fermions in chalcogenide ternary compounds, JEONGWOO KIM, JINWOONG KIM, SEUNG-HOON JHI, Pohang University of Science and Technology — Chalcogenide ternary compounds such as Ge₂Sb₂Te₅ are considered as superlattice of topological insulating layers and band insulating layers. Using first-principles methods and a model Hamiltonian, we study the topological phases of the chalcogen compounds arising from the interactions of Dirac fermions existing at the interfaces between the topological insulating and band insulating layers. We particularly investigate the interactions of Dirac fermions upon varying the thickness of band insulating layers or upon introducing magnetic impurities in the layers. We observe a jump of Dirac cones from one time-reversal invariant momentum to another when the thickness is changed. We also discuss the degree of freedom in the spin helicity of the Dirac fermions and how it limits the topological phases.
The space group classification of topological band insulators\(^1\), VLADIMIR JURICIC, Lorentz-Institute for Theoretical Physics, Leiden University, ROBERT-JAN SLAGER, Lorentz-Institute for Theoretical Physics, Leiden University, The Netherlands, ANDREJ MESAROS, Department of Physics, Boston College, USA, JAN ZAANEN, Lorentz-Institute for Theoretical Physics, Leiden University, The Netherlands — The existing classification of topological band insulators(TBIs) departs from time-reversal symmetry, but the role of the crystal symmetries in the physics of these topological states remains elusive. I will discuss the classification of TBIs protected not only by time-reversal, but also by space group symmetries [1]. I find three broad classes of topological states: (a) \(\Gamma\)-states robust against general time-reversal invariant perturbations; (b) Translationally-active states protected from elastic scattering, but susceptible to topological crystalline disorder; (c) Valley topological insulators sensitive to the effects of non-topological and crystalline disorder. These three classes give rise to 18 different two-dimensional, and, at least 70 three-dimensional TBIs. I will show how some of these topological states can be realized in two dimensions when tight-binding M-B model, originally introduced for HgTe quantum wells, is generalized to include longer-range hoppings. Finally, experimental implications of our classification scheme with an emphasis on topological states in Sn-based materials will be discussed.

1\(^{\text{V. J. acknowledges the support of the Netherlands Organization for Scientific Research (NWO).}}\)

Why is the bulk resistivity of topological insulators so small?\(^2\), TIANRAN CHEN, BRIAN SKINNER, BORIS SHKLOVSKII, Fine Theoretical Physics Institute, University of Minnesota — As-grown topological insulators (TIs) are typically heavily-doped \(n\)-type crystals. Compensation by acceptors is used to move the Fermi level to the middle of the band gap, but even then TIs have a frustratingly small bulk resistivity. We show that this small resistivity is the result of band bending by poorly screened fluctuations in the random Coulomb potential. Using numerical simulations of a completely compensated TI, we find that the bulk resistivity has an activation energy of just 0.15\(\times\) the band gap, in good agreement with experimental data. At lower temperatures activated transport crosses over to variable range hopping with a relatively large localization length.


Detection and interrogation of biomolecules via nanoscale probes: From fundamental physics to DNA sequencing\(^3\), MICHAEL ZWOLAK\(^4\), Oregon State University — A rapid and low-cost method to sequence DNA would revolutionize personalized medicine [1], where genetic information is used to diagnose, treat, and prevent diseases. There is a longstanding interest in nanoribbons as a platform for rapid interrogation of single DNA molecules. I will discuss a sequencing protocol based on the measurement of transverse electronic currents during the translocation of single-stranded DNA through nanoribbons. Using molecular dynamics simulations coupled to quantum mechanical calculations of the tunneling current, I will show that the DNA nucleotides are predicted to have distinguishable electronic signatures in experimentally realizable systems. Several recent experiments support our theoretical predictions. In addition to their possible impact in medicine and biology, the above methods offer ideal test beds to study open scientific issues in the relatively unexplored area at the interface between solids, liquids, and biomolecules at the nanometer length scale [1].

1\(^{\text{M. Zwolak and M. Di Ventra, \textit{Physical Approaches to DNA Sequencing and Detection}, Rev. Mod. Phys. 80, 141 (2008).}}\)

3:06PM W9.00002 Single Molecule Electrical Sequencing of DNA and RNA, MASATERU TANIGUCHI, The Institute of Scientific and Industrial Research, Osaka University — Gating nanopore devices are composed of nanopores with embedded nanoelectrodes, and they are expected to be one of the core devices used to realize label-free, low-cost DNA sequencing, subsequently leading to \$1000\text{-}\text{genome sequencing technology.} The operating principle of these nanopores is based on identifying single base molecules of single DNA passing through a nanopore using a tunneling current between nanoelectrodes. We successfully identified single base molecules of DNA and RNA using tunneling currents. To make gating nanopore devices fit for practical use, core technologies should be integrated on one device chip. One core technology is the identification of single DNA and RNA composed of many base molecules using tunneling currents. We have succeeded in the single-molecule electrical sequencing of DNA and RNA formed by 3 and 7 base molecules, respectively, using a hybrid method of identifying single base molecules via a tunneling current and random sequencing. A method that controls the speed of a single DNA passing through a nanopore is one core technology that determines the speed and accuracy of sequencing. We successfully developed a method that controls the translocation speed of a single DNA by three orders of magnitude using a voltage between nanoelectrodes.

3:42PM W9.00003 DNA Electronic Fingerprints by Local Spectroscopy on Graphene\(^1\), ALEXANDER BALATSKY\(^2\), Los Alamos National Laboratory, NORDITA — Working and scalable alternatives to the conventional chemical methods of DNA sequencing that are based on electronic/ionic signatures would revolutionize the field of sequencing. The approach of a single molecule imaging and spectroscopy with unprecedented resolution, achieved by Scanning Tunneling Spectroscopy (STS) and nanopore electronics could enable this revolution. We use the data from our group [1] and others in applying this local scanning tunneling microscopy and illustrate possibilities of electronic sequencing of freeze dried deposits on graphene. We will present two types of calculated fingerprints: first in Local Density of States (LDOS) of DNA nucleotide bases (A,C,G,T) deposited on graphene[2]. Significant base-dependent features in the LDOS in an energy range within few eV of the Fermi level were found in our calculations. These features can serve as electronic fingerprints for the identification of individual bases in STS. In the second approach we present calculated base dependent electronic transverse conductance as DNA translocates through the graphene nanopore. Thus we argue that the fingerprints of DNA-graphene hybrid structures may provide an alternative route to DNA sequencing using STS.

1\(^{\text{Work supported by US DOE, NORDITA.}}\)

Our work paves the way towards the experimental study and control of Andreev bound states in ultracold atomic gases. In the presence of spin imbalance, the mass enhancement is more than fifty times larger than expectations from mean-field Bogoliubov-de Gennes theory.

Solitons in relativistic quantum field theory, and the spinless charged solitons responsible for the high conductivity of polymers. However, the free motion of fermions that often play a crucial role for the system’s transport properties. Famous examples are Andreev bound states inside vortex cores, fractionally charged leptons, etc. Here, solitons in strongly interacting quantum many-body systems play an important role, and the study of solitons is crucial.

Topological excitations are found throughout nature, in proteins and DNA, as dislocations in crystals, as vortices and solitons in superfluids and superconductors, and generally in the wake of symmetry-breaking phase transitions. In fermionic systems, topological defects may provide bound states for fermions that often play a crucial role for the system’s transport properties. Famous examples are Andreev bound states inside vortex cores, fractionally charged solitons in relativistic quantum field theory, and the spinless charged solitons responsible for the high conductivity of polymers. However, the free motion of topological defects in electronic systems is hindered by pinning at impurities. We have created long-lived solitons in a strongly interacting fermionic superfluid by imprinting a phase step into the superfluid wavefunction, and directly observed their oscillatory motion in the trapped superfluid. As the interactions are tuned from the regime of Bose-Einstein condensation (BEC) of tightly bound molecules towards the Bardeen-Cooper-Schrieffer (BCS) limit of long-range Cooper pairs, the effective mass of the solitons increases dramatically to more than 200 times their bare mass. This signals their filling with Andreev states and strong quantum fluctuations. For the unitary Fermi gas, the mass enhancement is more than fifty times larger than expectations from mean-field Bogoliubov-de Gennes theory. Our work paves the way towards the experimental study and control of Andreev bound states in ultracold atomic gases. In the presence of spin imbalance, the solitons created in our experiment represent one limit of the long sought-after Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state of mobile Cooper pairs.

In the presence of spin imbalance, the mass enhancement is more than fifty times larger than expectations from mean-field Bogoliubov-de Gennes theory.

Funding provided by the Swedish Research Council (VR), the Swedish Foundation for International Cooperation in Research and Higher Education (STINT), and the Carl Trygger Foundation for Scientific Research.
The dynamics of the center-of-mass dipole oscillation is studied in a broad parameter region as a function of spin-orbit coupling parameters as well as the oscillation amplitude. The anharmonic properties beyond the effective-mass approximation are revealed, such as the amplitude-dependent frequency and finite oscillation frequency at a place with a divergent effective mass. These anharmonic behaviors agree quantitatively with variational wave-function calculations. Moreover, we experimentally demonstrate a unique feature of the spin-orbit coupled system predicted by a sum-rule approach, stating that spin polarization significantly affects the THz emission efficiency. Therefore, the THz radiation from topological insulators can be used to ascertain the existence and characteristics of the Dirac-cone surface states.

2:42PM W13.00002 THz generation and the detection on the Dirac-cone surface states in topological insulator Bi$_2$Se$_3$\textsuperscript{1}

C. H. ZHANG, Peking University, FAN MING QU, Institute of Physics, Chinese Academy of Science — The topological insulator material Bi$_2$Se$_3$ is known to suffer from a non-insulating bulk due to doping caused by selenium vacancies. We present results on the synthesis and characterization of pure undoped Bi$_2$Se$_3$ crystals that exhibit nonmetallic transport behavior over the entire measured temperature range, from room temperature down to at least 2 K. Measurements of longitudinal transport and Hall effect are used to characterize the transport temperature and magnetic field dependences, carrier sign and density, and sensitivity to air exposure.

3:06PM W13.00004 Bulk versus surface contributions to the Shubnikov-de Haas Effect\textsuperscript{1}

E. MANIV, M. PETRUSHESKY, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel, A. RON, I. NEDER, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel, S. WIEDMANN, V.K. GUDURU, U. ZEITLER, J.C. MAAN, High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University Nijmegen, The Netherlands, K. CHASHKA, A. KANIGEL, Department of Physics, Technion-Israel Institute of Technology, Israel, Y. DAGAN, Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Israel — Among the bulk materials that are considered as experimental realizations of topological insulators Bi$_2$Se$_3$ is of particular interest due to its large bulk band gap and surface states with a single Dirac cone. It has been recently shown that Bi$_2$Se$_3$ can become superconducting when Cu intercalation is introduced (Hor, Y. S.; Williams, A. J. et al. Phys. Rev. Lett. 2010, 104, 057001). We report on transport measurements of cleaved flakes ~1–100 μm thick of Cu intercalated Bi$_2$Se$_3$. Clear Shubnikov-de Haas oscillations are observed. We study the temperature and angular dependence of these oscillations together with the Hall coefficient at low temperatures for various Cu concentrations. We discuss possible contributions from bulk and the protected surface states to the various transport channels.

3:18PM W13.00005 Modification of topological insulator transport properties by electron beam irradiation\textsuperscript{1}

ZILONG JIANG, ZHIYONG WANG, TAO LIN, JING SHI, Department of Physics and Astronomy, University of California, Riverside, CA, 92521 — Topological insulators (TI) are predicted to present a variety of interesting surface transport phenomena. However, in TI devices, the metallic bulk conduction usually overshadows the surface transport. In this work, we first fabricate TI devices based on our high bulk resistivity material (~5 Ω cm) Bi$_2$Sb$_2$Te$_3$ using ebeam lithography. Then we expose the devices with an electron beam to introduce disorders to localize the bulk carriers. The devices are ~100-200 nm in thickness and the resistivity is weakly temperature dependent. Upon initial low-energy exposures, we find that the resistance of device decreases and reaches a saturation state at the dosage increases. We attribute this decrease in resistivity to an increased electron density in the devices. As we ramp up the energy of the electron beam, the resistance starts to increase, showing the effect of additional scattering. At low temperatures, the resistance rapidly increases in a diverging trend. At 4 K, the magnetoresistance starts to display oscillatory features that are likely the Shubnikov-de Haas oscillations from the surface states. We believe that the disorders introduced by the electron beam play an important role in modifying the transport of the bulk carriers. More detailed experimental results and discussions will be presented.

\textsuperscript{1}This work was supported in part by DOE and UC-Lab Fees program.
3:30PM W13.00006 Topological Spin-Polarized Electron Layer above the Surface of Ca-Terminated Bi$_2$Se$_3$¹, XIAOXIONG WANG, College of Science, Nanjing University of Science and Technology, Nanjing 210094, China, GUANG BIAN, TOM MILLER, TAIChANG CHIANG, Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, USA — Spin-polarized gapless surface states on the boundary of topological insulators are of interest for spintronic applications. First-principles calculations show that adsorption of a Ca monolayer on films of the prototypical topological insulator, Bi$_2$Se$_3$, yields a substantial enhancement of the surface-state spin polarization, despite the low atomic mass of Ca and its weak spin-orbit coupling. Much of the topological surface electron distribution is transferred outside the Ca to form a polarized electron layer out in vacuum; this spatial separation from the substrate minimizes scattering by defects in Bi$_2$Se$_3$ and is very desirable for spin transport.

¹This work was supported by the National Natural Science Foundation of China (No. 11204133), the Jiangsu Province Natural Science Foundation of China (No. BK2012393), and the Young Scholar Project of NUST (No. AB41382).

3:42PM W13.00007 Strong single-ion anisotropy and anisotropic interactions of magnetic adatoms induced by topological surface states¹, ZHENGLU LI, JIHUI YANG, GUOHONG CHEN, Department of Physics, Fudan University, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, HONGJUN XIAN, XINGAO GONG, Department of Physics, Fudan University — The nature of the magnetism brought about by Fe adatoms on the surface of the topological insulator Bi$_2$Se$_3$ was examined in terms of density functional calculations. The Fe adatoms exhibit strong easy-axis magnetic anisotropy in the dilute adsorption limit due to the topological surface states (TSS). The spin exchange J between the Fe adatoms follows a Ruderman-Kittel-Kasuya-Yosida behavior with substantial anisotropy, and the Dzyaloshinskii-Moriya interaction between them is quite strong with $|D/J| \approx 0.3$ under the mediation by the TSS, and can be further raised to 0.6 by an external electric field. The apparent single-ion anisotropy of a Fe adatom is indispensable in determining the spin orientation.

¹NSFC, FANEDD, Pujiajiang Plan, Eastern Scholar

3:54PM W13.00008 The Fermi Surface of Highly Doped Bi$_2$Se$_3$ and the Implications for Superconductivity in CuBi$_2$Se$_3$, ELIAS LAHOUD, AMIT KANGEL, MUNTASER NAAMNEH, AMIT RIBAK, HANAN CHASKA, Technion-Israel Institute of Technology, MICHAL PETRUSHEVSKY, ERAN MANIV, YORAM DAGAN, Tel-Aviv University, KANGIEL GROUP TEAM, DAGAN GROUP TEAM — The 3D Fermi-surface (FS) mapping of Bi$_2$Se$_3$ for different samples with carrier-density ranging from $10^{17}$ to $10^{20}$ cm$^{-3}$ was made using Angle Resolved Photoemission Spectroscopy. While in the low carrier density samples a closed FS was observed, in high carrier density superconducting Cu$_x$Bi$_2$Se$_3$ samples the FS was found to be open. The open FS puts constraints on the possible order-parameters in this system.

4:06PM W13.00009 Scanning tunneling microscopy of defects and electronic fluctuations in Cu-doped Bi$_2$Se$_3$, CHRISTOPHER MANN, University of Texas at Austin, DAMIEN WEST, Rensselaer Polytechnic Institute, IRENEUSZ MIOTKOWSKI, YONG CHEN, Purdue University, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, CHIH-KANG SHIH, University of Texas at Austin — We report scanning tunnel microscopy and spectroscopy studies of the topological insulator Cu$_x$Bi$_2$Se$_3$. We have identified five different atomic-resolution signatures of Cu dopant-related point defects and correlated several of them to density functional theory simulations of the defects. Most interestingly, by investigating the dI/dV images of the known Bi$_{25}$ antisite defects as a function of bias, we show that local electronic structure can vary substantially over a length scale of 30nm, with amplitudes as large as ±50meV. The strong fluctuations appear to be caused by a variety of defects and may have consequences for the topological surface state, as revealed by quasiparticle scattering studies. Correlation of quasiparticle scattering with the various defects indicates that the surface state is robust to backscattering, though detailed analysis shows that some defects are more effective in producing stationary scattering states than others.

4:18PM W13.00010 Probing the pairing symmetry of candidate topological superconductor Cu$_x$Bi$_2$Se$_3$ via point contact spectroscopy, XUNCHI CHEN, CHAO JUAN, Georgia Institute of Technology, YEW SAN HOR, Missouri University of Science and Technology, CARLOS SA DE MELO, ZHIGANG JIANG, Georgia Institute of Technology — We perform point contact spectroscopy measurements on the candidate topological superconducting material, Cu$_x$Bi$_2$Se$_3$, using a normal-metal gold tip or an s-wave superconductor niobium tip. For the Au- Cu$_{25}$Bi$_2$Se$_3$ interface, we observe a marked zero-bias conductance peak in the point contact spectra on the superconducting area of the sample, indicative of unconventional superconducting pairing symmetry. The point contact spectra also exhibit a pronounced linear background, which we attribute to inelastic scattering at the tip-sample interface. We compare the background subtracted spectra to a single-band p-wave model. For the Nb- Cu$_{25}$Bi$_2$Se$_3$ interface, we observe a two-gap-like feature in the spectra, corresponding to the superconducting gap of the niobium and the sample, respectively. In addition, we find that the spectra are highly dependent on the interface barrier strength, and exhibit non-monotonic temperature dependence at zero bias, possibly owing to the incompatibility of the pairing symmetries between the Nb tip and the sample. Our results signify the unconventional superconductivity in Cu$_x$Bi$_2$Se$_3$.

4:30PM W13.00011 Quantum oscillations in topological superconductor candidate Cu$_x$Bi$_2$Se$_3$, BENJAMIN LAWSON, GANG LI, Physics Dept., Univ. of Michigan, YEW SAN HOR, Physics Dept., Missouri S&T, LU LI, Physics Dept., Univ. of Michigan — In Cu$_x$Bi$_2$Se$_3$, a candidate to be a 3-dimensional topological superconductor, it is of high interest to study how its bulk electronic structure differs from Bi$_2$Se$_3$, since the nature of the emergent bulk superconducting order puts constraints on the possible surface state. The de Hass-van Alphen effects is observed on a single crystals of Cu$_{25}$Bi$_2$Se$_3$ using sensitive torque magnetometry. Our results show that the Cu doping in Bi$_2$Se$_3$ increases the carrier density and the effective mass, without increasing the scattering rate or decreasing the mean free path. In addition, the Fermi velocity remains the same in copper doped samples, indicative of unconventional superconducting pairing symmetry. The point contact spectra also exhibit a pronounced linear background, which we attribute to inelastic scattering at the tip-sample interface. We compare the background subtracted spectra to a single-band p-wave model. For the Nb- Cu$_{25}$Bi$_2$Se$_3$ interface, we observe a two-gap-like feature in the spectra, corresponding to the superconducting gap of the niobium and the sample, respectively. In addition, we find that the spectra are highly dependent on the interface barrier strength, and exhibit non-monotonic temperature dependence at zero bias, possibly owing to the incompatibility of the pairing symmetries between the Nb tip and the sample. Our results signify the unconventional superconductivity in Cu$_x$Bi$_2$Se$_3$.

4:42PM W13.00012 Gapped Dirac surface states in In doped topological insulator Bi$_2$Se$_3$, WEIDA WU, QUANTONG SHEN, XUEYUN WANG, SANG-WOOK CHEONG, Rutgers Center for Emergent Materials & Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, 08854 — Topological insulators host helical Dirac surface states which linearly disperse through the bulk band gap. The unusual helical surface states are protected by time reversal symmetry, and therefore believed to be robust against disorders that do not break time reversal symmetry. It has been debated whether massive Dirac surface states (i.e., a gap at the Dirac point) are experimentally observed in doped topological insulators [1-3]. Herein, we report the observation of a spectroscopic gap of topological surface states in Bi$_{25}$In$_{25}$Se$_3$ using low temperature scanning tunneling microscopy and spectroscopy (LT-STM/STS). The tunneling spectroscopic maps suggest that the interactions between In dopants effectively change the topological class of local band structure, resulting in a nanoscale mixture of topologically trivial and nontrivial states. This electronic inhomogeneity poses a nanoscale spatial confinement to the Dirac surface states so that the long wavelength surface states near the Dirac point are suppressed, i.e. a gap is opened at the Dirac point.


[1] This work is supported by NSF DMR grant 0848807.
4:54PM W13.00013 Topological phase transition in the (Bi$_{1-x}$In$_x$)$_2$Se$_3$ system investigated via STM. WENWEN ZHOU, YOSHINORI OKADA, ZHENSONG REN, DANIEL WALKUP, STEPHEN WILSON, VIDYA MADHAVAN, Boston College — Transport and photoemission measurements on (Bi$_{1-x}$In$_x$)$_2$Se$_3$ have shown that the system transforms from a pure (x=0) topological insulator (TI) into a topologically trivial material (x > 0.07) through a topological phase transition. Indium (In) substitution for heavier Bismuth is expected to have a large effect on the electronic properties of TIs and is a very sensitive way to tune spin-orbit coupling while maintaining the same lattice structure. In this talk we present scanning tunneling microscopy measurements of the surface state and electronic structure of (Bi$_{1-x}$In$_x$)$_2$Se$_3$ single crystals over a wide range of In concentrations. We identify the local density signature of the In impurities and use these local measurements to determine the actual doping levels. Using spectroscopy and Fourier transform maps we then trace the evolution of the topological insulator into the trivial phase, thereby providing insights into the nanoscale evolution of this process.

This work is supported by the US Department of Energy under grant DE-FG05-91ER40627.

5:06PM W13.00014 Topological-Metal to Band-Insulator Transition in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ Thin Films. MATTHEW BRAHLEK, NAMRATA BANSAL, NIKESH KOIRALA, Rutgers University Physics and Astronomy Department, SU-YANG XU, MAD-HAB NEUPANE, CHANG LIU, M. ZAHID HASAN, Princeton University Physics Department, SEONGSHIK OH, Rutgers University Physics and Astronomy Department — By combining transport and photoemission measurements on (Bi$_{1-x}$In$_x$)$_2$Se$_3$ thin films, we report that this system transforms from a topologically nontrivial metal into a topologically trivial band insulator through three quantum phase transitions. At x \approx 3\%-7\%, there is a transition from a topologically nontrivial metal to a trivial metal. At x \approx 15\%, the metal becomes a variable-range-hopping insulator. Finally, above x \approx 25\%, the system becomes a true band insulator with its resistance immeasurably large even at room temperature. This material provides a new venue to investigate topologically tunable physics and devices with seamless gating or tunneling insulators.

5:18PM W13.00015 Theoretical study of topological phase transitions in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ and (Bi$_{1-x}$Sb$_x$)$_2$Se$_3$. JIANPENG LIU, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — We use first-principles calculations to study the phase transition from a topological to a normal insulator with concentration x in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ and (Bi$_{1-x}$Sb$_x$)$_2$Se$_3$ in the Se$_3$ crystal structure. The spin-orbital coupling (SOC) strength is similar in In and Sb, which have similar atomic numbers, so that if the topological transitions in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ and (Bi$_{1-x}$Sb$_x$)$_2$Se$_3$ are purely driven by the decrease of SOC strength, we would expect to see similar critical concentrations x_c in the two systems. However, based on our preliminary calculations, x_c is much lower in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ than in (Bi$_{1-x}$Sb$_x$)$_2$Se$_3$, indicating that different mechanisms control the behavior in the two cases. Specifically, in (Bi$_{1-x}$Sb$_x$)$_2$Se$_3$ we find that the phase transition is mostly dominated by the decrease of SOC. However, for (Bi$_{1-x}$In$_x$)$_2$Se$_3$, the In 5s orbitals also play an important role, both in the phase-transition behavior and in determining the indirect bulk band gap. Finally, we discuss the accuracy of the energy-level position of the In 5s orbitals in (Bi$_{1-x}$In$_x$)$_2$Se$_3$ as predicted by density-functional theory and more advanced methods.


2:30PM W19.00001 Spin and holographic metals. VICTOR ALEXANDROV, PIERS COLEMAN, Rutgers University — We examine the spin structure of the Green’s function of the holographic metal, demonstrating that the excitations of the holographic metal are “chiral,” lacking the inversion symmetry of a conventional Fermi surface, with only one spin orientation for each point on the Fermi surface aligned parallel to the momentum. This implies that ferromagnetic spin fluctuations are absent from the holographic metal, leading to a complete absence of Pauli paramagnetism. The talk will discuss a possibility of going to a 3-dimensional holographic metal, where electrons should have both left- and right-handed chiralities.


3 This work is supported by the US Department of Energy under grant DE-FG05-91ER40627.
3:30PM W19.00006 Metal-Insulator Transition from Holography. SEAN HARTNOLL, Stanford University, ARISTOMETENIS DONOS, Imperial College London — The holographic correspondence allows theoretical control of certain phases of matter that do not admit a quasiparticle description. This approach has proved helpful for the description of quantum critical transport. I will present holographic results for transport away from particle-hole symmetry. This requires explicit inclusion of lattice effects to render the conductivity finite. I will show that the holographic system undergoes a metal-insulator transition as a function of the strength of the lattice. This results implies that holography is capable of describing localization physics in strongly interacting systems. I will present results for the optical conductivity, exhibiting a transition from a metallic drude peak to Mott insulating behavior.

3:42PM W19.00007 Multipoint correlators of conformal field theories: implications for quantum critical transport. PHILIPP STRACK, DEBANJAN CHOWDHURY, Harvard, SUVRAT RAJU, Bangalore, SUBIR SACHDEV, Harvard, AJAY SINGH, Waterloo — We relate three-point correlators between the stress-energy tensor and conserved currents of conformal field theories (CFTs) in 2+1 dimensions to observables of quantum critical transport. We first compute the correlators in the large-flavor-number expansion of conformal gauge theories and then do the computation using holography. In the holographic approach, the correlators are computed from an effective action on 3+1 dimensional anti-de Sitter space (AdS3), and depend upon the co-efficient, $\gamma$, of a four-derivative term in the action. We find a precise match between the CFT and the holographic results, thus fixing the values of $\gamma$. The CFTs of free fermions and bosons take the values $\gamma = 1/12$, $-1/12$ respectively, and so saturate the bound $|\gamma| \leq 1/12$ obtained earlier from the holographic theory: the correlator of the conserved gauge flux of U(1) gauge theories takes intermediate values of $\gamma$. The value of $\gamma$ also controls the frequency dependence of the conductivity, and other properties of quantum-critical transport at non-zero temperatures. Our results for the values of $\gamma$ lead to an appealing physical interpretation of particle-like or vortex-like transport near quantum phase transitions of interest in condensed matter physics.

3:54PM W19.00008 The quasi-normal modes of quantum criticality$^1$. WILLIAM WITCZAK-KREMPA, Perimeter Institute, SUBIR SACHDEV, Harvard University — We study the general features of charge transport of quantum critical points described by CFTs in 2+1D. We use an effective field theory on an asymptotically AdS spacetime, expanded to fourth order in spatial and temporal gradients. The presence of a horizon at non-zero temperatures implies that this theory has quasi-normal modes with complex frequencies. The quasi-normal modes determine the poles and zeros of the conductivity in the complex frequency plane, and so fully determine its behavior on the real frequency axis, at frequencies both smaller and larger than the temperature. We describe the role of particle-vortex or S-duality on the conductivity, specifically how it maps poles to zeros and vice versa. These analyses motivate two sum rules obeyed by the quantum critical conductivity. Finally, we compare our results with the analytic structure of the O(N) model in the large-N limit, and other CFTs.

$^1$Supported by Walter Sumner Foundation, NSF, ARO.

4:06PM W19.00009 FFLO States in Holographic Superconductors. GEORGE SIOPSIS$^2$, University of Tennessee, JAMES ALSUP, University of Michigan - Flint, ELEFTHERIOS PAFANTONOPOULOS, National Technical University of Athens — We discuss a novel mechanism to set up a gravity dual of FFLO states in strongly coupled superconductors. The gravitational theory utilizes two $U(1)$ gauge fields and a scalar field coupled to a charged AdS black hole. The first gauge field couples with the scalar sourcing a charge condensate below a critical temperature, and the second gauge field provides a coupling to spin in the boundary theory. The scalar is neutral under the second gauge field. By turning on an interaction between the Einstein tensor and the scalar, it is shown that, in the low temperature limit, an inhomogeneous solution possesses a higher critical temperature than the homogeneous case, giving rise to FFLO states.

$^2$Supported by the US Department of Energy under Grant No. DE-FG05-91ER40627.

4:18PM W19.00010 Study of Higgs mode near quantum critical points. YEJIN HUH, SUBIR SACHDEV, Harvard University — We present a study of Higgs excitation mode in different quantum theories in 2 space dimensions. $O(N)$ theory and $CP^N$ theory near the quantum critical points will be discussed for zero and finite temperature. Electron systems with fermi surfaces will be studied under this framework.

4:30PM W19.00011 Superconductivity in a model involving transverse gauge bosons$^1$. IPSITA MANDAL, SUDIP CHAKRABARTY, SUK BUM CHUNG, University of California Los Angeles — It has been known for some time that a system of fermions interacting with transverse gauge bosons does not behave like a Fermi liquid and provides a bona fide model for a non-Fermi liquid. Here we study superconductivity in this model. Preliminary calculations show explicitly that a superconducting gap exists only for couplings greater than a threshold. It is hoped that a proper elucidation of this problem would lead to insights that may be useful in developing effective low energy theories of realistic physical problems, such as the normal state of high temperature superconductors, the state of half-filled quantum Hall systems, or the color superconductivity in the quark-gluon system, or even in the effects of disorder in a non-Fermi liquid system that could provide a new paradigm.

$^1$This work is being supported by NSF under Grant number DMR-1004520.

4:42PM W19.00012 Detection of Higgs mode in D-wave Superconductors. YAFIS BARLAS, CHANDRA VARMA, University of California at Riverside — Higgs modes, which are collective excitations of the amplitude of the order parameter, have zero spin and no charge, do not couple directly to experimental probes. They are, however, linearly coupled to excitations which shake the ground state and therefore appear as poles or branch-cuts in their self-energy. In the superconducting state the Higgs modes can be distinguished from other excitations because they can only appear as satellites which steal all their spectral weight from excitations which promote superconductivity. This is an observable effect if such excitations and the Higgs modes are not too far separated in energy. We show that the Higgs mode in the $\Delta_{1g}$ Raman scattering channel appears as a sharp resonance below $\Delta$ in the spectral weight of excitations responsible for superconductivity in Cuprates in a class of theories. Comparison is made with existing experiments and further experiments to confirm or rule out the idea are proposed.
under pressures up to a maximum of \( \approx 1.4 \) GPa. For \( P \), we also observe a broad hump in \( \partial \rho / \partial T \) at a temperature \( T^* \), which increases with increasing \( P \). We will compare these measurements to expectations for prototypical felectron quantum critical point (QCP) systems (e.g., CeRhIn\(_5\) and CeRh\(_2\)Si\(_2\)) and the iron arsenide high temperature superconductors (e.g., CaFe\(_2\)As\(_2\), SrFe\(_2\)As\(_2\), and BaFe\(_2\)As\(_2\)) and discuss implications for studying a possible d-electron QCP in the absence of superconductivity.

Anomalous thermodynamic power laws in nodal superconductors\(^1\). JORGE QUINTANILLA, University of Kent and ISIS Facility, STFC Rutherford Appleton Laboratory, BAYAN MAZIDIAN, University of Bristol and ISIS Facility, STFC Rutherford Appleton Laboratory — Unconventional superconductors are frequently identified by the observation of power law behaviour on low temperature thermodynamic properties such as specific heat. These power laws generally derive from the linear spectrum near points or lines of zeros, or nodes, in the superconducting energy gap on the Fermi surface. Here we show that, in addition to the usual point and line nodes, a much wider class of different nodal types can occur. Some of these new types of nodes typically occur when there are transitions between different types of gap node topology, for example when point or line nodes first appear as a function of some physical parameter. We derive anomalous, non-integer thermodynamic power laws associated with these new nodal types and predict their occurrence in iron pnictide superconductors and in the noncentrosymmetric system Li\(_2\)Pd\(_3\)\(_2\)Pt\(_3\).  

\(^1\) This work was supported by EPSRC and STFC (U.K.) J.Q. gratefully acknowledges funding from HEFCE and STFC through the South-East Physics network (SEPnet).

Anomalous angular dependence of the upper critical induction of orthorhombic ferromagnetic superconductors with completely broken \( p \)-wave symmetry. CHRISTOPHER LÖRSCHER, University of Central Florida, JINGCHUAN ZHANG, QIANG GU, University of Science and Technology Beijing, RICHARD KLEMM, University of Central Florida — We calculate the angular dependence of the upper critical field, \( H_{c2}(\theta, \phi, T) \), for an orthorhombic ferromagnetic superconductor with a general ellipsoidal Fermi surface with effective masses \( m_1 \), \( m_2 \), and \( m_3 \) in which we have \( p \)-wave parallel-spin pairing that is locked onto the \( z \)-axis direction. We report anomalous angular dependence of \( H_{c2} \) for fixed \( 3 < m_1 (m_1 \cos^2 \theta + m_2 \sin^2 \theta) \), for which we observe a peak in \( H_{c2} \) for some angle \( 0^\circ < \theta < 90^\circ \), providing a sensitive test of the order parameter symmetry in materials such as URhGe. This technique can be generalized to other order parameter symmetries. We have also made relevant predictions about the angular dependence of \( H_{c2} \) for the low-field superconducting phase of URhGe.
— We solve a theoretical problem about the upper critical magnetic field, parallel to a conducting axis of a layered quasi-one-dimensional superconductor. In particular, we consider the case, where triplet superconducting order parameter is not sensitive to the Pauli destructive effects against superconductivity and has no zeros on two quasi-one-dimensional pieces of the Fermi surface. We demonstrate [1] that in this case the orbital destructive effects against superconductivity can destroy superconducting state at magnetic fields much higher than the so-called Clogston-Chandrasekhar paramagnetic limit. Comparison of our theoretical results with the very recent experimental data [2] is in favor of a triplet superconducting pairing in the layered quasi-one-dimensional superconductor Li$_{0.9}$Mo$_6$O$_{17}$.


1This work was supported by the NSF under Grant DMR-1104512.

3:30PM W35.00006 Triplet Nodeless Superconductivity Scenario in the Quasi-One-Dimensional Layered Conductor Li$_{0.9}$Mo$_6$O$_{17}$

3:42PM W35.00007 Ferromagnetism in CuFeSb: Evidence of competing magnetic interactions in Fe-based superconductors

4:06PM W35.00009 Physical properties of Kx(Ni,Fe)2-ySe2 single crystal alloys

4:18PM W35.00010 Physical and magnetic properties of LaFe$_{0.6}$Sb$_{1.4}$

1Research supported by a DOD National Security Science and Engineering Faculty Fellowship via the AFOSR.
4:30PM W35.00011 Quasi-two-dimensional non-collinear magnetism in the Mott insulator Sr$_2$Fe$_2$FeO$_6$[1]. SHAN WU, C. BROHOLM, Johns Hopkins University, LIANG L. ZHAO, JIAKUI K. WANG, E. MOROSAN, Rice University, J.P. HODGES, Oak Ridge National Laboratory. JOHNS HOPKINS UNIVERSITY TEAM, RICE UNIVERSITY COLLABORATION — We study the magnetism of Sr$_2$Fe$_2$FeO$_6$ through neutron powder diffraction and thermodynamic and transport measurement. Quasi-two-dimensional magnetic order develops below $T_N=106K$ with an in-plane correlation length exceeding 310 Å and an out-of-plane correlation length of only 17(3) Å. The data are well described by a two-k structure with $k_1=(1/2,0,1/2)$ and $k_2=(0.1,2/1,2)$. The ordered moment is 3.3(1) $\mu_B$ oriented along the in-plane components of k. This structure is composed of orthogonal AFM chains intersecting at super-exchange mediating O sites. The Density Function Theory (by Liang L. Zhao, Jiakui K. Wang, etc.) also leads to this structure and a narrower Fe 3d band than for the iron pnictides from which electronic correlations produce a Mott insulator.

1This research was supported by the U.S. DoE under award DE-FG02-08ER46544 and contract DEAC05-00OR22725 with UT-Battelle, LLC. The work at Rice University was supported by AFOSR-MURL.

4:42PM W35.00012 Functional interfaces in La$_2/3$Ca$_{1/3}$MnO$_3$ / YBa$_2$Cu$_3$O$_{7-x}$ heterostructures[1]. TRA VU THANH, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, YING-JIUN CHEN, HONG-JI LIN, National Synchrotron Radiation Research Center, Hsinchu 30010, Taiwan, YU-JUAN LIN, Institute of Physics, National Chiao Tung University, Hsinchu 30010, Taiwan, YING-HAO CHU, Department of Materials Science and Engineering, National Chiao Tung University Hsinchu 30010, Taiwan — Interfaces have emerged as one of the focal points of current condensed matter science. In complex, correlated oxides, heterointerfaces provide a powerful route to create and manipulate the charge, spin, orbital, and lattice degrees of freedom. In this study, epitaxial bilayers of ferromagnetic of La$_2/3$Ca$_{1/3}$MnO$_3$ (LCMO) and superconducting YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) with two distinct interfaces have been fabricated to understand the effects of these two distinct interfaces. X-ray absorption near edge spectroscopy (XANES) was applied to characterize the interfaces and also provided direct evidence of the charges transfer at these interfaces. The studies of the macroscopic properties, such as the transport and magnetic properties, established the connection between macroscopic properties and the interface structures. This present study opens new venue to design the functional interfaces.

1This work was supported by National Science Council of Taiwan, ROC

4:54PM W35.00013 Superconducting interface in cuprate p-n heterostructures[1], MAXIME DION, LAURENT OLIVIER, GUILLAUME HARDY, SÉBASTIEN GODIN-PROULX, PATRICK FOURNIER, Université de Sherbrooke — In this explorative work, we combined two kinds of non-superconducting cuprates: over-doped Pr$_{2-x}$Ce$_x$CuO$_4$ and under-doped La$_{2-x}$Sr$_x$CuO$_4$ in the same p-n heterostructures in order to generate new behaviors through the interplay between the two materials. We will show that a thin superconducting layer (< 10 nm) arise at the interface between these two compounds. We will discuss its actual location, its unexpected occurrence and its origin which is partly compatible with a charge transfer scenario that takes place in similar p-p cuprate heterostructures [1,2].

1Supported by NSERC, FQRNT and CIFAR

5:06PM W35.00014 Electron Doping by Charge Transfer at LaFeO$_3$/Sm$_2$CuO$_4$ Epitaxial Interfaces, JACOBO SANTAMARIA, F.Y. BRUNO, GFMC. Dpt. Applied Physics. U. Complutense, M. VARELA, Materials science and Technology Div. Oak Ridge National Laboratory. Tn 37831-6071, J. GARCIA-BARRIOCANAL, A. RIVERA, R. SCHMIDT, C. LEON, GFMC. Dpt. Applied Physics. U. Complutense, P. THAKUR, J.C. CEZAR, N.B. BROOKES, European Synchrotron Radiation Facility (ESRF), P. 220 Grenoble Cedex 38043 France, M. GARCIA HERNANDEZ, Instituto de Ciencia de Materiales ICMM CSIC 28049 Madrid, E.R. DAGOTTO, S.J. PENNYCOOK, Materials science and Technology Div. Oak Ridge National Laboratory. Tn 37831-6071 — We examine the interfacial charge transfer in epitaxial heterostructures formed between Mott insulating Sm$_2$CuO$_4$ (SCO) and charge transfer insulator LaFeO$_3$ (LFO) in LFO/SCO superlattices. High resolution EELS measurements at the O-K edge have provided evidence for 0.09/-0.01 extra electrons in the SCO d- band as revealed by a reduction of the Cu oxidation state. The transfer of electrons from LFO to SCO is further supported by the spectroscopic signature of Cu$^{+1}$ as obtained from XAS measurements. Transport measurements have evidenced a metallic state at the interface between these two nominally insulating materials. Dielectric spectroscopy measurements have allowed ascribing the metallic state to the LFO/SFO interfaces, consistent with DC measurements. When lowering the temperature a metal to insulator transition occurs at 120 K, indicating, in accordance with the phase diagram, an insufficient doping level to enter a superconducting state.

Friday, March 22, 2013 8:00AM - 11:00AM — Session Y1 DCMP: Invited Session: New Perspectives on Kondo Systems Ballroom I - David Goldhaber-Gordon, Stanford University

8:00AM Y1.00001 Frustration & Order in Kondo Lattice Systems, MEIGAN ARONSON, Stony Brook University — No abstract available.

8:36AM Y1.00002 Visualizing heavy fermions emerging in a quantum critical Kondo lattice[1], PEGOR AYNAJIAN, Princeton University — In solids containing elements with $f$ orbitals, the interaction between $f$-electron spins and those of itinerant electrons leads to the development of low-energy fermionic excitations with a heavy effective mass. These excitations are fundamental to the appearance of unconventional superconductivity and non-Fermi-liquid behavior observed in actinide- and lanthanide-based compounds. We use spectroscopic mapping with the scanning tunneling microscope to detect the emergence of heavy excitations with lowering of temperature in a prototypical family of cerium-based heavy-fermion compounds. We demonstrate the sensitivity of the tunneling process to the composite nature of these heavy quasiparticles, which arises from quantum entanglement of itinerant conduction and $f$ electrons. Scattering and interference of the composite quasiparticles is used to resolve their energy–momentum structure and to extract their mass enhancement, which develops with decreasing temperature. The lifetime of the emergent heavy quasiparticles reveals signatures of enhanced scattering and their spectral lineshape shows evidence of energy–temperature scaling. These findings demonstrate that proximity to a quantum critical point results in critical damping of the emergent heavy excitation of our Kondo lattice system.

1This work is funded by a DOE-BES grant. Partial support for instrumentation is provided by NSF-DMR, Keck Foundation, and NSF-MRSEC. PA also acknowledges support of a fellowship through the PCCM funded by NSF MERSEC.
9:12AM Y1.00003 Observation of Majorana-like Behavior at the Quantum Critical Point in a Resonant Level Coupled to a Dissipative Environment. GLEB FINKELSTEIN, Duke University — We investigate tunneling through a resonant level embedded in a dissipative environment, which suppresses tunneling rates at low temperatures. Specifically, the resonant level is formed in a carbon nanotube quantum dot, and the dissipative environment is realized by fabricating resistive leads. For the symmetric coupling of the resonant level to the two leads, we find that the resonant peak reaches the unitary conductance $e^2/h$ despite the presence of dissipative modes. Simultaneously, the width of the resonance tends to zero as a non-trivial power of temperature. We draw a connection between our system and a resonant tunneling in a Luttinger liquid and interpret the observed unitary resonance of vanishing width in terms of a quantum critical point (QCP). We further investigate an exotic state of electronic matter obtained by fine-tuning the system exactly to the QCP and report on several transport scaling laws both near and far from equilibrium. Particularly striking is a quasi-linear non-Fermi liquid scattering rate found at the QCP, interpreted in terms of a model with Majorana modes at the resonant level. Although unlikely to be practical for fault-tolerant quantum computing, our device constitutes a viable alternative to topological superconductors as a platform for studying strong correlation effects within Majorana physics.

1This work was supported by the DOE and done in collaboration with H. T. Mebrahtu, I. V. Borzenets, H. Zheng, D. E. Liu, Y. V. Bomze, A. I. Smirnov, S. Florens, and H. U. Baranger.

9:48AM Y1.00004 Nonequilibrium Kondo model: Real-time RG study of crossover from weak to strong coupling. MIKHAIL PLETYUKHOV, Institute for Theory of Statistical Physics, RWTH Aachen University — We analyze the nonequilibrium Kondo model at finite voltage and temperature by using a new formulation [1] of the real-time renormalization group [2] with the Laplace variable as the flow parameter. We evaluate the energy-dependent spin relaxation rate and nonlinear conductance, and derive an approximate form for the universal line shape for the latter in the whole crossover regime from weak to strong coupling (that is, from high to low energy scales). The results are shown to agree well with exact methods and the numerical renormalization group in equilibrium, Fermi liquid theory, weak-coupling expansions, and recent experiments [3].

References:

10:24AM Y1.00005 Quantum quench of Kondo correlations in optical absorption. ANDREAS WEICHELBAUM. Ludwig Maximilians University — Absorption spectra of individual semiconductor quantum dots tunnel-coupled to a degenerate electron gas in the Kondo regime have recently become accessible to the experiment [1]. The absorption of a single photon leads to an abrupt change in the system Hamiltonian, which can be tailored such that it results in a quantum quench of the Kondo correlations. This is accompanied by a clear signature in the form of an Anderson orthogonality catastrophe, induced by a vanishing overlap between initial and final many-body wave functions and with power-law exponents that can be tuned by an applied magnetic field. We have modeled the experiment in terms of an Anderson impurity model undergoing an optically induced quench, and studied this Kondo exciton in detail using both analytical methods and the Numerical Renormalization Group (NRG). Our NRG results reproduce the measured absorption line shapes very well, showing that NRG is ideally suited for the study of Kondo excitons. In summary, the experiments demonstrate that optical measurements on single artificial atoms offer new perspectives on many-body phenomena previously studied using transport spectroscopy only.


Friday, March 22, 2013 8:00AM - 11:00AM — Session Y2 DCMP: Invited Session: Magnetism and non-Fermi Liquid in Heavy Fermion Metals

8:00AM Y2.00001 Dimensionality and quantum criticality in heavy fermion metals. SILKE PASCHEN, Vienna University of Technology — Heavy fermion compounds are at the forefront of research on quantum criticality. This is due to the fact that many of these materials can be tuned to a quantum critical point (QCP) by readily accessible values of the control parameters magnetic field, pressure or substitution/doping. In recent years efforts are being made to classify the different kinds of quantum critical behavior experimentally observed, to test the extent to which heavy fermion quantum criticality is universal. We have identified a cubic heavy fermion material, Ce$_2$Pd$_{20}$Si$_6$, as exhibiting a field-induced quantum phase transition as the lower of two consecutive phase transitions is suppressed to zero. This transition is accompanied by an abrupt change of Fermi surface [1], reminiscent of what happens across the field-induced antiferromagnetic to paramagnetic transition in tetragonal YbRh$_2$Si$_2$ [2]. In Ce$_2$Pd$_{20}$Si$_6$, the QCP separates two different ordered phases. In fact, a Kondo destruction QCP [3] has been theoretically predicted to exist in the ordered portion of a global phase diagram for quantum critical heavy fermion compounds [4]. We conclude that dimensionality is an effective way to tune through such a global phase diagram and that the cubic material studied here is situated in the barely explored three-dimensional portion of this phase diagram. We believe that this finding will guide the search for further experimental anchoring points in the global phase diagram, and for a unified theoretical description.


1We acknowledge financial support from the European Research Council (ERC Advanced Grant No 227378).
8:36AM Y2.00002 From incommensurate correlations to mesoscopic spin resonance in YbRh2Si2. COLIN BROHOLM, Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University — Spin fluctuations are reported near the magnetic field driven quantum critical point in YbRh2Si2 [1]. On cooling, ferromagnetic fluctuations evolve into incommensurate correlations with a characteristic in-plane wave vector of \(q_{\|} = (\delta, \delta)\) with \(\delta = 0.14 \pm 0.04\) r.l.u. At low temperatures, an in plane magnetic field induces a sharp intra doublet resonant excitation at an energy \(\epsilon_{2g} B_{\perp} H\) with \(\epsilon_{2g} = 3.8 \pm 0.2\). The intensity is localized at the zone center and has a width in momentum space indicating precession of spin density extending \(\xi = 6 \pm 2\) Å beyond the 4f site.


1Work at IQM was supported by DoE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Award DE-FG02-08ER46454.

9:12AM Y2.00003 Critical quasi-particle theory and scaling near a Quantum Critical Point of Heavy Fermion metals. PETER WÖLFLE, ITKM and INT, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — We recently developed a theory of the critical properties of a heavy fermion metal near an antiferromagnetic (AFM) quantum phase transition governed by three-dimensional spin fluctuations. The critical spin fluctuations induce critical behavior of the electron quasi-particles (qp) as seen in a diverging effective mass, leading, e.g., to a diverging specific heat coefficient. This in turn gives rise to a modification of the spin excitation spectrum [1]. We use that the concept of electron quasi-particles is well-defined as long as the qp width is less than their excitation energy, which is still the case in the so-called non-Fermi liquid regime. Impurity scattering [1,2] and/or higher order loop processes in the clean system [3] cause a redistribution of the critical scattering at the hot lines all over the Fermi surface, leading to a weakly momentum dependent critical self-energy. We derive a self-consistent equation for the qp effective mass which allows for two physical solutions: the usual weak coupling spin density wave solution and a strong coupling solution featuring a power law divergence of the effective mass as a function of energy scale. The resulting spin excitation spectrum obeys \(E/T\) scaling with dynamical exponent \(z=4\) and correlation length exponent \(\nu = 1/3\), in excellent agreement with data for YbRh2Si2 [1,2]. Results of our theory applied to three-dimensional metals featuring quasi-two-dimensional spin fluctuations will be presented with the aim of explaining the observed properties of the AFM quantum critical point of CeCu6−xAlx, in particular the \(E/T\) scaling exhibited by inelastic neutron scattering data. In that case we find \(z=8/3\) and \(\nu = 3/7\) [3]. Finally, the microscopic underpinning of our theory will be addressed, including the issues of qp renormalization, vertex corrections, interaction of bosonic fluctuations in the renormalization group sense, and higher loop corrections [3].


9:48AM Y2.00004 Ferromagnetic quantum criticality in heavy fermion systems1, MANUEL BRANDO, Max Planck Institute for Chemical Physics of Solids, Noethnitzer Strasse 40, 01187 Dresden, Germany — Heavy fermion (HF) systems are metals where the weak hybridisation between nearly localized \(f\)-electrons and the mobile conduction electrons, i.e., the Kondo effect, leads to a Fermi liquid (FL) ground state with narrow bands and quasiparticles with strongly enhanced effective electronic masses. When the magnetic RKKY interaction becomes comparable to the Kondo interaction, magnetic order can appear, mostly at very low \(T\). The magnetic order can be suppressed by an external parameter, e.g. pressure or magnetic field, inducing a quantum phase transition (QPT) at \(T = 0\). If this QPT is continuous, the associated quantum critical point (QCP) is surrounded by a non-FL regime of quantum critical fluctuations where unconventional superconductivity or novel phases of matter may arise [1]. The unambiguous observation of antiferromagnetic (AFM) QCPs in HF systems [2] has led to an increasing number of theoretical and experimental works in order to understand QPTs as deeply as their classical counterpart. Although it has been demonstrated that in antiferromagnets QCPs exist, in ferromagnets there is still no clear evidence. Intensive investigations have shown that metallic ferromagnets are inherently unstable [3,4] and do not exhibit a FM QCP. However, in the recently discovered HF system YbNi1−xP2, a quasi-1D ferromagnet with a remarkably-low \(T_C = 0.15\) K [5], the \(T\)-divergence in the Grüneisen ratio points to the presence of a FM QCP. I will present a general overview of the state of the art of quantum criticality in HF systems, discussing in particular the cases of YbNi1−xP2, CeFePO, CePd1−xRh3, as well as the AFM system YbRh2Si2 where FM order is induced by chemical pressure.


1Part of this work has been supported by the DFG Research Unit 960 “Quantum Phase Transitions”


Friday, March 22, 2013 8:00AM - 11:00AM –
Session Y3 DCMP DCOMP: Invited Session: New Directions in Fractional Quantum Hall Phenomena Ballroom III - Mansour Shayegan, Princeton University

8:00AM Y3.00001 Local thermometry and compressibility measurements as new probes of strongly correlated states. AMIR YACOBOY, Harvard University — Electrons in two dimensions and strong magnetic fields can form an insulating two-dimensional system with conducting one-dimensional channels along the edge. Electron interactions in these systems can have fractionalized charge excitations and chiral edges with independent transport of charge and heat, even in opposite directions. Here, we use a quantum dot as a local thermometer to explore such heat transport along the edge at filling factor one and 2/3 in a GaAs 2DEG. Moreover, using a scanning quantum dot as a local charge sensor allows us to extract the charge of elementary excitations at filling factor 5/2 as well as to observe a delicate sequence of fractional quantum Hall states in suspended graphene.

8:36AM Y3.00002 Quantum Hall Transitions and Quantum Number Fractionalization in Trapped Cold Atom Systems. KUN YANG, Florida State University — Recently there have been experimental attempts to realize quantum Hall physics in trapped cold atom systems, either through rotation or synthetic gauge fields. This can potentially open up a completely new direction in the study of quantum Hall effects. In this talk I will discuss possible quantum phase transitions between integer and fractional quantum Hall states, driven by attractive interactions between fermionic atoms. Such transitions have no counterparts in electronic quantum Hall liquids, but are related to fractionalization transitions studied in other strongly correlated systems. In one of these examples charge fractionalization is associated with the confinement-deconfinement transition of the (2+1D) Z2 gauge theory, which is in the Ising universality class.
9:12AM Y3.00003 Fractional Quantum Hall in the Diluted Magnetic Semiconductor CdMnTe

9:48AM Y3.00004 Tunable interactions and the fractional quantum Hall effect

Friday, March 22, 2013 8:00AM - 11:00AM – Session Y5 DCMP: Graphene: Transport and Optical Phenomena: Heterostructures 301 - Sufei Shi, University of California, Berkeley

8:00AM Y5.00001 Plasmons and Coulomb drag in Dirac/Schroedinger hybrid electron systems

8:12AM Y5.00002 Enhancement of Coulomb drag in double-layer graphene structures by plasmons and dielectric background inhomogeneity
8:24AM Y5.00003 Energy-driven drag in Graphene, JUSTIN SONG, Harvard University/MIT, LEONID LEVITOV, MIT — When solid surfaces slide against each other they experience friction which can be enhanced by inserting molasses between them or reduced by using a lubricant. In the same way, two spatially conducting layers that are placed in close proximity with each other feel friction because the long-ranged Coulomb interaction allows electrons in adjacent layers to “rub shoulders at a distance.” Recent measurements of Coulomb drag in Graphene by Gorbachev and co-workers from Manchester (doi:10.1038/nphys2441) have found that it is dramatically enhanced near the Dirac point, in stark contradiction with earlier theories predicting vanishing drag. We argue that a new kind of drag develops when heat transport in the two layers becomes strongly coupled due to efficient energy transfer between the layers. As a result, spatial charge inhomogeneity couples the motion of the electron liquid with heat transport through it, damping motion of electron flow in one layer by heat dissipation in the other. Interestingly, and somewhat paradoxically, this leads to strong drag without momentum transfer between layers. We predict distinct experimental signatures and discuss its magnetic field dependence.

8:36AM Y5.00004 Hydrodynamical Modes and New Transport Phenomena in Graphene: Nonlocality and Anomalous Drag, LEONID LEVITOV, MIT — The semimetal band structure of graphene gives rise to an unusually strong coupling between electrical currents and charge-neutral currents. This coupling leads to new transport phenomena mediated by neutral modes. This talk will highlight two examples connected with ongoing experiments. One is giant nonlocality observed in electric measurements.[1] This effect was explained by spin transport made possible by novel spin-Hall response near the Dirac point.[2] Another example is anomalous drag observed at charge neutrality which was attributed to the effects mediated by energy transfer in graphene heterostructures.[3,4] Drag measurements thus afford a unique probe of energy transfer at the nanoscale, a fundamental process which is not easily amenable to more conventional techniques such as calorimetry, and is key for the physics of strong interactions that occur near neutrality.

[1] D. A. Abanin et al, Science 332, 328-330 (2011);

8:48AM Y5.00005 Insulating behavior at the neutrality point in dual-gated single-layer graphene, FRANCOIS AMET, JAMES WILLIAMS, DAVID GOLDBER-GORDON, Stanford University — The conductivity at the neutrality point in single-layer graphene is known to saturate on the order of $e^2/h$ due to disorder-induced density fluctuations. In this study, we report contrasting results using dual-gated graphene devices with a boron nitride back-gate dielectric and a suspended top-gate, allowing for carrier mobilities over 100 000 cm$^2$/Vs. As the temperature is lowered, the peak resistivity at the charge-neutrality point unexpectedly diverges with a power-law behavior and becomes as high as several meghohms per square. As a transverse magnetic field is applied, our device remains insulating and directly transitions to the $\nu=0$ quantum Hall state. We discuss possible origins for this insulating behavior.

9:00AM Y5.00006 Broken Symmetry Quantum Hall states in Dual Gated ABA Trilayer Graphene, YONGJIN LEE, University of California Riverside, JAIRO VELASCO JR., University of California Berkeley, DAVID TRAN, University of California Riverside, FAN ZHANG, University of Pennsylvania, WENZHONG BAO, LEI JING, KEVIN MYHRO, University of California Riverside, DMITRY SMIRNOV, National High Magnetic Field Laboratory, JEANIE LAU, University of California Riverside — We perform low temperature transport measurements on dual-gated suspended trilayer graphene in the quantum Hall (QH) regime. We observe QH plateaus at filling factors $\nu = -8, -2, 2, 6$, and $10$, in agreement with the full-parameter tight binding calculations. In high magnetic fields, odd-integer plateaus are also resolved, indicating almost complete lifting of the 12-fold degeneracy of the lowest Landau levels (LL). Under an out-of-plane electric field E$_\perp$, we observe degeneracy breaking and transitions between QH plateaus. Interestingly, depending on its direction, E$_\perp$ selectively breaks the LL degeneracies in the electron-doped or hole-doped regimes.

9:12AM Y5.00007 Comparison of mobility at the top and bottom surfaces of multilayer graphene placed on SiO$_2$ substrate, AWINOBU KANDA, YOUSUKE NUKUI, HIKARI TOMORI, HIDENORI GOTO, YOUII OOTUKA, University of Tsukuba — It is known that charged impurities attached to the surface of graphene films are the main source of deteriorating mobility in graphene flakes obtained by the mechanical exfoliation. There are several origins for charged impurities: charges in the substrate, to which the bottom surface of the graphene films faces, the adsorbed molecules and contaminants due to chemicals (resist residues and so on) mainly attached to the top surface of graphene. This paper aims to evaluate the influence of the charged impurities on the top and bottom surfaces separately. For this purpose, we used dual-gated multilayer graphene with a contactless top gate. We developed a method of estimating the mobility of the top and bottom surfaces of multilayer graphene (MLG), from the top- and bottom-gate voltage dependence of the conductivity. We find that in thick MLG, mobility of the top surface is more than three times larger than that of the bottom surface. This indicates that the influence of the SiO$_2$ substrate on the mobility is stronger than that of adsorbates and contaminations on the top surface of the MLG.

9:24AM Y5.00008 Electric charge and potential distribution in twisted multilayer graphene, NATALYA ZIMBOVSKAYA, University of Puerto Rico-Humacao, EUGENE MELE, University of Pennsylvania — The specifics of charge screening and electrostatic potential spatial distribution in rotationally faulted multilayered graphene films with decoupled layers placed in between charged substrates is theoretically analyzed. The analysis is carried out using a nonlinear Thomas-Fermi approach. It is shown that by varying the areal charge densities on the substrates and/or the thickness of the graphene pack one may tune the screening length in the graphene pack. When the charge densities on the substrates are weak, the screening length is of the same order as the pack thickness, which agrees with semimetallic properties of graphene. When the amount of the donated charge is sufficiently large the screening length reduces indicating the transition to a metallic-like behavior of the graphene layers. The transition is shown to turn on rather quickly, and in occurs when the charge on the substrate/external electric field reaches a certain crossover magnitude. The possibilities for experimental observation of the predicted transition are discussed.

3This work was partly supported by NSF-DMR-PREM 0353730.

9:36AM Y5.00009 Tunable van Hove Singularities and Optical Absorption of Twisted Bilayer Graphene, YUFENG LIANG, LI YANG, Washington University in St. Louis — We perform the first-principles GW-Bethe-Salpeter Equation (BSE) simulation to study the optical absorption spectra of isolated twisted bilayer graphene (TBLG). The twisting generates new van Hove singularities (VHS), and these VHSs and corresponding optical absorption peaks can be tuned in a wide range by the twist angle. Enhanced electron-electron and electron-hole interactions are shown to be important to understand both optical absorption peak positions and their line shapes. With these many-electron effects included, our calculation satisfactorily explains recent experimental measurements.
Gate tunable quantum transport in double layer graphene heterostructures

KOSTYANTYN KECHEDZHI, EUYHEON HWANG, SANKAR DAS SARMA, CMT, Department of Physics, University of Maryland College Park — Motivated by the recently observed highly resistive state in double layer graphene heterostructures [1] we consider a system of two layers of graphene, “studied” and “control,” separated by an insulating layer. We theoretically analyze the effect of additional screening provided by Dirac electrons in the “control” graphene layer on the transport characteristics of the “studied” graphene layer. We find that in a typical device geometry fabricated on top of SiO2 substrate [1] the suppression of charge inhomogeneity is less efficient than initially expected and is limited by about a factor of 2. We also analyze the effect of additional screening on the quantum correction to the conductivity of the “studied” layer in this system in the metallic regime. We find that “control” layer screening is very efficient at suppressing electron-electron interactions in the “studied” layer which results in improved coherence and a novel gate tunable quantum correction to conductivity. The results of this work are summarized in [2].


This work is supported by US-ONR.

10:00AM Y5.00011 Transport properties of monolayer and bilayer graphene supported by hexagonal boron nitride

JING LI, KE ZOU, DONALD SEIWELL, JUN ZHU, Department of Physics, Pennsylvania State University — We present transport studies on hexagonal boron nitride (h-BN) supported monolayer and bilayer graphene. Following the method introduced by Dean et al, we first exfoliate thin sheets of h-BN (15-20 nm) to SiO2/Si substrate then align and transfer exfoliated graphene flakes onto the h-BN sheets. E-beam lithography is used to process the samples into Hall bar devices. We find that current annealing at low temperature can increase the mobility of as-fabricated devices but often introduces large density inhomogeneity at the same time. AFM images of annealed devices reveal the limitations of this technique. In comparison, thermal annealing is much more reliable in improving the sample quality. Bilayer devices annealed in a flow of Ar/H2 at 450°C for 5 hours show high mobility of 30,000 cm²/Vs at low temperature. We observe high-quality Shubnikov-de Hass (SdH) oscillations and degeneracy-lifted Landau levels in these samples. We extend existing measurements of the electron and hole effective mass in bilayer graphene [1] to lower carrier density regimes and discuss the implications of the results. [1] K. Zou, X. Hong, and J. Zhu, Phys. Rev. B 84, 085408 (2011).

1Department of Applied Physics, Yale University

10:12AM Y5.00012 Ground state of double layer graphene heterostructures in the presence of charged impurities

MARTIN RODRIGUEZ-VEGA, JONATHAN FISCHER, ENRICO ROSSI, College of William and Mary — A graphene double layer heterostructure is formed by two sheets of graphene separated by a thin dielectric film. Using the Thomas-Fermi-Dirac theory we have studied the carrier density profile in the presence of charged impurities. In this talk I will present our results for the case of heterostructures formed by two sheets of single-layer-graphene (SLG) and two sheets of bilayer-graphene (BLG). As for isolated layers, we find that the presence of charged impurities induces strong carrier density inhomogeneities, especially at low dopings where the density landscape breaks up in electron-hole puddles. We find that the amplitude of the carrier density inhomogeneities in double layers can be much lower than in isolated layers due to the better screening properties of double layer systems. I will then present results for the case of “hybrid” structures formed by one sheet of SLG and one sheet of BLG.

1Work supported in part by the Jeffress Memorial Trust, Grant No. J-1033.

10:24AM Y5.00013 Electronic and thermolectric transport in graphene double layer structures with boron nitride spacers

JIUNING HU, TAILUNG WU, JIFA TIAN, YONG CHEN, Purdue University — Recently, much attention has been devoted to electrically isolated graphene-graphene double layers in which interaction-driven novel physics such as exciton condensation are predicted. We have used polyvinyl alcohol (PVA) based carrier films and a micro-manipulator to transfer mechanically exfoliated flakes onto desired locations with accuracy of ~1 μm. We have fabricated graphene/boron nitride (BN)/graphene stacking structures on BN substrates to study their electronic and thermoelectric transport properties. We observed the low temperature mobility of graphene as high as 75000 cm²/V·s. We have performed Coulomb drag measurements and observed the sign and magnitude dependence of the drag resistivity on the carrier types and densities of both graphene layers, consistent with the previous reports. We also performed thermolectric transport measurements in such graphene double layer structures, especially in the complementary doped regime (so called excitonic regime) with one layer of electrons and the other layer of holes. Our approach may be useful to probe exciton condensation and other novel physics driven by electron-electron interactions in graphene double layers.

10:36AM Y5.00014 Photo doping effect in graphene/BN heterostructure

LONG JU, JAIO VELASCO JR., EDWIN HWANG, JONGHWA KIM, FENG WANG, UC Berkeley — Boron nitride has been demonstrated as an ideal substrate to achieve high mobility in graphene. At the same time We observed strong change of graphene transport properties by shining light on graphene/BN heterostructure. This is attributed to photo doping effect induced by impurity excitation in BN. Optical spectroscopy based on this photo-doping effects enables us to probe impurities in crystalline BN. Such information will be important for potential applications based on graphene/BN heterostructures. The potential of applying similar technique to probe defects in other insulators and semiconductors will also be discussed.

10:48AM Y5.00015 Photon Induced Transport in Graphene-Boron Nitride-Graphene Heterostructures

NITYAN NAIR, NATHANIEL GABOR, QIONG MA, Massachusetts Institute of Technology, KENJI WATANABE, TAKASHI TANIGUCHI, National Institute for Materials Science, Japan, WENJING FANG, JING KONG, PABLO JARILLO-HERRERO, Massachusetts Institute of Technology — Monolayer graphene, an atomically thin sheet of hexagonally oriented carbon, is a zero band gap conductor that exhibits strong electron-electron interactions and broadband optical absorption. By combining MLG and hexagonal boron nitride into ultrathin vertical stacks, experiments have demonstrated improved mobility, Coulomb drag, and field-effect tunneling across few-layer boron nitride barriers. Here, we report on the photon-induced transport of charge carriers through a graphene-boron nitride-graphene heterostructure. The dependence of the generated photocurrent on photon energy and interlayer bias voltage is studied. The photocurrent is found to depend strongly on both these parameters, showing several interesting features. We consider several processes that may serve to explain the rich dependence of photocconductance on applied bias voltage and photon energy.

Friday, March 22, 2013 8:00AM - 10:48AM –
Session Y6 DCMP: Nanotubes and Nanowires (non-carbon): Transport and Optical Phenomena 302 - Jonathan Spanier, Drexel University
During the past half century, feature-size of electronic elements has been reduced dramatically. Semiconductor industry expects this down-scaling to be continued for at least next decade. Among different approaches proposed for reducing the size of electronic elements, is nanowire (NW) based elements such as nanowire field effect transistor (NW-FET). NW approach offers a coaxial gate-dielectric-channel geometry that has advantage of electrostatic control in down-scaling the transistor channel. However, fundamental mechanisms for how such passivations alter the electronic properties of NW-FETs have not been rigorously scrutinized. In this work, we address this issue through first-principles calculations on CH₃, fluorine (F) and hydrogen (H) passivated [110] and [111] SiNWs. In comparison to H passivation, we explain how CH₃- and F-passivations cause significant band gap reductions in [110] SiNWs, through strain and quantum confinement respectively. Furthermore, we discuss how structural differences in [111] SiNWs mitigate these effects, thereby giving the electronic properties of [111] SiNWs greater stability against various surface passivations than those of [110] SiNWs.

8:12AM Y6.00002 Axial Si/Ge hetero-nanowires for tunneling transistors, SON LE, Department of Physics and School of Engineering, Brown University, DANIEL PEREA, Environmental and Molecular Sciences Laboratory, Pacific Northwest National Laboratory, POOYAN JANNATY, XU LUO, Department of Physics and School of Engineering, Brown University, SHADI DAYEH, Department of Electrical and Computer Engineering, University of California, ALEXANDER ZASLAVSKY, Department of Physics and School of Engineering, Brown University, THOMAS PIRRAUX, Center for Integrated Nanotechnologies, Los Alamos National Laboratory — Modern vapor-liquid-solid (VLS) growth based on alloy catalysts can grow SiGe heteronanowires (hetero-NWs) with controlled axial heterojunction abruptness [1] combined with simultaneous control of material composition (Si and Ge) and doping profile. Previously, we reported on axial in-situ doped Ge NW pn junction tunneling field effect transistors (TFETs) with effective backgate control of the tunneling current [2]. In this presentation, we report on tri-gated p-Ge/i-Si/n-Si axial hetero-NWs TFET with on-state tunneling occuring in the Ge drain section and off-state leakage dominated by the Si junction in the source. The devices have high Ion of 2 µA/µm, suppressed ambipolarity, and a sub-threshold slope of 50 mV/decade over 4 decades of current with lowest SS of 50 mV/decade. Device operation in the tunneling mode is confirmed by three-dimensional TCAD simulation. In addition, our devices work standard as NW FETs with good Ion/Ioff ratio when the source-drain junction is forward-biased [3]. [1] D. E. Perea et al., Nano Lett 11, 3117 (2011). [2] Son T. Le et al., Appl. Phys. Lett. 96, 262102 (2010). [3] Son T. Le et al., accepted to Nano Lett. (10/2012).

8:24AM Y6.00003 Probing Interface Band Edge Discontinuity in Single Core-shell Nanowire by Photocurrent Spectroscopy, GUANNAN CHEN, Department of Materials Science & Engineering, Drexel University, GUAN SUN, YUJIE DING, Department of Electrical & Computer Engineering, Lehigh University, ILIO MACCOLI, NICO LOVERGINE, Department of Innovation Engineering, University of Salento, Italy, PAOLA PRETE, IMM-CNR, Lecco, Italy, JONATHAN SPANIER, Department of Materials Science & Engineering, Drexel University — Group III-V co-axial core-shell semiconductor nanowire (NW) heterostructures possess unique advantages over their planar counterparts in logic, photovoltaic and light-emitting devices. Dimensional confinement of electronic carriers and interface complexity in NWs are known to produce local electronic potential landscapes along the radial direction that deviate from those along the normal to planar heterojunction interfaces. However, understanding of electronic and optoelectronic transport properties and device characteristics remains lacking without a direct measurement of band alignment in individual NWs. Photocurrent spectroscopy has proven to be effective in investigating the effects of quantum confinement and surface related properties such as bandgaps, surface adsorption/desorption, and polarization anisotropy. Here, we report on, using the GaAs/AlGaAs core-shell NW system (x = 0.24 and 0.33), how photocurrent and photoluminescence spectroscopies can be used together to construct a band diagram of an individual heterostructure NW with high spectral resolution. This approach and results are relevant for the study of tunable hot electron transfer across NW core-shell interfaces.

8:36AM Y6.00004 Capacitance of Nanowire with different cross sections and materials at different frequencies¹, ABBAS ARAB, QILIANG LI, Dept. of ECE, George Mason University, GEORGE MASON UNIVERSITY TEAM — During the past half century, feature-size of electronic elements has been reduced dramatically. Semiconductor industry expects this down-scaling to be continued for at least next decade. Among different approaches proposed for reducing the size of electronic elements, is nanowire (NW) based elements such as nanowire field effect transistor (NW-FET). NW approach offers a coaxial gate-dielectric-channel geometry that has advantage of electrostatic control in down-scaling the electronic elements. NWs can be grown in different cross sections depending on the material used as the core of the coaxial structure. Despite so much interest and research on this field, a complete set of study on nanowire capacitance will be very useful for nanoelectronics. In this work, we are going to study different NW structures with different materials and cross sections including: square, triangular, circular and hexagonal in different frequencies. We will study the effect of oxide thickness, oxide material and rotation of cross section, in cases that are not symmetric to rotation, on NW behavior.

¹Supported by NSF Career grant 0846649.

8:48AM Y6.00005 ABSTRACT WITHDRAWN —  

9:00AM Y6.00006 Discrete random distribution of source dopants in nanowire tunnel transistors (TFETs)¹, SOMAIA SYLVIA, University of California Riverside, M. ABUL KHAYER, Intel Corporation, KHAIRUL ALAM, East West University, Dhaka, Bangladesh, HONG-HYUN PARK, Samsung Semiconductor Inc., GERHARD KLIMECK, Purdue University, ROGER LAKE, University of California Riverside — InAs and InSb nanowire (NW) tunnel field effect transistors (TFETs) require highly degenerate source doping to support the high electric fields in the tunnel region. For a target on-current of 1 µA, the doping requirement may be as high as $1.5 \times 10^{20}$ cm$^{-3}$ in a NW with diameter as low as 4 nm. The small size of these devices demand that the dopants near tunneling region be treated discretely. Therefore, the effects resulting from the random distribution of dopant atoms in the source of a TFET are studied for 30 test devices. Comparing with the transfer characteristics of the same device simulated with a continuum doping model, our results show (1) a spread of $I$ vs $V$ toward the positive gate voltage axis, (2) the same average threshold voltage, (3) an average 62% reduction in the on current, and (4) a slight degradation of the subthreshold slope. Random fluctuations in both the number and placement of dopants will have significant effects on [110] SiNWs through strain and quantum confinement respectively. Therefore, a comparison of materials is also performed, showing their ability to block direct tunneling for sub-10 nm channel FETs and TFETs.

¹This work was supported in part by the Center on Functional Engineered Nano Architectonics and the Materials, Structures and Devices Focus Center, under the Focus Center Research Program, and by the National Science Foundation under Grant OCI-0749140.
9:12AM Y6.00007 Observation of defect-induced Photoresponse and charge carrier transport in single GeSe2 nanobelt devices. BUBLU MUKHERJEE, ENG SOON TOK, CHORNG HAUR SOW, National University of Singapore — Single crystal GeSe2 nanobelts were grown using chemical vapor deposition techniques. Morphology of the nanostructures was characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM), X-ray diffractionmetry (XRD) and Raman spectroscopy. Electronic transport properties, impedance spectroscopy, photoconductive characteristics and temperature-dependent electrical resistivity measurements were carried out on individual GeSe2 nanobelt devices. The photosensitivity of single GeSe2 nanobelt (NB) devices was examined with two different excitation wavelengths of laser beams with photon energies above band gap and at sub-band gap of the NB. A maximum photoconductive gain 10^4 % was achieved at a wavelength of 808 nm. The magnitude of the photocurrent and response time of the individual GeSe2 NB device indicate that the photoresponse could be attributed to the presence of isolated mid band gap defect levels. Temperature dependent photocurrent measurements indicate the rough estimation of the energy levels for the defect states. Localized photostudy shows that the large photoresponse of the device primarily occurs at the metal-NB contact regions.

1Department of Physics, 2 Science Drive 3, National University of Singapore (NUS), Singapore 117542

9:24AM Y6.00008 Finite Element Analysis of lateral charge distribution in ZnO nanowire. JAVAD USEFIE MAFAHIM, ARKADIY KROKHIN, ARUP NEOGI, University of North Texas — The coupling of piezoelectric and semiconducting properties in zinc oxide creates a strain field and charge separation across a nanowire (NW) as a result of an external or internally induced strain. The potential drop along the transverse section of a hexagonal ZnO NW is simulated by the finite element analysis method. The NW is considered to be fixed at one end and laterally deflected at the other with a uniform force on a constant area of cross-section. We numerically simulate the potential drop across a direction transverse to the growth of the NW attached to the substrate. The piezoelectric potential differences is analyzed as a function of the lateral force, thickness, and aspect ratio of the NW. It is observed that due to a change in the component of the shear force in the transverse direction with respect to the length of the NW, a significant variation of strain in observed in the direction of the lateral force. Our analysis explains previously observed experimental results. It is also shown that the potential difference is influenced by the changing aspect ratio. The charge distribution is also analyzed in a fluid medium with a lateral flow of the liquid. Our results can be used for the design of novel biosensors.

9:36AM Y6.00009 Tailoring electronic properties of SnO2 nanobelts via thermal annealing. TIMOTHY KEIPER, JORGE BARREDA, JOON-IL KIM, Department of Physics, Florida State University. JIM P. ZHENG, Electrical and Computer Engineering, FAMU/FSU College of Engineering, PENG XIONG, Department of Physics, Florida State University — Metal oxide semiconductors nanowires are a viable option for the fabrication of transistors with desirable characteristics for nanoelectronic and sensing applications. SnO2 nanobelts (NBs) have been synthesized using catalyst-free chemical vapor deposition. The growth parameters have been explored, producing NBs as long as millimeters. These NBs have been demonstrated as effective channel-limited gas [1], pH [2] and protein [3] field-effect transistor (FET) sensors. Through modification of O2 and vacuum thermal annealing conditions, we investigate the control and optimization of the electronic properties of the NBs to achieve desired device characteristics for sensing applications. A pronounced increase in conductance, up to the order of microsiemens, has been observed in annealed NBs under O2 environment at elevated temperatures above 600°C. We also examine the properties of the electrical contacts with different metalization and varying NB conductivity. Optimal device characteristics for various sensing applications will be tested and discussed.


9:48AM Y6.00010 Gated nonlocal transport in sketched oxide nanostructures. SHICHENG LU, GUANGLIE CHENG, JOSHUA P. VEAEZY, PATRICK IRVIN, FENG BI, MENGCHEN HUANG, JEREMY LEVY, University of Pittsburgh, CHUNG-WUNG BARK, SANGWOO RYU, KWANG-HWAN CHO, CHANG-BEOM EOM, University of Wisconsin-Madison — The oxide heterostructure LaAlO3/SrTiO3 supports a two-dimensional electron liquid (2DEL) with a variety of competing phases including magnetism, superconductivity and weak antilocalization due to Rashba spin-orbit coupling. Further confinement of this 2DEL into quasi-one-dimensional regime can provide insight into the underlying physics of this system and reveal new behavior. Prior magnetotransport experiments on narrow LaAlO3/SrTiO3 structures created by a conductive atomic force microscope lithography technique have revealed large nonlocal resistances [as large as 10^4Ω], with separations between current and voltage that are large compared to the 2D mean-free path. To help understand the origin of this remarkable behavior, we perform electric gating of nanowire structures in order to vary the carrier density and possibly other interactions such as spin-orbit coupling strength.

1This work is supported by AFOSR FA9550-10-1-0524 (J.L., C.B.E.), ARO W911NF-08-1-0317 (J.L.), NSF DMR-1104191 (J.L.), and DMR-0906443 (C.B.E).

10:00AM Y6.00011 ABSTRACT WITHDRAWN —

10:12AM Y6.00012 ABSTRACT WITHDRAWN —

10:24AM Y6.00013 Atomic Hydrogen and Oxygen Adsorptions in Single-Walled Zigzag Silicon Nanotubes. HAO LIANG CHEN, ASOK RAY, University of Texas at Arlington — Ab initio calculations have been performed to study the electronic and geometric structure properties of zigzag Si nanotubes. Full geometry and spin optimizations have been performed without any symmetry constraints with an all electron 3-21G* basis set and the B3LYP functional. The largest zigzag silicon nanotube (12, 0) studied has a binding energy per atom of 3.584eV. Atomic hydrogen and oxygen adsorption on (9, 0) and (10, 0) nanotubes have been studied by optimizing the distances of the adatoms from both inside and outside the tube. The adatom can be placed initially in four adsorption sites- parallel bridge, zigzag bridge, hollow, and on-top site. The on-top site is the most preferred site for hydrogen atom adsorbed on (9, 0) with an adsorption energy of 3.0eV and an optimized distance of 1.49 Å. For oxygen adsorption on (9, 0), the most preferred site is the zigzag bridge site with an adsorption energy of 5.987eV. For atomic hydrogen adsorption on (10, 0), the most preferred site is also the on-top site with an adsorption energy of 2.974eV and an optimized distance of 1.49 Å. For adsorption of atomic oxygen on (10, 0), the most preferred site is parallel bridge site with an adsorption energy of 6.275eV.

1Work partially supported by the Welch Foundation. (Grant No. Y-1525)
10:36AM Y6.00014 Topological Effect to Surface Plasmon Excitation in Topological Insulator Nanowires, MINGDA LI, MIT, WENPING CUI, University of Benn, JU LI, MIT, YIMEI ZHU, LIJUN WU, QINGPING MENG, BNL, WEISHU LIU, ZHIFENG REN, Boston College, FERHAT KATMIS, PENG WEI, JACADEESH MOODERA, YONG ZHANG, MIT, LI GROUP, MIT TEAM, CFN, BNL COLLABORATION1, FBML, MIT COLLABORATION2, CMSE, MIT COLLABORATION3, REN GROUP, BC COLLABORATION4 — We present a theoretical investigation of the surface plasmon at the interface between topologically non-trivial cylindrical core and topologically trivial surrounding material, from the axion electrodynamics and modified constitutive relations. We find that the topological effect lowers the SP energy in any case, while as the diameter of the core becomes smaller, the topological modification to SP energy is reduced. A qualitative picture based on perturbation theory of shifted boundary is given to explain these phenomena, from which we also infer that in order to amplify the topological effect, the difference between the inverse of dielectric constants of two materials must be increased. We also find that when the surrounding material goes magnetic, the magnetism overcomes topological effect, makes the latter seemingly suppressed. What’s more, bulk plasmon energy at 17.5 ± 0.2eV for semiconducting Bi2Se3 nanoparticle is observed from high-resolution Electron Energy Loss Spectrum Image measurements.

Friday, March 22, 2013 8:00AM - 10:36AM – Session Y8 DCMP: Electron-electron Interactions and Unconventional Structures 307 - Sumit Mazumdar, University of Arizona


1Work supported by the Australian Research Council

8:12AM Y8.00002 Charge-Carrier Screening in Single-Layer Graphene, DAVID SIEGEL, University of California, Berkeley / Sandia National Laboratories, WILLIAM REGAN, University of California, Berkeley, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, University of California, Berkeley / Lawrence Berkeley National Laboratory — Unlike normal metals that have a true Fermi surface, the pointlike Fermi surface of undoped graphene allows for long-ranged coulomb interactions to be unscreened by free charges, leading to singular behaviors. Therefore, the introduction of charge to a neutral graphene sheet can have a profound effect on transport properties and device performance. In this talk I will demonstrate the effects of charge-carrier screening of the electron-electron and electron-impurity interactions on the electronic properties of graphene, as we have observed through angle-resolved photoemission spectroscopy (ARPES). These observations help us to understand the basis for the transport properties of graphene, and shed light on the fundamental physics in the vicinity of the Dirac point crossing.

8:24AM Y8.00003 Evidence for strong electron correlations in graphene molecular fragments: Theory and experiments on two-photon absorptions1, KARAN AARYANPOUR, Department of Physics, University of Arizona, ADAM ROBERTS, U.S. Army AMRDEC, Redstone Arsenal AL, ARVINDER SANDHU, Department of Physics and Optical Sciences Center, University of Arizona, ALEX ZETTL, ALEXEI FEDOROV, Lawrence Berkeley National Laboratory, ALEX ZETTL, ALESSANDRA LANZARA, University of California, Berkeley / Lawrence Berkeley National Laboratory — Organometallic molecules with a 3d metal center carrying a spin offers many interesting properties, e.g., existence of multiple spin states [1]. A recent interest has been in understanding the magnetic exchange interaction between these organometallic molecules and magnetic substrates both from experiments and theory [2]. In this work, we will show by calculations based on density functional theory how the exchange interaction is mediated via graphene in a geometry containing iron porphyrin(Fep)/graphene/Ni(111). The exchange interaction varies from a ferromagnetic to an antiferromagnetic one depending on the lattice site and type of defect in the graphene lattice along with the switching of spin state of Fe in FeP between S=1 and S=2, which should be detectable by x-ray magnetic circular dichroism experiments. This scenario of complex magnetic couplings with large magnetic moments may offer a unique spintronic logic device. [1] S. Bhandary, S. Ghosh, H. Herper, H. Wende, O. Eriksson and B. Sanyal, Phys. Rev. Lett. 107, 257202 (2011). [2] H. Wende et al., Nat. Mater. 6, 516 (2007).

3We acknowledge NSF-CHE-1151475 grant as our funding source.

8:36AM Y8.00004 Manipulating molecule-substrate exchange interactions via graphene1, SUMANTA BHANDARY, OLLE ERIKSSON, BIPLAB SANYAL, Dept. of Physics and Astronomy, Uppsala University, Sweden — Organometallic molecules with a 3d metal center carrying a spin offers many interesting properties, e.g., existence of multiple spin states [1]. A recent interest has been in understanding the magnetic exchange interaction between these organometallic molecules and magnetic substrates both from experiments and theory [2]. In this work, we will show by calculations based on density functional theory how the exchange interaction is mediated via graphene in a geometry containing iron porphyrin(Fep)/graphene/Ni(111). The exchange interaction varies from a ferromagnetic to an antiferromagnetic one depending on the lattice site and type of defect in the graphene lattice along with the switching of spin state of Fe in FeP between S=1 and S=2, which should be detectable by x-ray magnetic circular dichroism experiments. This scenario of complex magnetic couplings with large magnetic moments may offer a unique spintronic logic device. [1] S. Bhandary, S. Ghosh, H. Herper, H. Wende, O. Eriksson and B. Sanyal, Phys. Rev. Lett. 107, 257202 (2011). [2] H. Wende et al., Nat. Mater. 6, 516 (2007).

3We acknowledge financial support from the Swedish Research Council, KAW foundation and the ERC(project 247062 - ASD).
8:48AM Y8.00005 Giant capacitance of a plane capacitor with a two-dimensional electron gas in a magnetic field. BRIAN SKINNER, BORIS SHKLOVSKII, University of Minnesota — If a clean two-dimensional electron gas (2DEG) with small concentration comprises one (or both) electrodes of a plane capacitor, the resulting capacitance can be larger than the “geometric capacitance” defined by the physical separation between electrodes. Such capacitance enhancement is a hallmark of the positional correlations that arise between electrons within the 2DEG at low electron density. Here we show that in the presence of a strong perpendicular magnetic field, such correlations are enhanced, leading to unusually large capacitance even for systems where the effective Bohr radius is large. The effect is perhaps most dramatic for ultrathin graphene-based capacitors, where strongly-correlated electron states appear at small filling factors, even though in the absence of magnetic field such correlated states are normally precluded by graphene’s Dirac-like kinetic energy spectrum.

9:00AM Y8.00006 Electron-electron Interaction and Thermoelectricity in Graphene. FERESHTEH GHARHARI, YURI ZUEV, CARLOS FORSYTHE, Physics Department, Columbia University, KENJI WATANABE, TAKASHI TANIGUCHI, Advanced Materials Laboratory, National Institute for Materials Science, Japan, PHILIP KIM, Physics Department, Columbia University — In this presentation, we report thermoelectric power (TEP) measurements on graphene samples deposited on hexagonal boron nitride substrates where drastic suppression of disorder is achieved. Our results show that at high temperatures where the inelastic scattering rate due to electron-electron (e-e) interactions is higher than the disorder induced elastic scattering rate, the measured TEP deviates from the Mott relation, and can be explained by a non-relativistic hydrodynamic flow of electrons. We also investigated TEP in the quantum Hall regime at a high magnetic fields, where we observed symmetry broken integer quantum Hall due to the strong e-e interactions. The field dependence of TEP at these states reveals the important role that exchange interactions play.

9:12AM Y8.00007 Interface Inducing Interesting Effects on Thermal Transport in Graphene Based Systems1. HAIYUAN CAO, HONGJUN XANG, XINGAO GONG, Fudan University — Using nonequilibrium molecular dynamics method (NDEM), we have studied how the interface affecting the thermal conductivity in multilayer graphene nanoribbons and the graphene grain boundaries. In multilayer graphene nanoribbons, the monotonous decrease of the thermal conductivity with the increase of the number of layers can be attributed to the phonon resonant effect of out-of-plane phonon modes. The reduction of thermal conductivity is proportional to the layer size, which is caused by the increase of phonon resonance. The results clearly show the dimensional evolution of thermal conductivity from quasi-one dimension to higher dimensions in graphene nanoribbons. The thermal transport across the asymmetric tilt grain boundary between armchair and zigzag graphene has also been investigated by simulations. We have observed significant temperature drop and ultra-low temperature-dependent thermal boundary resistance. More importantly, we find an unexpected thermal rectification phenomenon. The thermal conductivity and Kapitza conductance is direction-dependent. The effect of thermal rectification could be amplified by increasing the difference of temperature imposed on two sides. Our results show the interface phonon coupling could greatly change the thermal conductivity. Besides that, we have proposed a new promising kind of thermal rectifier and phonon diode based on the asymmetric interface in graphene.

9:24AM Y8.00008 Direct visualization of reversible dynamics in a Si₆ magic cluster in a graphene pore1. JAEKWANG LEE, Oak Ridge National Laboratory, WU ZHOU, Vanderbilt University, STEPHEN PENNYCOOK, JUAN-CARLOS IDROBO, Oak Ridge National Laboratory, SOKRATES PANTELIDES, Vanderbilt University — Clusters containing only a handful of atoms have been the subject of extensive theoretical and experimental studies, but direct imaging of their structure and dynamics has not been possible so far, with information provided mainly by theory. We report a direct atomically-resolved observation of a single Si₆ magic cluster trapped in a graphene nanopore. We report a sequence of images that show a reversible, oscillatory, conformational change: one of the Si atoms jumps back and forth between two different positions. Density functional theory shows that the cluster is exploring metastable configurations under the influence of the beam providing direct information on the atomic-scale energy landscape. The capture of a magic cluster in a graphene nanopore suggests the possibility of patterning nanoflakes or assembling atomic clusters with a potential for applications.

9:36AM Y8.00009 ABSTRACT WITHDRAWN

9:48AM Y8.00010 Brownian Dynamics Simulations of Dispersed Graphene Sheets. YUEYI XU, MICAH GREEN, Department of Chemical Engineering, Texas Tech University — Past simulations of the dynamics of dispersed graphene sheets are limited to static fluids on small timescales, with little attention devoted to flow dynamics. To address this need, we investigated how flow fields affect graphene morphology dynamics using a coarse-grained model; this relatively untouched area is critical given the importance of graphene solution-processing of multifunctional devices and materials. In particular, we developed a Brownian Dynamics (BD) algorithm to study the morphology of sheetlike macromolecules in dilute, flowing solutions. We used a bead-rod lattice to represent the mesoscopic conformation of individual two dimensional sheets. We then analyzed the morphology dynamic modes (stretching, tumbling, crumpling) of these molecules as a function of sheet size, Weisenberg number, and bending stiffness. Our results indicate the model can successfully simulate a range of dynamic modes in a given flow field and yield fundamental insight into the flow processing of graphene sheets.

10:00AM Y8.00011 Temperature-dependent levitation of a graphene flake due to Casimir forces1. ANH PHAN, DAVID DROSDOFF, LILIA WOODS, Department of Physics, University of South Florida, Tampa, Florida 33620, USA, IGOR BONDAREV, Physics Department, North Carolina Central, Durham, North Carolina 27707, USA, NGUYEN VIET, Institute of Physics, 10 DaoTan, BaDinh, Hanoi, Vietnam — We present theoretical investigations of temperature-dependent Casimir interactions of a graphene flake between substrates in a fluid. By properly choosing the materials, we propose that the graphene can be suspended in the fluid due to the balance between the Casimir, buoyancy and gravitational forces. The graphene properties, such as the Dirac-like nature of the carriers and universal optical conductivity, have a profound effect on the Casimir force making it completely thermal at room temperature. Since thermal contributions to the Casimir interaction in most materials are usually small, the graphene system offers a unique opportunity to demonstrate such effects without going to extreme temperatures. We show that the equilibrium position of the suspended flake is temperature dependent. We suggest that this maybe a promising system for observing thermal Casimir effects via levitation.

1This research was supported in part by the Department of Energy Basic Energy Sciences, Materials Science and Technology directorate.

9:36AM Y8.00009 ABSTRACT WITHDRAWN

10:00AM Y8.00011 Temperature-dependent levitation of a graphene flake due to Casimir forces. ANH PHAN, DAVID DROSDOFF, LILIA WOODS, Department of Physics, University of South Florida, Tampa, Florida 33620, USA, IGOR BONDAREV, Physics Department, North Carolina Central, Durham, North Carolina 27707, USA, NGUYEN VIET, Institute of Physics, 10 DaoTan, BaDinh, Hanoi, Vietnam — We present theoretical investigations of temperature-dependent Casimir interactions of a graphene flake between substrates in a fluid. By properly choosing the materials, we propose that the graphene can be suspended in the fluid due to the balance between the Casimir, buoyancy and gravitational forces. The graphene properties, such as the Dirac-like nature of the carriers and universal optical conductivity, have a profound effect on the Casimir force making it completely thermal at room temperature. Since thermal contributions to the Casimir interaction in most materials are usually small, the graphene system offers a unique opportunity to demonstrate such effects without going to extreme temperatures. We show that the equilibrium position of the suspended flake is temperature dependent. We suggest that this maybe a promising system for observing thermal Casimir effects via levitation.

1This work is supported by NSF of China, the Special Funds for Major State Basic Research, the Research Program of Shanghai municipality.
10:12AM Y8.00012 Properties of field-effect transistors of CVD grown MoS$_2$ single atomic layers on CVD grown hexagonal Boron Nitride . NIHAR PRADHAN, DANIEL RHODES, QIU ZHANG, National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA, ANA ELIAS, N. LOPEZ, Department of Physics, The Pennsylvania State University, University Park, PA, USA, ZHENG LIU, SINA NAJMEI, JUN LOU, Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX, USA, SAIKAT TALAPATRA, Department of Physics, Southern Illinois University, Carbondale, IL, USA, MAURICIO TERRONES, Department of Physics, The Pennsylvania State University, University Park, PA, USA, PULICKEL AJAYAN, Department of Mechanical Engineering & Materials Science, Rice University, Houston, TX, USA, LIU WU BAILING, NA XIAO, High Magnetic Field Laboratory, Florida State University, Tallahassee, FL, USA — Two-dimensional crystalline layered materials such as MoS$_2$, WS$_2$, have recently become an intense focus of research activities due to their exceptional electronic and optical properties. A single- or a few atomic layers of these materials show quite promising charge conduction characteristics, such as large mobility or fast on/off switch ratios, which lead to a few recent examples of integrated circuits based on these materials. Here, we will present a comparison among the electronic transport properties of, either mechanically exfoliated or CVD grown MoS$_2$ under different substrates, i.e. on SiO$_2$, on exfoliated or on CVD grown h-BN, and suspended. We will also discuss results obtained from back and top gated configurations with different dielectrics.

10:24AM Y8.00013 Nanochannel Device with Embedded Nanopore: a New Approach for Single-Molecule DNA Analysis and Manipulation , YUNING ZHANG, WALTER REISNER, Department of Physics, McGill University — Nanopore and nanochannel based devices are robust methods for biomolecular sensing and single DNA manipulation. Nanopore-based DNA sensing has attractive features that make it a leading candidate as a single-molecule DNA sequencing technology. Nanochannel based extension of DNA, combined with enzymatic or denaturation-based barcoding schemes, is already a powerful approach for genome analysis. We believe that there is a revolutionary potential in devices that combine nanochannels with embedded pore detectors. In particular, due to the fast translocation of a DNA molecule through a standard nanopore configuration, there is an unfavorable trade-off between signal and sequence resolution. With a combined nanochannel-nanopore device, based on embedding a pore inside a nanochannel, we can in principle gain independent control over both DNA translocation speed and sensing signal, solving the key drawback of the standard nanopore configuration. We demonstrate that we can optically detect successful translocation of DNA from the nanochannel out through the nanopore, a possible solution to select a given barcode for further analysis. In particular, we show that in equilibrium DNA will not escape through an embedded sub-persistence length nanopore, suggesting that the pore could be used as a nanoscale window through which to interrogate a nanochannel extended DNA molecule. Furthermore, electrical measurements through the nanopore are performed, indicating that DNA sensing is feasible using the nanochannel-nanopore device.

Friday, March 22, 2013 8:00AM - 11:00AM
Session Y11 DCMP: Glassy and Amorphous Systems, Including Quasicrystals followed by Epitaxial Growth and Structure of Oxides 310 - Punit Boolchand, University of Cincinnati

8:00AM Y11.00001 Hydrogen microstructure of amorphous silicon via inversion of nuclear magnetic resonance spectra: A moment-based approach . PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAJENDRA TIMILSINA, The University of Tennessee at Knoxville — We present an inverse approach for reconstructing hydrogen microstructure in amorphous silicon (a-Si). The approach consists of generating a prior distribution (of spins) by inverting experimental nuclear magnetic resonance (NMR) data, which is subsequently superimposed on a network of a-Si. The resulting network is then relaxed using a total-energy functional to obtain a stable, low-energy configuration such that the initial spin distribution is minimally disturbed. The efficacy of this approach is demonstrated by generating model configurations that not only have the correct NMR spectra but also satisfy simultaneously the experimental structural, electronic and vibrational properties of hydrogenated amorphous silicon.

8:12AM Y11.00002 Antiferromagnetic order in the Cd$_6$R ($R=$ rare earth) quasicrystal approximants$^1$ . ALAN GOLDMAN, MIN GYU KIM, Ames Laboratory and Iowa State University, GUILLAUME BEUTIER, SIMaP, UMR 5266 CNRS Grenoble-INP UJF, ANDREAS KREYSSIG, Ames Laboratory and Iowa State University, TAKANOBU HIROTO, TSUNETOMO YAMADA, Tokyo University of Science, JONG WOO KIM, Argonne National Laboratory, MARC DE BOISSIEU, SIMaP, UMR 5266 CNRS Grenoble-INP UJF, RYUJI TAMURA, Tokyo University of Science — Many theoretical treatments of spins on aperiodic lattices support the notion of long-range antiferromagnetic order. However, to date, there has been no experimental confirmation of long-range magnetic order in quasicrystalline systems. The absence of long-range magnetic order extends to crystalline approximant phases of the icosahedral structures as well. Surprisingly, the 1/1 approximant to the Cd$_6$Mg$_8$R icosahedral phases, Cd$_6$R$_8$, appears to be an exception to the rule. Here, we report on the results of x-ray resonant magnetic scattering measurements on Cd$_6$R$_8$ approximants which show that long range antiferromagnetic order is, indeed, realized. For $R=$ Tb and Ho, viewing the structure as a body-centered cubic packing of Tsai clusters, we find that the $R$ ions associated with the icosahedral cluster at the corner of the unit cell are antiferromagnetically correlated with the $R$ ions associated with the icosahedral cluster at the body-center of the unit cell.

1Work at the Ames Laboratory was supported by the Division of Materials Sciences and Engineering, Office of Basic Energy Sciences, US Department of Energy. Work at the Tokyo University of Science was supported by KAKENHI (Grant No. 20045017)

8:24AM Y11.00003 Fragility, slow homogenization and Intermediate Phase in the Si$_x$Ge$_{1-x}$Te$_{100-2x}$ ternary$^1$ . K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, S. MAMEDOV, Horiba Jobin Yvon Inc. — Small sized (0.5g) melts were synthesized by reacting pure elements in 5mm ID quartz tubes at 950C, and examined after 1 week and then 2 weeks of reaction. Bulk glass formation is realized in 6%<x<16% range with T$_g$(x) increasing linearly in 6%<x<12% range, and decreasing thereafter (x>12%). The enthalpy of relaxation at T$_g$ shows a flat bottomed minimum in 7.5%<x<9.0% range with the term increasing sharply at x>9% and at x<7.5%. We identify the 7.5%<x<9.0% range with the Intermediate Phase. Fragility(m) of melts were established in complex Cp measurements, and show a global minimum (m=30) in the IP range, and a value of m=20 at x=8.5%. The slow homogenization of Telluride melts results from the strong character of IP melts. Raman scattering, excited using low power density of 785nm radiation, shows evidence of a broad mode near 1600cm$^{-1}$ (characteristic of a-Te chains) and a narrower one near 127cm$^{-1}$ (group IV crosslinking units). The scattering strength of the 127cm$^{-1}$ mode increases at the expense of the 1600cm$^{-1}$ mode as x increases. The nature of structure evolution with glass composition will be commented upon.

1Supported by NSF grant DMR 08-53957
8:36AM Y11.00004 Slow kinetics of melt homogenization and strong nature of intermediate phase melts in chalcogenides, P. BOOLCHAND, K. GUNASEKERA, University of Cincinnati; S. BHOSLE, IM Flash Technologies — The strong-fragile classification of melts is manifested in the T-dependence of viscosity. Strong (fragile) melts possess a T-independent (dependent) activation energy of viscosity leading to an Arrhenian (non-Arrhenian) behavior reflecting the robust (weak) nature of network structure. We have now measured [1] complex C_n of binary Ge_x Se_{100-x} glasses as a function of x, and find that in dry and homogeneous melts, fragility (m(x)) shows a global minimum (m < 20) in the Intermediate Phase (IP) compositions (19.5% < x < 26%) but increases rapidly outside the IP. These findings have a direct bearing on synthesis of non-stoichiometric melt compositions at elevated temperatures in which IP melt compositions serve as a bottleneck [1] to homogenize [2] batches globally. The physical properties of dry and homogeneous glasses differ significantly from their inhomogeneous counterparts, and have led, in general, to differences in results reported by various groups.


3Supported by NSF grant DMR08-53957.

8:48AM Y11.00005 Fragility and slow kinetics of melt homogenization in the As-Se binary, SRIRAM RAVINDREN, KAPILA GUNASEKERA, PUNIT BOOLCHAND, University of Cincinnati — Two gram sized As_x Se_{100-x} batches at various As content x were synthesized using pure Se and As_x Se_{100-x} as starting materials that were reacted at 700°C. Such melts typically took 3-12 days to homogenize, as monitored in punctuated, off-line FT-Raman line profiling experiments. We have now undertaken mDSC experiments as a function of modulation frequency to establish the compositional dependence of complex C_n(x), and deduce the variation of fragility m(x). We find the fragility to be rather low, m < 20, across the 22% < x < 38% range, and to rapidly increase at x > 22% to acquire a value of 43 near x = 3%. We show that the slow melt homogenization is a direct consequence of the “strong” character of melts that serves as a bottleneck in melt-mixing at high temperatures. Once homogenized, physical properties of glasses, such as density, glass transition temperature T_g(x), the Intermediate phase, and variation of enthalpy of relaxation at T_g(x) differ significantly from their inhomogeneous counterparts.

3This work is supported by NSF grant DMR 08-53957.


9:00AM Y11.00006 Quantitative description of orientational order in non-graphitic carbons, ENSHI XU, VINCENT CRESPI, Department of Physics, Penn State University — The key factor that determines the ability to graphitize of a non-graphitic material is believed to be the level of orientational disorder which indicates how well the elemental structures are aligned. To characterize the disorder, we have developed a correlation function with multiple variable dependencies, such as radial distance and zenith angle. Through the characteristic parameter of the function, the ability to graphitize can be determined given the structure of a carbon material. The model is applied to a set of non-graphitic structures, which is generated systematically in non-conventional methods that emphasize to represent the orientational order of the carbon material rather than to match the radial distribution function.

9:12AM Y11.00007 Localization and percolation in random elastic networks, JACOB KRICH, University of Ottawa, ARIEL AMIR, Harvard University, VINCENTZO VITELLI, Leiden University, YUVAL OREG, YOSEPH IMRY, Weizmann Institute of Science — We consider a minimal model for a disordered phonon system that shows rich behavior in the localization properties of the phonons. We use a percolation analysis to argue for a localization/delocalization transition of the phonon modes and predict the speed of sound in the delocalized region, with comparison to numerics. We show that in contrast to the behavior in electronic systems (cf. Anderson localization), the transition exists for arbitrarily large disorder, albeit with an exponentially small critical frequency. The structure of the modes reflects a divergent percolation length that arises from the disorder in the springs without being explicitly present in the definition of our model. We calculate the critical frequency as a function of density and test the prediction numerically using a recursive Green function method. We further explore the existence of delocalized states in the two-dimensional version of this model.

9:24AM Y11.00008 Stoichiometric SrTiO3 Films via High Pressure Oxygen Sputter Deposition, PALAK AMBWANI, BHARAT JALAN, CHRIS LEIGHTON, Department of Chemical Engineering and Materials Science, University of Minnesota, USA — Defect management in epilayers of semiconducting complex oxides such as SrTiO3 is a topic of considerable contemporary interest. Recent work has shown that sufficiently precise control over stoichiometry and defects in SrTiO3 enables facile-type doping, record high mobilities, and even simultaneous observation of quantum oscillations and superconductivity. Such progress has typically been made using techniques such as oxygen/LAZER MBE or high-temperature PLD. In this work we demonstrate, via homoepitaxy on SrTiO3(001), that RF high pressure oxygen sputtering from a ceramic target is similarly capable of growth of high-quality, stoichiometric SrTiO3 films. We show that optimization of the deposition temperature (above 750 °C) and oxygen pressure (above 2.5 mBar) leads to the deposition of films indistinguishable from the substrate via grazing incidence and wide-angle x-ray scattering. The importance of a pre-treatment of the substrates in oxygen above 900 °C is emphasized. The defect density/stoichiometry was further probed via the transport properties of vacuum annealed samples with controlled O vacancy density. Finally, we also demonstrate that the stoichiometry and defect density of films deposited under non-optimal conditions can be remarkably improved via post-deposition heat treatment.

3Work supported by NSF DMR and NSF MRSEC.

9:36AM Y11.00009 Time-resolved in-situ X-ray Study of Homoepitaxial SrTiO3 Growth Using Reactive Molecular-Beam Epitaxy, I.C. TUNG, Advanced Photon Source, Argonne National Laboratory; Department of Materials Science and Engineering, Northwestern University; Z.Z. LUO, Materials Science Division, Argonne National Laboratory; National Synchrotron Radiation Laboratory, University of Science and Technology of China. J.H. LEE, H. HONG, Advanced Photon Source, Argonne National Laboratory, S.H. CHANG, J.A. EASTMAN, Materials Science Division, Argonne National Laboratory, M.J. BEDZYK, Department of Materials Science and Engineering, Northwestern University, J.W. FREELAND, Advanced Photon Source, Argonne National Laboratory, D.D. FONG, Materials Science Division, Argonne National Laboratory — Functional materials based on complex oxides in thin film form offer new and exciting strategies for meeting many energy challenges. Unfortunately, synthesis of such oxide films can be a major challenge even when utilizing reactive molecular-beam epitaxy (MBE). To understand the fundamental physics of complex oxide thin film growth, we have developed the world’s first reactive MBE system with in-situ synchrotron x-ray scattering capability at the Advanced Photon Source (APS). Here we present the results of in-situ surface x-ray scattering measurements taken during homoepitaxial growth of SrTiO3 on (001) SrTiO3 substrates. We compare the shuffled growth technique with codoposition to understand the nature of the distinctly different approaches. Work at the APS, Argonne is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.
9:48AM Y11.00010 STMs of Sub-monolayer SrO and LaAlO$_3$ Film Growth on SrTiO$_3$(001) Substrate Surfaces, TAKEO OHSAWA, KATSUYA IWAYA, RYOTA SHIMIZU, SUSUMU SHIRAKO, TARI HIOTOSUGI, Advanced Institute for Materials Research (WPI-AIMR), Tohoku University. — We report atomic-scale observations of initial growth of sub-monolayer SrO and LaAlO$_3$ (LAO) films on the atomically-ordered (1-T$ar{1}$3-v1 T$ar{3}$)-R33.7° SrTiO$_3$ (STO) (001) substrate surfaces using scanning tunneling microscopy/spectroscopy (STM/STS). We found that the growth processes depend strongly on the film compositions and the investigations unveil complex chemistry of thin-film oxides. These findings will provide microscopic insights into the understanding of transport properties at the LAO/STO interface, which is known to exhibit conducting behavior depending on the termination structures of STO substrates, namely, whether “TiO$_2$-” or “SrO-terminated” surfaces, respectively. Controlling the interface structure genuinely with atomic precision will eventually lead to the creation of exotic electronic phenomena and functionalities at the complex oxide interfaces.

10:00AM Y11.00011 In-situ Surface X-ray Diffraction Study of Ruddlesden-Popper Series Thin Film Growth, JUNE HYUK LEE, SEO HYOUNG CHANG, ZHENLIN LUO, Argonne National Laboratory, I-CHENG TUNG, Northwestern University, MILIND MALSHE, JULIUS JELLINEK, JEFF EASTMAN, HAWOONG HONG, DILLON FONG, FREELAND JOHN, Argonne National Laboratory. — The layered Ruddlesden-Popper phases of $A_nB_{n+1}O_{3n+2}$, such as Sr$_2$TiO$_4$ and La$_2$NiO$_4$, have attracted much attention as potential materials for solid-oxide fuel cell cathodes and thermoelectrics. To understand the fundamentals of this class of layered oxide thin films, we studied the growth of (001)-oriented Sr$_2$TiO$_4$ and La$_2$NiO$_4$ on SrTiO$_3$ substrates by using atomic molecular beam epitaxy with in-situ surface x-ray diffraction. For Sr$_2$TiO$_4$, the synthesis of the double SrO layer followed by TiO$_2$ dynamically reconstructs back into the SrTiO$_3$ phase, which demonstrates that during thin film deposition other pathways under growth conditions can give rise to new structural arrangements. In contrast with Sr$_2$TiO$_4$, the growth of La$_2$NiO$_4$ involves the stacking of polar LaO$^+$ and NiO$_2^-$ layers. This raises the question of how polarity mismatch at the interface with the SrTiO$_3$ substrate will influence the growth process. A detail comparison of these two cases will be discussed. Work at the Advanced Photon Source, Argonne is supported by the U.S. Department of Energy, Office of Science, and Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

10:12AM Y11.00012 Atomic Resolution and First Principles Study of the Electronic Structure at SrTiO$_3$/GaAs Hetero-interfaces, QIAO QIAO, ROBERT KLIE, SERDAR OGU'T, University of Illinois at Chicago, RAVI DROOPAD, ROCIO CONTRERAS-GUERRERO, Texas State University. — We examined ultra-thin SrTiO$_3$ films deposited on As-terminated GaAs (001) using molecular beam epitaxy under various O$_2$ partial pressures. Atomic-resolution Z-contrast images of different SrTiO$_3$ films were obtained using the aberration-corrected JEOL JEM-ARM200CF operated at 80 kV. Using atomic-column resolved EELS, our analysis of the Ti and O near-edge fine structure reveals different bonding configurations at the interface resulting from different growth methods. These results strongly suggest that a Ti pre-layer deposition alleviates the oxidation of the substrate and consequently the Fermi level pinning at the interface, as reported before. We also examined BaTiO$_3$ thin films grown on GaAs (001) with an ultrathin SrTiO$_3$ buffer layer. Interfacial charge distribution related to the polarization of BaTiO$_3$ thin film will be studied using atomic-resolution Z-contrast images, annular bright field images and EELS. Using first-principles DFT calculations, we analyze the formation energies of Ti-related impurity defects in different GaAs surface reconstructions to help interpret the electron microscopy experiments.

10:24AM Y11.00013 Temperature-driven irreversible phase transition of Sr template for epitaxial SrTiO$_3$ growth on vicinal Si (001), KRISTY KORMONDY, AGHAM POSADAS, ALEXANDER DEMKOV, University of Texas at Austin. — Strontium titanate (STO) grown epitaxially on Si has been an area of interest both for its own properties as a high-k dielectric and its capacity to act as a substrate for other crystalline oxides. In this study, we investigate STO growth on a 4° miscut Si (001) surface with double atomic steps to enhance our understanding of submonolayer Sr deposition and STO growth. It is well-known that a half-ML of Sr on the Si surface is a necessary prerequisite for crystalline growth; however, detailed study of reflection high-energy electron diffraction (RHEED) pattern during Sr deposition at various substrate temperatures reveals two distinct surface reconstructions at half-ML coverage. At temperatures below 350°C, the 2x1 pattern is nearly identical to that of clean Si, but as the temperature is increased, we see the irreversible appearance of a 2x spot parallel to the step edge while the 2x spot perpendicular to the step edge dims. We also find that crystalline STO can be grown on both of these high- and low-temperature templates, with identical RHEED and band alignment as determined by XPS, showing that this previously unexplored low-temperature template can provide an alternative route for STO growth on Si.

10:36AM Y11.00014 Correlation effects on the different crystal structures of AO$_2$ (A=Na, K, and Ba), MINJAE KIM, CHANG-JONG KANG, B.I. MIN, Pohang University of Science and Technology (POSTECH). — In alkali superoxide (A=Na, K, and Ba), the structural phase transition from high to low symmetry structures occurs upon cooling. On the other hand, in BaO$_2$ peroxide, the crystal structure is always the high symmetry tetragonal structure of KO$_2$, independent of temperature. To resolve these different crystal structures of AO$_2$ (A=Na, K, and Ba), we have calculated phonon dispersions of AO$_2$, assuming the high symmetry tetragonal structure of KO$_2$ with first-principle band structure method in the generalized gradient approximation (GGA) incorporating the Coulomb interaction U (GGA+U). From softened phonon modes, we have shown that, in KO$_2$ and NaO$_2$, the degeneracy of the incomplete pi anti-bonding level is lifted with the symmetry lowering such as Jahn-Teller effect with help of Coulomb correlation U. In contrast, in BaO$_2$, the pi anti-bonding level of the peroxide is completely filled without degeneracy. Thus, U is not effective on the phonon structure where the structural instability does not occur in BaO$_2$.

10:48AM Y11.00015 Fragility, Intermediate Phase and Polaronic conductivity in heavy metal oxides, SHIBALIK CHAKRABORTY, KAPILA GUNASEKERA, PUNIT BOOLCHAND, University of Cincinnati, MOHAMMED MALKI, Polytech’ Orleans, MATTTHIEU MICOUVALUT, UPMC-University Paris 6. — The ($B_2O_3$)$_x$(TeO$_2$)$_1-x$($V_2O_3$)$_x$ ternary forms bulk glasses over a wide range of compositions, 25% $< x < 25$%. Complex C$_p$(T) measurements as a function of modulation frequency reveal that melt fragility (m) show a global minimum (m = 52(2)°) in the 23% $< x < 26$% range with m = 65 outside that window. These results suggest more stable network structure in the window than outside it. The fragility window coincides with a global minimum of the non-reversing enthalpy of relaxation at T_g, the reversibility window (23% $< x < 27$%), a behavior also found in chalcogenide glasses. Conductivity ($\sigma$) data show three regimes of variation; a low $\sigma$ at $x < 23$, a plateau in 23% $< x < 27$, and an exponential increase at $x > 27$. The reduced activation energy for conductivity at $x > 27$% is consistent with increased polaronic mobility as the network becomes flexible. These findings show glasses at $x < 23$% are stressed-rigid, in 23% $< x < 27$% range in the Intermediate Phase, and at $x > 27$% to be flexible.

1Supported by NSF grant DMR 08-53957.

Friday, March 22, 2013 8:00AM - 11:00AM – Session Y13 DCMP: Topological Insulators: Thin Films and Interfaces 315 - Fazel Fallah Tafiti, Universite de Sherbrooke
8:00AM Y13.00001 An Infrared Study of Bi2Se3 Thin Films

KIRK POST, BRIAN CHAPLER, University of California - San Diego, LIANG HE, XUFENG KOU, University of California - Los Angeles, ALEX SCHAFGANS, None, KANG WANG, University of California - Los Angeles, DMITRI BASOV, University of California - San Diego — The experimental observation of surface states present in Bi2Se3 has been limited by self-doping via selenium vacancies. We have explored this issue by probing the electronic structure of Bi2Se3 using a combination of variable angle spectroscopic ellipsometry (VASE) and Fourier transform infrared spectroscopy (FTIR). Specifically, we have measured Bi2Se3 thin films grown on Si (111) substrates, ranging from 15 to 99 quintuple layers (QL) thick. These results show that both the carrier density and the energy gap are inversely related to the thickness. Surprisingly, the energy gap in all but the 15QL samples was smaller than the bulk band gap. Furthermore, the energy gap varied by over 100 meV between the 15QL and 99QL sample. The features that we observed are consistent with a modified picture of the band structure of Bi2Se3 that includes an impurity band below the conduction band and a Fermi level that is inversely related to the thickness.

8:12AM Y13.00002 Impact of growth conditions on the MBE-grown topological insulator Bi2Se3 thin films1

Y. LIU, Y.Y. LI, S. RAJPUT, M. WEINERT, L. LI, University of Wisconsin, Milwaukee — Recently, molecular beam epitaxy (MBE) has been successfully applied to prepare atomically flat topological insulator thin films that exhibit helical Dirac states. In this work, we systematically investigate the effects of substrate temperature and Bi/Se flux ratio on the morphology and properties of Bi2Se3 thin films grown on graphene/SiC(0001) by MBE. Under optimal growth conditions, in situ scanning tunneling microscopy indicates spiral growth [1], characterized by atomically smooth terraces 10 to 50 nm in width, separated by steps that are one quintuple-layer in height. Ex situ Raman spectroscopy reveals two characteristic peaks at 130 and 171 cm−1, corresponding to the in-plane Eg and out-of-plane Ag vibrational modes, respectively. The close resemblance of the positions and line shapes of both these peaks to those of bulk Bi2Se3 attest to the high quality of the film. These results and the impact of growth spills on the properties of the topologically protected Dirac surface states of Bi2Se3 will be presented at the meeting.


1Supported by NSF (DMR-1105839).

8:24AM Y13.00003 Epitaxial Growth of Topological Insulators on Hexagonal Boron Nitride Nitride

CHRISTOPHER GUTIERREZ, WOO CHANG CHUNG, CHOICKALINGAM SUBBAIAH, Columbia University, MATTHEW BRAHLEK, SEONGSHIK OH, Rutgers University, ABBAY PASUPATHY, Columbia University — Topological insulators (TIs) have attracted much attention for exhibiting exotic, topologically-protected surface states consisting of massless Dirac fermions. Investigations on thin film TIs have primarily relied on those either grown by MBE or by mechanical exfoliation onto suitable target substrates. Taking a cue from the graphene community, hexagonal boron nitride (hBN) has proven to be an excellent insulating substrate since it is atomically flat with no surface dangling bonds. In this talk I will report on recent transport and scanning probe measurements on epitaxial thin films of bismuth selenide TI grown by MBE on hBN/SiOx.

8:36AM Y13.00004 Gate-tunable supercurrent in S-TI-S structures

VLADIMIR ORLYANCHIK, MARTIN STEHNO, CHRISTOPHER NUGROHO, DALE VAN HARLINGEN, University of Illinois at Urbana-Champaign, MATTHEW BRAHLEK, NAMRATA BANSAL, NIKESH KOIRALA, SEONGSHIK OH, Rutgers, the State University of New Jersey — Theoretical proposals for observation of the zero energy excitations (Majorana modes) involve coupling between the surface states of 3D topological insulators (TI) and s-wave superconductors (SC). A prerequisite for such experiments is a highly tunable topological phase which is decoupled from bulk charge carriers and non-topological surface states. Here we report on measurements performed using high-quality MBE-grown thin films of Bi2Se3 patterned to create planar Josephson devices with Nb leads and a metallic top gate. We present the dependence of the conductance and proximity-induced supercurrent on the junction geometry, temperature, and the gate voltage. By analyzing the gate voltage dependence, we deduce that there are contributions to the supercurrent from two channels - topological surface states and a conventional supercurrent from the bulk.

8:48AM Y13.00005 Terahertz dynamics of gated thin films of the topological insulator Bi2Se3

ANDREAS STIER, JAMES NEILSON, LIANG WU, Department of Physics and Astronomy, Johns Hopkins University, NAMRATA BANSAL, MATTHEW BRAHLEK, SEAN OH, Department of Physics and Astronomy, Rutgers, the State University of New Jersey, N. PETER ARMITAGE, Department of Physics and Astronomy, Johns Hopkins University — Topological insulators are a newly discovered class of materials, which in principle exhibit bulk insulating behavior and conducting surface channels with a Dirac like dispersion relation. Real materials, however, suffer from large residual bulk conductance due to donor defect sites. This places the chemical potential in the bulk bands. Ionic liquid gating techniques are capable of moving the chemical potential into the bulk band gap, making the exotic transport characteristics predicted for the surface states accessible. Here, we present terahertz time domain spectroscopy of gated thin films of the topological insulator Bi2Se3 utilizing an ionic liquid gel as a top gate. The evolution of the Drude like conductivity features as a function of gate bias show a sharp decrease in the scattering rate which we interpret as the chemical potential moving from the conduction band into the surface states. We also discuss efforts to optically observe potential axionic terms in the action governing Maxwell’s equations for this material class, which are reflected in a discontinuous evolution of the Faraday rotation.

9:00AM Y13.00006 Scanning tunneling spectroscopic (STS) studies of magnetically doped MBE-grown topological insulators (TIs)

HAO CHU, MARCUS TEAGUE, CHIEN-CHANG CHEN, NICHOLAS WOODWARD, NAI-CHANG YEH, California Institute of Technology, XUFENG KOU, LIANG HE, MURONG LANG, KANG LONG WANG, UCLA, CALTECH COLLABORATION, UCLA COLLABORATION — We conduct STS studies on MBE-grown heterostructures of non-magnetic TI (Bi2Se3) with a range of thicknesses (d = 1, 3, 5, 7 quintuple layers, QL) on top of 7-QL magnetically doped TI (Cr-doped Bi2Se3). For d = 1 and 3-QL, a spatially homogeneous magnetism-induced surface gap (as large as about 150 meV for d = 1-QL) is observed at 77 K, whereas gapless Dirac spectra are found for d = 5 and 7-QL, suggesting that the effective magnetic length for Cr-doped Bi2Se3 is approximately 4 ~ 5-QL. These findings are further corroborated by ARPES and bulk electrical transport measurements. The magnetism-induced surface gap differs from those found in pure Bi2Se3 and (Bi1-xSbx)2Te3 films of thicknesses smaller than 6-QL, because the latter are due to overlaps of wave functions between the surface and interface layers, which lead to Rashba-like spin-orbit splitting and spin-preserving quasiparticle interference wave-vectors. In contrast, STS studies of TIs with magnetism-induced surface gap do not yield any quasiparticle interferences for energies within the bulk Bi2Se3 gap. Finally, comparative STS studies of pure and magnetically doped TIs in high magnetic fields will be discussed.

1This work was funded by the Gordon and Betty Moore foundation.

2This work was supported by DARPA.
9:12AM Y13.00007 Thickness-Independent Transport Channels in Topological Insulator Bi2Se3 Thin Films, NAMRATA BANSAL, Rutgers University, YONG-SEUNG KIM, Sejong University, MATTHEW BRAHLEK, ELIY EDREY, NIKFESH KOIRALA, SEONGSHIK OH. Rutgers University — With high quality Bi2Se3 thin films grown on Al2O3(0001), we report thickness-independent transport properties over wide thickness ranges. Low temperature conductance remained nominally constant as the sample thickness changed from 256 to ~3QL (where QL refers to quintuple layer, QL=8nm). Two surface channels with very different behaviors were identified. The sheet carrier density of one channel remained constant at ~3x10^{13}cm^{-2} down to 2QL, while the other, which exhibited quantum oscillations, remained constant at ~8x10^{12}cm^{-2} only down to ~8QL. The weak antilocalization effect also exhibited similar thickness independence. These two channels are most consistent with the topological surface states and the surface accumulation layers, respectively. We will also discuss surface signatures present in Bi2Se3 thin films grown on Si(111) and amorphous SiO2.

9:24AM Y13.00008 An abrupt change in transport dynamics across the topological phase transition in the (Bi1-xInx),Se3, and ultra-thin Bi2Se3 systems, LIANG WU, ROLANDO VALDES AGUILAR, ANDREAS V. STIER, LUCAS S. BILBRO, YUVAL LUBASHESKY, N. PETER ARMITAGE, The Institute for Quantum Matter, Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218 USA, MATTHEW BRAHLEK, NAMRATA BANSAL, SEAN OH, Department of Physics and Astronomy, Rutgers the State University of New Jersey. Piscataway, NJ 08854 — We have utilized time-domain terahertz (THz) spectroscopy to investigate the low frequency optical conductivity in (Bi1-xInx),Se3 through its topological phase transition from the pure (x=0) compound to the topologically trivial strongly insulating material (x > 0.25). The thickness independent Drude peak shows only minor broadening at low In substitutions. However, above x ~ 0.05 we observe a sudden collapse in the transport lifetime. This substitution level closely coincides with a maximum in the mid-infrared (MIR) absorption coefficient which can be identified with the substitution level where the band gap closes, the band structure inverts, and hence the topological class changes. We therefore associate the collapse in the transport lifetime with the loss of topological protection of surface states as the system enters the topologically trivial phase.

9:36AM Y13.00009 Fabrication and transport measurements of stacked double layer topological insulator devices, TAI-LUNG WU, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, JIUNING HU, School of Electrical and Computer Engineering, Purdue University, West Lafayette, IN 47907, JIFA TIAN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, IRENEUSZ MITKOWSKI, Department of Physics, Purdue University, West Lafayette, IN 47907, YONG P. CHEN, Department of Physics and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907 — A double-layer structure, consisting of two separated two-dimensional electron systems close in proximity, has been an interesting system to study novel ground states and transport properties driven by electron-electron interaction, e.g. Coulomb drag, exciton condensation, and counterflow superfluidity. Recently, topological insulators (TI), such as Bi2Se3 and Bi2Te3, have attracted much attention due to their exotic topologically protected spin-helical and Dirac-particle surface states. Motivated by a recently proposed "topological exciton condensate" that may be formed in two interacting TI surfaces, we have fabricated stacking double-layer TI structures and studied their electrical transport properties. Using a polyvinyl alcohol (PVA) based support film and micro-manipulator, double layer TI structures (Bi2Se3/boron nitride/Bi2Se3) were fabricated with exfoliated Bi2Se3 separated by thin boron nitride flakes (~ 20 nm). We will present results from transport measurements including mutual-gated electrical field effect, Coulomb drag, and counterflow conductivity.

9:48AM Y13.00010 Angle-resolved photoemission spectroscopy study of the magnetic doped topological insulator ultra-thin film Bi2Fe3Se3, YI ZHANG, LBL/SIMES, BO ZHOU, Stanford/Oxford, YULIN CHEN, Oxford, SUNG-KWAN MO, ZAHID HUSSAIN, LBL, ZHI-XUN SHEN, SIMES/Stanford — Topological insulator is a new type of quantum matter with gapped bulk states coexisting with a gapless surface state (SS) that is protected by time reversal symmetry and robust against non-magnetic impurities. Researches have shown that there exist two routes to open a gap in the SS: doping with magnetic impurities and the coupling of SS on opposite surfaces in ultra-thin films. In order to study the mixing of these two types of gap-opening, we prepared ultra-thin Bi2Fe3Se3 films, grown by molecular beam epitaxy, with different Fe concentration and thickness. The spin polarization is large for larger wave-vectors or for momenta far from the center of the surface Brillouin zone. In addition, the polarization is observed to decrease significantly with enhanced tunneling realized systematically in thin insulating films. We present theoretical model calculations that qualitatively capture the delicate relationship between quantum tunneling and Fermi surface spin polarization.

10:00AM Y13.00011 Tunneling tuned spin modulations in ultrathin topological insulator films, MADHAB NEPANE, S.-Y. XU, N. ALIDOUST, I. BELOPOLSKI, CHANG LIU, Department of Physics, Princeton University, D.M. ZHANG, A. RICHARDELLA, Department of Physics, Penn State University, J. SANCHEZ-BARRIGA, D. MARCHENKO, A. VARYKHALOV, O. RADER, BESSY II, Germany, M. LEANDERSSON, T. BALASUBRAMANIAN, MAX-Labs, Sweden, L.A. WRAY, ALS, LBNL, T.-R. CHANG, National Tsing Hua University, Taiwan, H.-T. JENG, National Tsing Hua University and Academia Sinica, Taiwan, H. LIN, A. BANSIL, Department of Physics, Northeastern University, N. SAMARTH, Department of Physics, Penn State University, M.Z. HASAN, Department of Physics, Princeton University — Understanding the spin behavior of boundary modes in ultrathin topological insulator films is critically essential for the design and fabrication of functional nano-devices. We report tunneling-dependent evolution of spin configuration in topological insulator thin films across the metal-to-insulator transition. We observe that for a given film thickness of the prototype topological insulator Bi2Se3 ultrathin films, the spin polarization is large for larger wave-vectors or for momenta far from the center of the surface Brillouin zone. In addition, the polarization is observed to decrease significantly with enhanced tunneling realized systematically in thin insulating films. We present theoretical model calculations that qualitatively capture the delicate relationship between quantum tunneling and Fermi surface spin polarization.

10:12AM Y13.00012 Study of proximity effect in superconductor - topological insulator heterostructures by scanning SQUID microscope, ILYA SOCHNIKOV, ANDREW J. BESTWICK, JAMES R. WILLIAMS, THOMAS M. LIPPMAN, ANDREW S. BLEICH, JAMES G. ANALYTIKS, IAN R. FISHER, DAVID GOLDBAHER-GORDON, JOHN R. KIRTLEY, KATHRYN A. MOLER, Stanford University — A proximity induced superconducting state in topological insulators is potentially an enabling condition for exotic forms of superconductivity that may support Majorana fermions in some geometries. Initial studies of induced superconductivity in topological insulators have relied on transport measurements. We present a different contactless characterization approach based on a scanning SQUID microscope. We characterized AI superconducting rings with Josephson junctions made of Bi2Se3, long Al/Bi2Se3/Al Josephson junctions, and Bi2Se3/Al dots. We observe both induced proximity and inverse proximity effects in these heterostructures and each of the structures exhibit the proximity effect, such as the critical current, the magnetic field penetration depth, and the critical temperatures of the induced superconducting state. These measured parameters allow the determination of limits on contributions from the surface and the bulk to the proximity effects in the topological insulator Bi2Se3.
10:24AM Y13.00013 Local Magnetic Imaging of Proximity Effect-Induced Superconductivity at the Bi$_2$Se$_3$/Nb Interface , PHILIP KRATZ, JOHN KIRTHLEY, ILYA SOCHNIKOV, PHILLIP WU, ERIC SPANTON, KRISTIE KOSKI, YI CUI, ROBERT HAMMOND, MALCOLM BEASLEY, KATHRYN MOLER, Stanford University, USA — The interface between a topological insulator (TI) and an s-wave superconductor (SC) is predicted to host Majorana bound states analogous to vortices in a spinless p$_x$-ip$_y$ superconductor. For 3D TIs coupled to s-wave superconductors, the winding of the superconducting vortices can counteract the TI pi-Berry’s phase, resulting in zero-energy Majorana fermion excitations at the interface. Transport measurements of Bi$_2$Se$_3$ and Bi$_2$Te$_3$ superconducting junctions have shown Josephson junction effects[1,3,4] and established the existence of a supercurrent that is tunable with gate voltage [2], but the relative contributions of the bulk and bound states to the supercurrent is not well-understood. We report on measurements of the local superfluid density at the interface between Bi$_2$Se$_3$ nanoplatelets and Nb using a scanning SQUID microscope and quartz tuning fork sensor for simultaneous AFM characterization. We demonstrate that the local penetration depth measurements have increased accuracy and provide an experimentally tractable method for studying proximity effect-induced superconductivity at the SC-TI interface, which is a precursor for observation of the elusive Majorana fermion in Bi$_2$Se$_3$ and other 3D TIs.


10:36AM Y13.00014 Dirac cone shift and potential fluctuations in a passivated In$_2$Se$_3$/Bi$_2$Se$_3$ topological interface state$^1$. GREGORY S. JENKINS, A.B. SUSHKOV, D.C. SCHMADEL, M.-H. KIM, H.D. DREW, Department of Physics, University of Maryland at College Park, G. KOBLMUELLER, M. BICHLER, Walter Schottky Institut and Physik Department, Technische Universität München, N. BANSAL, M. BRAHLEK, S. OH, Department of Physics and Astronomy, The State University of New Jersey, Piscataway — The topological interface state of Bi$_2$Se$_3$ capped with In$_2$Se$_3$ is measured by gated THz cyclotron resonance. An observed shift of 70 meV in the position of the Dirac point towards mid-gap due to the physical properties of the trivial insulator In$_2$Se$_3$ on Bi$_2$Se$_3$ opens new possibilities in tailoring Dirac cone properties in topological insulators. Modulating and sweeping a semi-transparent gate while probing at terahertz frequencies in magnetic field enables characterization of the buried In$_2$Se$_3$/Bi$_2$Se$_3$ topological interface state, even in the presence of significant bulk conductivity. Near the Dirac point, the mobility is 3500 cm$^2$/V·s with potential fluctuations of 60 meV. The scattering rate shows a precipitous drop with Fermi energy indicating decoupling of the surface states from bulk states. At Fermi energies above the conduction band edge, a plateau is observed in the real part of the Faraday angle that is 80 times flatter than the step size expected from a single Landau Level, quantized in units of the fine structure constant.

$^1$The work at UMD is supported by NSF DMR-1104343 and DOE DE-SC0005436

10:48AM Y13.00015 Massive Dirac surface states in topological insulator/magnetic insulator heterostructures$^1$, WEIDONG LUO, Shanghai Jiao Tong University, XIAO-LIANG QI, Stanford University — We study the behavior of topological surface states in heterostructures formed by a topological insulator (TI) and a magnetic insulator (MI). Several MILs with compatible magnetic structure and relatively good lattice matching with TIs are identified, and the best candidate material is found to be MnSe, an anti-ferromagnetic insulator. We perform first-principles calculation in Bi$_2$Se$_3$/MnSe superlattices and obtain the surface state bandstructure. The magnetic exchange coupling with MnSe induces a gap of 54 meV at the surface states. In addition we tune the distance between Mn ions and TI surface to study the distance dependence of the exchange coupling. Finally, we study the band bending effect at the Bi$_2$Se$_3$/MnSe interface, and propose possible solutions to avoid band bending.

$^1$We acknowledge funding support from the Defense Advanced Research Projects Agency (DARPA).

Friday, March 22, 2013 8:00AM - 11:00AM — Session Y19 DCMP: Charge Density Wave Order 321 - David Hawthorn, University of Waterloo

8:00AM Y19.00001 Specific heat studies of the chiral phase transition in charge ordered 1T-TiSe$_2$ , XU LUO, Material Science Division, Argonne National Laboratory, Argonne, IL60439, J.-P. CASTELLAN, Karlsruhe Institute of Technology, D-76021, Karlsruhe, Germany, S. ROSENKRANZ, R. OSBORN, Q. LI, Material Science Division, Argonne National Laboratory, Argonne, IL60439, G. KARAPETROV, Department of Physics, Drexel University, Philadelphia, PA 19104, J.P.C. RUFF, CHESS, Cornell University, Ithaca, NY 14853, U. WELP, Material Science Division, Argonne National Laboratory, Argonne, IL60439, J. VAN WEZEL, H.H. Willis Physics Laboratory, University of Bristol, BSS ITL, UK — We use high-resolution steady-state ac-micro-calorimetry to investigate the transition of 1T-TiSe$_2$ into the charge-ordered state. A mean-field like step of ~ 0.4 J/molK in the specific heat C(T) near 193 K signals the transition into the commensurate CDW state. Upon further cooling, C(T) varies linearly in temperature until near 180 K a clear break in the slope of C(T) by 13 mJ/molK and possibly a small step indicate a second phase transition. Comparisons with theoretical predictions based on the Ginzburg-Landau free energy, with resistivity measurements, and with x-ray diffraction indicate that, at this transition, the commensurate CDW state changes into a helically ordered state along the crystal c-axis.

8:12AM Y19.00002 Electronic Properties of Cu$_3$TiSe$_2$ Single Crystals$^1$, PETRA HUSANIKOVA, Drexel University and IEE, Slovak Academy of Sciences, JAN FEDOR, JAN DERER, VLADIMIR CAMBEL, IEE, Slovak Academy of Sciences, GORAN KARAPETROV, Drexel University — We investigate the normal state and superconducting properties of 1T-TiSe$_2$ family of single crystals intercalated with different level of copper content. Magnetoresistance and Hall effect data indicate that 1T-TiSe$_2$ is a compensated narrow band-gap semiconductor or semimetal with small number of electron and hole carriers. We compare the influence of copper intercalant and titanium interstitials on the temperature evolution of charge density waves via resistivity and Hall effect measurements. Our findings indicate that the origin of the charge density waves in 1T-TiSe$_2$ is due to the combination of exciton and Jahn-Teller mechanisms. At higher copper concentrations we investigate the superconducting properties of Cu$_3$TiSe$_2$ in overdoped regime and find that the system is a single-gap strongly type-II superconductor with in-plane Ginzburg-Landau parameter reaching 50.

$^1$This work has been supported by Slovak Grant Agency APVV, project APVV-0036-11 (0.2), and by the Research & Development Operational Program funded by the ERDF, "HD Video", ITMS code 26240120043 (0.6) and "CENTE II", ITMS code 26240120019 (0.2).
The effect of dimensionality on the charge-density-wave phase in layered dichalcogenides 1. DARSHANA WICKRAMARATNE, PRADYUMNA GOLI, ALEXANDER BALANDIN, ROGER LAKE, University of California, Riverside — Transition-metal dichalcogenides exhibit a variety of conducting phases, which includes a charge-density-wave state (CDW). Exfoliation of these layered materials allows the effect of dimensionality on the CDW state to be studied. CDW collective states are currently being considered as an alternative state variable for information processing [1]. 2H-TaSe2 and 1T-TiSe2 are examples of layered transition metal dichalcogenides that undergo a CDW transition. Our recent experiments demonstrated an increase in the CDW transition temperature of TiSe2 with a decrease in film thickness [1]. This increase in temperature was attributed to the negative CDW transition temperature-pressure relationship. Here we present a density-functional theory investigation of the CDW instability in bulk, single and few-layer 1T-TiSe2 and other layered dichalcogenide materials. The effect of the film thickness on the atomic structure, electronic structure, electron-phonon coupling and the CDW transition temperature will be discussed for each material.


1 NSF and SRC-NRI project 2204.001: Charge-Density-Wave Computational Fabric (NSF-1124733)

A quantum phase transition from triangular to stripe charge order in NbSe2 1. ERIC HUDSON, Pennsylvania State University, ANJAN SOUMYANARAYANAN, M. M., YEE, YANG HE, Harvard University, D. J. RAHN, K. ROSSNÄGEL, University of Kiel, JASPER VAN WEZEL, M. R. NORMAN, Argonne National Laboratory, JENNIFER E. HOFFMAN, Harvard University — We use scanning tunneling microscopy to reveal a previously unknown unidirectional (stripe) charge density wave (CDW) smoothly interfacing with the familiar tridirectional (triangular) CDW on the surface of the stoichiometric superconductor NbSe2. Our low temperature measurements rule out thermal fluctuations, and point to local strain as the tuning parameter for this quantum phase transition. We use this discovery, in conjunction with bandstructure calculations, to resolve two longstanding debates about the anomalous spectroscopic gap and the role of Fermi surface nesting in the CDW phase of NbSe2. First, the 15% wavelength difference between the two CDWs demonstrates that Fermi surface nesting plays a minor role in determining the CDW wavevectors in NbSe2. Second, we disentangle a ∆ ∼ 12 meV particle-hole asymmetric CDW gap from a spectrum dominated by collective modes, resolving a longstanding debate regarding the nature of the gap previously observed by STM and ARPES. Our results highlight the importance of local strain in governing phase transitions and competing phenomena, and suggest a new direction of inquiry for resolving similarly longstanding debates in cuprate superconductors and other strongly correlated materials.

1Supported by NSF DMR-0847433 (Harvard), DOE, Office of Science DE-AC02-06CH11357 (Argonne) and DFG via SFB 855 (Kiel).

Role of impurities in the charge density wave state of transition metal dichalcogenides 1. JUNICHI OKAMOTO, ANDREW MILLIS, Columbia University — Motivated by recent scanning tunneling microscope (STM) measurements of NbSe2 which revealed the formation of charge density wave (CDW) droplets around impurities even at temperatures of the order of three times the transition temperature [1], we present a theory of impurity-induced CDW formation, and examine its consequences for the thermodynamic phase transition and low temperature ordered phases. Our fits to the STM measurements suggest that the CDW is strongly pinned by impurities, so that a standard theory predicts that even at lowest temperature the material should be in the disordered phase. We present a new theoretical picture explaining how to reconcile the experimental observation of a sharp transition with the strong pinning. [1] S. P. Chockalingam et al. (submitted to PNAS)

Electronic Structure and Charge-Density Wave Instabilities in Monolayers of Transition Metal Dichalcogenides 1. PIERRE DARANCECT, Dept of Applied Physics and Applied Mathematics, Columbia University, ANDREW J. MILLIS, Dept of Physics, Columbia University, CHRIS A. MARIANETTI, Dept of Applied Physics and Applied Mathematics, Columbia University — Transition metal dichalcogenides (TMD) are layered materials displaying a variety of charge-density-wave (CDW) instabilities and complex phase diagrams for group IV & V transition metals. Recent progress in mechanical exfoliation and device fabrication now allow for electrical characterization and gating of individual, 3-atom thick layers [1] of TMDs, providing new probes of the complex many-body interactions arising in these compounds. In this talk, I will present our investigations using density functional and dynamical mean-field theory regarding the electronic structure and electronic correlations arising in distorted monolayers, bilayers, and trilayers of octahedral group V TMDs. We will examine the importance of many-body interactions and their influence on the transport and optical properties of these materials upon distortion. [1] K. S. Novoselov et al., PNAS 102, 10451 (2005).

9:24AM Y19.00008 Role of Disorder in Atomic Scale Onset of Charge Density Waves. ERICK ANDRADE, CARLOS ARGUELLO, ETHAN ROSENTHAL, SUBBAIAH CHOCKALINGAM, LUIYAN ZHAO, CHRISTOPHER GUTIERREZ, WOO CHUNG, WENCEN JIN, PO-CHUN YEH, Columbia University, TONIČA VALLA, Brookhaven National Labs, RAFAEL FERNANDES, Columbia University, SHUANG JIA, Princeton University, RICHARD OSGOOD, ANDREW MILLIS, Columbia University, ROBERT CAVA, Princeton University, ABHAY PASUPATHY, Columbia University — How does strong disorder affect the electronic states of complex electronic materials? This question is of relevance to many quantum materials such as the cuprates and pnictides, where interesting electronic phases like superconductivity only arise in strongly disordered samples. The study of these materials is complicated by the presence of multiple electronic phases, which obscures the interpretation of local spectroscopic measurements. To gain insight into this problem, we study 2H-NbSe2, a relatively simple material with a 2D charge density wave ground state. To tune the disorder in the sample, we use sulfur substitution to go from weak (in pristine NbSe2) to strong disorder (in NbSe2−xSx). We use variable-temperature scanning tunneling microscopy and spectroscopy to visualize the electronic structure in real space. Strong changes in the local electronic spectrum are observed with the introduction of disorder, with a pseudogap appearing in the local density of states. We also observe strong changes in the quasiparticle interference from spectroscopic images. We will discuss the interpretation of quasiparticle interference in the limit of strong disorder, and its relevance to existing measurements in the cuprates and pnictides.
9:36AM Y19.00009 Charge Density Wave Disproportionation in Pd(III)-containing PdTe3

PATRICK COTTINGHAM, JOHN SHECKELTON, DAVID MILLER, JAMES NEILSON, TYRELL MCQUEEN, Johns Hopkins University — Exotic electronic properties in strongly correlated materials often emerge from the interplay of structure and charge. In most Pd3+-containing materials, Pd3+ statically disproportionates into Pd2+ (d7) and Pd4+ (d6) with square planar and octahedral geometries, respectively. However, high-resolution diffraction data acquired for PdTe indicate exclusively octahedral coordination of the Pd species within this compound. Temperature-dependent electrical resistivity measurements of this material performed in our lab show a hysteresis between T_{CDW1} \sim 120 K and T_{CDW2} \sim 50 K, indicative of a first-order phase transition. The most likely origin of this anomaly is the formation of a CDW involving partial, dynamic charge disproportionation of Pd3+. In addition, low-temperature diffraction data show a broadening of Bragg peaks on cooling which is indicative of strain or disorder concomitant with disproportion. In this presentation the temperature dependencies of the magnetic susceptibility, heat capacity, and electronic properties of PdTe will be discussed in the context of CDW formation.

9:48AM Y19.00010 Short-range CDW correlations in Co0.5NbSe2 and Mn0.5NbSe2

J. LEE, Physics Department, Temple University, Philadelphia, PA 19122, R. DI CAPUA, Dipartimento S.p.e.s., Universita degli Studi del Molise, Campobasso, and CNR-SPIN, Napoli, Italy, G. KARAPETROV, Physics Department, Drexel University, Philadelphia, PA 19104, T. NISHIZAKI, K. NOKAYASHI, Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan, M. IAVARONE, Physics Department, Temple University, Philadelphia, PA 19122 — Scanning tunneling microscopy and transport measurements were performed on NbSe2 and Co- and Mn-intercalated NbSe2 single crystals, to address the effect of disorder induced on the CDW structure by the effect of intercalation. We find that the CDW transition at T_{CDW} \sim 33 K in the pure compound is accompanied by a small anomaly in resistivity, a strong non linearity of the Hall effect, with a sign reversal occurring at CDW transition, and high magnetoresistance in agreement with previous reports. The system remains metallic below the CDW transition. Upon increase of disorder the anomaly in resistivity moves at a lower temperature and eventually disappears for higher doping levels. By increasing the disorder also the magnetoresistance decreases and the Hall effect does not show any sign reversal. STM measurements on a pure sample reveal that CDW phase is long-range ordered below T_{CDW}. For doped samples short range CDW correlations dominate a large part of the phase diagram.

10:00AM Y19.00011 Optical Excitation Spectrum in Ni- and Cu-doped ZrTe3

CHIARA MIRRI, ADAM DUSZA, LEONARDO DEGIORGi, Solid State Physics Laboratory, ETH Zurich, CH-8093 Zurich, Switzerland, CEDOMIR PETROVIC, Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton NY 11973, USA, BROOKHAVEN NATIONAL LABORATORY COLLABORATION — We report on an optical study performed on Cu0.5ZrTe3 and Ni0.5ZrTe3 single crystals. ZrTe3 was previously found to display a BCS-like CDW-gap opening in the optical spectra along the direction orthogonal to the Zr-chains and to undergo a filamentary superconducting transition below a T_c of about 2 K. The intercalation by Cu and Ni between the ZrTe3 layers partially fills the CDW gap and induces bulk superconductivity coexisting with the CDW state below T_c. Here we show the effect of Cu and Ni intercalation on the reflectivity and optical conductivity above and below the CDW phase-transition temperature. Furthermore, we analyze the optical spectral weight, providing equivalent information in both compounds about the partial gapping of the Fermi surface and the overall redistribution of spectral weight across the CDW phase transition.

10:12AM Y19.00012 Interplay between electron-electron and electron-lattice interactions in the RTe3 compounds

ALEXANDER KEMPER, Lawrence Berkeley National Laboratory, H.-M. EITER, M. LAVAGNINI, R. HACKL, Walther Meissner Institut, Bayerische Akademie der Wissenschaften, E.A. NOWADNICK, T.P. DEVEREAUX, J.-H. CHU, J.G. ANALYTIS, I.R. FISHER, Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, L. DEGIORGi, Laboratorium für Festkörperphysik, ETH - Zürich — Charge and spin density waves, periodic modulations of the electron and magnetization densities, respectively, are among the most abundant and non-trivial low-temperature ordered phases in condensed matter. The ordering direction is widely believed to result from the Fermi surface topology. However, several recent studies indicate that this common view needs to be supplemented. Here, we show how an enhanced electron-lattice interaction can contribute to or even determine the selection of the ordering vector in the model charge density wave (CDW) system ErTe3. We show how the electron-photon coupling in the vicinity of band degeneracy points. The proposal shown here for CDW formation, may be of more general relevance in multi-band systems for driving phase transitions into other broken-symmetry ground states.

The authors acknowledge support from the US DOE, the DFG and the Swiss National Foundation for Scientific Research.

10:24AM Y19.00013 Charge density wave formation in multi-band systems

RUDI HACKL, HANS-MARTIN EITER, MICHELA LAVAGNNI, Walther Meissner Institut, 85748 Garching, Germany, ELIZABETH A. NOWADNICK, ALEXANDER F. KEMPER, THOMAS P. DEVEREAUX, JIUN-HAW CHU, JAMES G. ANALYTIS, IAN R. FISHER, Stanford University, Stanford CA 94305, USA, LEONARDO DEGIORGi, ETH Zurich, 8093 Zurich, Switzerland — Charge and spin density waves are among the most abundant and non-trivial low-temperature ordered phases in condensed matter. The Fermi surface topology is widely believed to determine the ordering direction. However, several recent experimental and theoretical studies show that nesting is only one out of various other driving forces behind these instabilities. We use Raman scattering to demonstrate in which way an enhanced electron-lattice interaction can contribute to or even determine the selection of the ordering vector in the model charge density wave (CDW) system ErTe3 and other rare-earth tri-tellurides. In our joint experimental and theoretical study we exploit the symmetry properties of the electron-photon and electron-phonon coupling vertex and establish a relation between the selection rules of the electronic light scattering spectra and the enhanced electron-phonon coupling in the vicinity of band degeneracy points. The proposal shown here for CDW formation, may be of more general relevance in multi-band systems for driving phase transitions into other broken-symmetry ground states. For example, the iron-based superconductors exhibit a similar phenomenology close to the intersection points of the Fermi surface and the overall redistribution of spectral weight across the CDW phase transition.

10:36AM Y19.00014 Charge-density wave transitions of rare-earth tritellurides investigated by femtosecond electron crystallography

TZONG-RU HAN, ZHENSHENG TAO, SUBHENDRA D. MAHANTI, KISEOK CHANG, CHONG-YU RUAN, Physics and Astronomy Department, Michigan State University, East Lansing, Michigan 48824, USA, CHRISTOS D. MALLIAKAS, MERCOURI G. KANATZIDIS, Department of Chemistry, Northwestern University, Evanston, Illinois 60208, USA, CHONG-YU RUAN TEAM, MERCOURI G. KANATZIDIS TEAM — The electron-phonon mechanism that gives rise to various charge-ordered systems depends on the topology of the Fermi surface that is subjective to the influence of hybridization, nesting, and electron correlation at low dimensions. Rare-earth tritellurides are ideal systems to investigate the two-dimensional charge-density wave density wave (CDW) formation as both nesting and hybridization are at play to select the unidirectional CDW at different temperatures. Using fs electron crystallography, we investigate the noncooperative suppression of the structural order parameters following ultrafast electronic quenching and correlate electronic and ionic evolutions based on a framework of three-temperature model and nons isotropic fluctuational analysis. We show that a joint consideration of the couplings between the lattice phonons, the CDW collective modes, and the corresponding electronic subsystem is required to account for the various novel structural dynamics features.

1This work is supported by DOE under DE-FG02-06ER46309 and NSF under DMR 0702911.
10:48AM Y19.00015 1/f noise anomalies in nanoribbons of charge density wave materials

1 Now at RWTH Aachen

8:00AM Y20.00001 Flux-dependent effects in degenerate and symmetric double dot Aharonov-Bohm interferometer with and without interactions

**Authors acknowledge support from NSERC**

8:12AM Y20.00002 Optical phonon lasing in transport through semiconductor quantum dots

**8:24AM Y20.00003 Quantum Confined Silicon Clathrate Quantum Dots**

8:36AM Y20.00004 Excess current noise in electrically conductive, crack-free, nanopatterned films of semiconductor nanocrystals

8:48AM Y20.00005 Energy spectrometry of electrons ejected from dynamic quantum dots driven up a potential slope by a surface acoustic wave

Friday, March 22, 2013 8:00AM - 11:00AM – Session Y20 DCMP: Focus Session: Electron, Ion, Exciton Transport in Nanostructures: Quantum Dots and Low-dimension Structures

Session Y20 DCMP: Focus Session: Electron, Ion, Exciton Transport in Nanostructures: Quantum Dots and Low-dimension Structures

322 - Seungbum Hong, Argonne National Laboratory

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9:00AM Y20.00006 Measurement of Valley Kondo Effect in a Si/SiGe Quantum Dot1, MINGYUN YUAN, ZHEN YANG, CHUNYANG TANG, A.J. RIMBERG, Department of Physics and Astronomy, Dartmouth College, R. JOYNT, D.E. SAVAGE, M.G. LAGALLY, M.A. ERIKSSON, University of Wisconsin-Madison — The Kondo effect in Si/SiGe QDs can be enriched by the valley degree of freedom in Si. We have observed resonances showing temperature dependence characteristic of the Kondo effect in two consecutive Coulomb diamonds. These resonances exhibit unusual magnetic field dependence that we interpret as arising from Kondo screening of the valley degree of freedom. In one diamond two Kondo peaks due to screening of the valley index exist at zero magnetic field, revealing a zero-field valley splitting of $\Delta \approx 0.28$ meV. In a non-zero magnetic field the peaks broaden and coalesce due to Zeeman splitting. In the other diamond, a single resonance at zero bias persists without Zeeman splitting for non-zero magnetic field, a phenomenon characteristic of valley non-conservation in tunneling.

1 This research is supported by the NSA and ARO.

9:12AM Y20.00007 The impact of finite-area inhomogeneities on resistive and Hall measurement, DANIEL KOON, St. Lawrence University — I derive an iterative expression for the electric potential in an otherwise homogeneous thin specimen as the result of a finite-area inhomogeneity in either the direct conductance, the Hall conductance, or both. This expression extends to the finite-area regime the calculation of the effect of such inhomogeneities on the measurement error in the sheet resistance and Hall sheet resistance. I then test these results on the exactly-solvable case of a circular inhomogeneity equally distant from the four electrodes for either a square four-point-probe array on an infinitely large conducting specimen or a circular van der Pauw specimen with symmetrically-placed electrodes.

9:24AM Y20.00008 Quasibound States and Evidence for a Spin 1 Kondo Effect in Asymmetric Quantum Point Contacts1, HAO ZHANG, Duke University, PHILLIP WU, Stanford University, ALBERT CHANG, Duke University — Linear conductance below $2e^2/h$ shows resonance peaks in highly asymmetric quantum point contacts (QPCs). As the channel length increases, the number of peaks also increases. At the same time, differential conductance exhibits zero bias anomalies (ZBAs) in correspondence with every other peak in the linear conductance. This even odd effect, observable in the longer channels, is consistent with the formation of quasi-localized states within the QPC. In rare cases, triple peaks are observed, indicating the formation of a spin one Kondo effect when the electron filling number is even. Changing the gate voltage tunes this spin triplet to a singlet which exhibits no ZBA. The triple-peak provides the first evidence suggestive of a spin singlet triplet transition in a QPC, and the presence of a ferromagnetic spin interaction between electrons.

1 Work supported by NSFDMR-0701948

9:36AM Y20.00009 Enhancement of the excition emission in ZnO nanowires1, ANDREW EPPS2, JAMIE NOWALK3, MARIAN TZOLOV1, Lock Haven University — The ZnO nanowires were grown by the chemical vapor transport method using a thin gold film as a catalyst. Their light emission in the visible and near UV spectral range was excited by continuous wave and pulsed UV light and by electrons within an SEM. The emission spectrum consists typically of the exciton emission band and a band in the green spectral range related to structural defects. We have followed the evolution of the ratio between the exciton and green band between our samples. The highly localized excitation by the electron beam allowed the profiling of the emission spectrum across the thickness of nanowire samples. We demonstrate that the tips of the nanowires show substantially higher excitation emission. Depth of excitation was varied independently by the electron accelerating voltage. The results have been interpreted within a model accounting for the surface effects and associated band bending at the surface.

1AE acknowledges the financial support from the NSF
2Undergraduate
3Undergraduate
4Professor

9:48AM Y20.00010 BEC-BCS crossover of a dipolariton condensate in a semiconductor microcavity, JUNG-JUNG SU, E. L. Ginzton Lab., Stanford Univ.; Dept. of Electrophys. Natl. Chiao Tung Univ., Taiwan, NA YOUNG KIM, E. L. Ginzton Lab., Stanford Univ; YOSHIHISA YAMAMOTO, E. L. Ginzton Lab., Stanford Univ; Natl. Inst. of Informatics, Japan, ALLAN H. MACDONALD, Dept. of Phys., Univ. of Texas at Austin — We study the electron-tunnel-coupling condensation of dipolar exciton-polariton (dipolariton) at the BEC-BCS crossover. An exciton-polariton (EP) is an extremely light bosonic quasiparticle composed of excitons and photons and can condense a temperatures as high as room temperature. Electron tunneling between nearby quantum wells can coupled spatially direct and indirect excitons and therefore also the corresponding exciton-polaritons; the indirect EPs in particular carry the interesting dipolar nature. We use a fermionic mean-field theory to examine the influence of this coupling on EP condensates from the dilute BEC to the dense BCS limits. A wide variety of distinct states are found, including mixed direct and indirect EP condensates, and metallic condensates, depending on particle-densities and on the relative positions of the quantum well states in different wells. Possible experimental manifestations of these phenomena will be discussed.

10:00AM Y20.00011 Strain-controlled band engineering and Self-doping in Ultrathin LaNiO3 films, X. LIU, E.J. MOON, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701. J.M. RONDINELLI, Department of Materials Science and Engineering, Drexel University, Philadelphia, Pennsylvania 19104. N. PRASAI, Department of Physics, University of Miami, Coral Gables, Florida 33124, B.A. GRAY, M. KAREEV, J. CHAKHALIAN, J. CHAKHALIAN, Department of Physics, University of Miami, Coral Gables, Florida 33124; J.L. COHN, Department of Physics, University of North Carolina at Charlotte, Charlotte, North Carolina 28223. YUAN, ZHEN YANG, CHUNYANG TANG, A.J. RIMBERG, Department of Physics and Astronomy, Dartmouth College, R. JOYNT, D.E. SAVAGE, M.G. LAGALLY, M.A. ERIKSSON, University of Wisconsin-Madison — The Kondo effect in Si/SiGe QDs can be enriched by the valley degree of freedom in Si. We have observed resonances showing temperature dependence characteristic of the Kondo effect in two consecutive Coulomb diamonds. These resonances exhibit unusual magnetic field dependence that we interpret as arising from Kondo screening of the valley degree of freedom. In one diamond two Kondo peaks due to screening of the valley index exist at zero magnetic field, revealing a zero-field valley splitting of $\Delta \approx 0.28$ meV. In a non-zero magnetic field the peaks broaden and coalesce due to Zeeman splitting. In the other diamond, a single resonance at zero bias persists without Zeeman splitting for non-zero magnetic field, a phenomenon characteristic of valley non-conservation in tunneling.

10:12AM Y20.00012 Monte Carlo simulations of electron transport for electron beam-induced deposition of nanostructures, FRANCESC SALVAT-PUJOL, HARALD O. JESCHKE, ROSER VALENTI, Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt, Germany — Tungsten hexacarbonyl, W(CO)6, is a particularly interesting precursor molecule for electron beam-induced deposition of nanoparticles, since it yields deposits whose electronic properties can be tuned from metallic to insulating. However, the growth of tungsten nanostructures poses experimental difficulties: the metal content of the nanostructure is variable. Furthermore, fluctuations in the tungsten content of the deposits seem to trigger the growth of the nanostructure. Monte Carlo simulations of electron transport have been carried out with the radiation-transport code Penelope in order to study the charge and energy deposition of the electron beam in the deposit and in the substrate. These simulations allow us to examine the conditions under which nanostructure growth takes place and to highlight the relevant parameters in the process.
10:24AM Y20.00013 Monte Carlo simulations of neon versus helium ion beam induced deposition, sputtering and etching. RAJENDRA TIMILSINA, DARYL SMITH, The University of Tennessee at Knoxville, Tennessee and Center for Nanophase Materials Sciences Oak Ridge National Laboratory, Oak Ridge. — The ion beam induced nanoscale synthesis of PtCx (where x < 5) using the trimethyl(methylcyclopentadienyl)platinum(IV) (MeCpPtIVMe5) precursor is investigated by performing Monte Carlo simulations of helium and neon ions. The helium beam leads to more lateral growth relative to the neon beam because of its larger interaction volume. The lateral growth of the nanopillars is dominated by molecules deposited via secondary electrons in the both simulations. Notably, the helium pillars are dominated by SE-I electrons whereas the neon pillars by SE-II electrons. Using a low precursor residence time of 70µs resulting in an equilibrium coverage of ~ 4%, the neon simulation has a lower deposition efficiency (3.5%) compared to that of the helium simulation (6.5%). At larger residence time (10ms) and consequently larger equilibrium coverage (85%) the deposition efficiencies of helium and neon increased to 49% and 21%, respectively; which is dominated by increased lateral growth rates leading to broader pillars. The nanoscale growth is further studied by varying the ion beam diameter at 10 ms precursor residence time. The study shows that total SE yield decreases with increasing beam diameters for the both ion types. However, the helium has the larger SE yield as compared to that of neon in the both low and high precursor residence time, and thus pillars are wider in all the simulations studied.

10:36AM Y20.00014 Electron field emission from freestanding Diamond nanomembranes and Application to time-of-flight mass spectrometry. HYUNSEOK KIM, University of Wisconsin, Madison, JONGHOO PARK, Kyungpook National University, Daegu, Korea, HYUNCHEOL SHIN, ROBERT H. BLICK, University of Wisconsin, Madison — We introduce a prototype of a freestanding diamond nanomembrane for large protein detection in time-of-flight mass spectrometry. Doped diamond as a material for mass spectroscopy is extremely interesting due to its mechanical and electrical properties. The freestanding diamond nanomembranes are able to fabricate lateral extensions of 400µm × 400µm with a thickness of 100nm. We employ optical lithography and a Buffered Oxide Etch (BOE) of SiO2 followed by anisotropic etching of the substrate silicon using TMAH solution and finally removing SiO2. The electron field emission from the surface of the membrane is traced in the IV characteristics at room temperature. The membrane is then applied for detection of the large ionized proteins using time-of-flight mass spectrometry. Ion detection is demonstrated in our nanomembrane MALDI-TOF analysis of Insulin (5,735 Da). That is when the ions with a large kinetic energy bombard the membrane their energy is thermalized upon impact into phonons. The phonons give a thermal energy to the electrons with the membrane, which are then excited to higher energetic states. Given an extraction voltage this leads to electron field emission from the membrane which we labeled phonon-assisted field emission (PAFE). In other words, the MALDI mass spectra are obtained by exploiting ballistic phonon propagation and quasi-diffusive phonon propagation.

Friday, March 22, 2013 8:00AM - 11:00AM
Session Y22 DCMP: Quantum Solids - He4

8:00AM Y22.00001 Dissipative superfluid mass flux through solid 4He1, YEGOR VEKHOV, ROBERT HALLOCK, Dept. of Physics, Univ. of Mass. Amherst. — The thermo-mechanical effect in superfluid helium is used to create a chemical potential difference, ∆µ, across a liquid or solid 4He sample and induce a mass flux. With an improved technique, measurements of the mass flux, F, through a solid-filled sample cell at several fixed helium sample temperatures, T, have been done as a function of ∆µ. And, measurements of F (in the range 100 < T < 550 mK) have been done as a function of temperature for several fixed values of ∆µ. The temperature dependence of the flow through solid helium above 100 mK is confirmed to show a reduction of the flux with increasing temperature, while for liquid helium there is no marked temperature dependence in the temperature range studied. The dependence of F on ∆µ documents in some detail the dissipative nature of the flow for the case of a solid helium-filled sample cell. In the case of solid helium we observe a kink in the ∆µ/F graph with b ≈ 0.3, which is consistent with expectations for 1D superfluidity. The relationship between this work and the various torsional oscillator NCRI results is not clear. We may be exploring different phenomena.

8:12AM Y22.00002 Exact Solution for Vortex Dynamics in Temperature Quenches of Two-Dimensional Superfluids, ANDREW FORRESTER, HAN-CHING CHU, GARY WILLIAMS, UCLA. — An exact analytic solution for the dynamics of vortex pairs is obtained for rapid temperature quenches of a superfluid film starting from the line of critical points below the critical temperature T_{KT}. An approximate solution for quenches at and above T_{KT} provides insights into the origin of logarithmic transients in the vortex decay, and are in general agreement with recent simulations of the quenched XY model. These results confirm that there is no "creation" of vortices whose density increases with the quench rate as predicted by the Kibble-Zurek theory, but only monotonic decay of the thermal vortices already present at the initial temperature. The problem in the Kibble-Zurek argument is the artificial restriction to measuring the vortex density only at the "freezeout" sampling time, which increases with the quench rate. But since the the pairs continually decay, of course this will always result in lower vortex densities for a longer quench time and hence a later sampling time. But in fact the vortex densities can be measured at all times, and it then becomes quite clear that there is an instantaneous superfluid quench has the lowest vortex density at all times of any quench rate, since it most rapidly gets to the lowest temperature.

1This work is supported by the Welch Foundation, Houston, Texas (Grant No. Y-1525), the Repperger Fellowship Program and the Air Force Office of Scientific Research.


3NSF DMR 07-57701, 08-55954

4Work supported by the NSF, Grant DMR 09-06467
8:24AM Y22.00003 Elasticity, Plasticity and Supersolidity in Solid Helium. JOHN BEAMISH, University of Alberta, ARIEL HAZIOT, ANDREW FEFFERMAN, XAVIER ROJAS, SEBASTIEN BALIBAR, Laboratoire de Physique Statistique de l’ENS — The frequency of a torsional oscillator containing solid helium depends on the helium’s elastic properties, as well as its inertia. Mobile dislocations reduce the helium’s shear modulus, but they are pinned at low temperatures. The resulting increase in shear stiffness raises the TO frequency and can mimic mass decoupling in a superfluid. The size of this elastic effect depends on the geometry of the oscillator and on the magnitude of the modulus changes. We recently showed that the elastic effect can be large enough to explain the apparent mass decoupling in some oscillators whose torsion rods have a central hole to admit the helium, suggesting that the apparent supersolidity is an artifact due to elastic changes. We have observed extremely large modulus changes in high quality single crystals. We were able to identify the dislocations responsible for the elastic changes and to show that they were arranged in a network with very large pinning lengths. The large modulus changes reflect the dislocations’ extremely high mobility at low temperatures, which produces a “giant plasticity” in this quantum crystal.

3 This work was supported by grants from ERC (AdG 247258) and NSERC Canada.

8:36AM Y22.00004 The giant plasticity in 4He crystals, ARIEL HAZIOT, ANDREW FEFFERMAN, XAVIER ROJAS, Ecole Normale Superieure, JOHN BEAMISH, University of Alberta, SEBASTIEN BALIBAR, Ecole Normale Superieure — We have applied very small shear stresses (down to 1 nanobar) to oriented single 4He crystals, and directly measured their response as a function of temperature (from 15 mK to 1 K), orientation, crystal quality, 4He concentration, frequency and shear stress magnitude. For particular orientations, we have found a giant plasticity that is reversible, associated with the elastic coefficient c_{44} which nearly vanishes around 200 mK. Other elastic coefficients show no measurable anomaly. The strong reduction of (80% in high quality crystals without impurities) shows that dislocations glide in the basal plane of the hexagonal structure with no dissipation. This plasticity disappears as soon as traces of 4He impurities bind to the dislocations (at low T) or if their motion is damped by collisions with thermal phonons (at higher T). It has no equivalent in classical crystals.

8:48AM Y22.00005 Dislocation densities and lengths in solid 4He from elastic measurements, ANDREW FEFFERMAN, ARIEL HAZIOT, Laboratoire de Physique Statistique de l’ENS, JOHN BEAMISH, University of Alberta, SEBASTIEN BALIBAR, Laboratoire de Physique Statistique de l’ENS — Elastic measurements on solid 4He show large softening of the shear modulus due to motion of dislocations, behavior which has been described as quantum plasticity. Dislocation networks may also be responsible for the unusual behavior seen at low temperatures in torsional oscillator and flow experiments. However, existing estimates of dislocation densities in helium crystals vary by many orders of magnitude. By measuring the temperature and frequency dependence of the elastic dissipation, we have determined dislocation densities and network lengths in both single crystals and polycrystals of 4He. The dislocation lengths are much longer than previous estimates, meaning that they are less connected than previously thought. Even in polycrystals, we find no evidence for the large densities of well-connected dislocations which would be needed to explain mass decoupling in torsional oscillators in terms of superfluidity in a dislocation network.

3 This work was supported by grant ERC-AdG 247258 SUPERSOLID and by a grant from NSERC Canada.

9:00AM Y22.00006 Solid 4He probed by both torsional oscillator and ultrasound, HARRY KOJIMA, Rutgers University, IZUMI IWASA, Kanagawa University, JOHN GOODKIND, UCSD — The interpretation of observed anomalous increases in the frequencies of torsional oscillators (TO) containing solid 4He confined in Vycor nanopores as evidence for emergence of a supersolid phase has been met recently by conflicting experiments. Yet questions remain on the origin of the observed TO anomalies in bulk solid 4He samples. To search for the origin, we are carrying out simultaneous measurements of 10 MHz longitudinal ultrasound and TOs (250~1100 Hz) on identical solid 4He samples. Temperature dependence of velocity and attenuation of ultrasound and that of amplitude and frequency of TO are measured. At the temperatures, where TO anomalies occur, anomalies in sound velocity and attenuation also appear. When solid 4He is doped with 20 ppm 3He, the temperature of TO anomaly tracks that of ultrasound. Interpretation of these observations in terms of the motion of dislocation lines will be presented.

1 Research supported by NSF.

9:12AM Y22.00007 Excitations of Amorphous Solid Helium, JACQUES BOSSY, Institut Néel, CNRS-UJF, BP 166, 38042 Grenoble Cedex 9, France, JACQUES OLLIVIER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, HELMUT SCHOFER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, Université Joseph Fourier, UFR de Physique, F38041 Grenoble Cedex 9, France, HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware — We present neutron scattering measurements of the dynamic structure factor, S(Q,ω), of amorphous solid helium confined in 47 Å pore diameter MCM-41 at pressure 48 kbar. At low temperature, T = 0.05 K, we observe S(Q,ω) of the confined quantum amorphous solid plus the bulk polycrystalline solid of the MCM-41 powder grains. No liquid-like phonon-roton modes, other sharply defined modes at low energy (ω < 1.0 meV) or modes unique to a quantum amorphous solid that might suggest superflow are observed. Rather the S(Q,ω) of confined amorphous and bulk polycrystalline solid appear to be very similar. At higher temperature (T > 1 K), the amorphous solid in the MCM-41 pores melts to a liquid which has a broad S(Q,ω) peaked near ω ≈ 0 characteristic of normal liquid 4He under pressure. Expressions for the S(Q,ω) of amorphous and polycrystalline solid helium are presented and compared. In previous experiments of liquid 4He confined in MCM-41 at lower pressure the intensity in the liquid roton mode decreases with increasing pressure until the roton vanishes at the solidification pressure (38 bars), consistent with no roton in the solid observed here.

9:24AM Y22.00008 Plasticity and dislocation-induced anomalous softening of solid helium under DC shear, IRENE BAYERLEIN, CAIZHI ZHOU, Los Alamos National Laboratory, JUNG-JUNG SU, Stanford University, MATTHIAS GRAF, CHARLES REICHHARDT, ALEXANDER BALATSKY, Los Alamos National Laboratory — The classical model of gliding dislocation lines in slip planes of crystalline solid helium leads to plastic deformation even at temperatures far below the melting temperature and strongly affects elastic properties. In this work, we propose that the gliding of dislocations and plasticity may be the origin of many observed elastic anomalies in solid He-4, which have been argued to be connected to supersolidity. We present and propose a dislocation motion model that describes the stress-strain τ–ε curves and work-hardening rate τ/dε of a DC shear experiment to be performed at constant strain rate in solid helium. The calculated τ/dε exhibits strong softening with increasing temperature owing to the motion of dislocations, which mimics anomalous softening of the elastic shear modulus μ. In the same low-temperature region the classical motion of dislocations causes dissipation with a prominent peak [1] [1] C. Zhou et al., Philos. Mag. Lett. 92 (2012) 608
9:36AM Y22.00009 Simultaneous measurements of the torsional oscillator and shear modulus of solid 4He diluted with various 3He concentration1, JAEHO SHIN, WONSIUK CHOI, JAEWON CHOI, SEONG JANG, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, Republic of Korea, KEIYA SHIRAHAM, Department of Physics, Keio University, Yokohama 223-8522, Japan, EUNSEONG KIM, Center for Supersolid & Quantum Matter Research and Department of Physics, KAIST, Daejeon 305-701, Republic of Korea — In 2004, Kim and Chan observed the non-classical rotational inertia (NCRI) of solid helium-4 by using a torsional oscillator (TO). Below 200mK, the resonance period of solid helium dropped, which was originally interpreted as the mass decoupling of the fraction of solid helium. Recently, anomalous increase in the shear modulus of solid helium was found and showed striking similarity in temperature, frequency, 3He concentration, and drive dependence to those of the NCRI [2]. To understand the connection between the NCRI and the shear modulus anomaly, we simultaneously measure the change in the resonance frequency and the stiffness of solid helium below 200mK. The torsion cell contains a pair of the concentric piezoelectric transducers (PZT) which defines an annular channel for the simultaneous measurements. We will report the interference between the motion of the TO at resonance and AC motion of the PZT in solid 4He with different 3He concentration.

1We gratefully acknowledge the financial support by the National Research Foundation of Korea through the Creative Research Initiatives.

9:48AM Y22.00010 4He adsorption on α-graphyne1, YONGYUNG KWN, HOONKYUNG LEE, Konkuk University, Seoul, KOREA, DAVID M. CEPERLEY, University of Illinois at Urbana-Champaign, IL61801, U.S.A. — Path-integral Monte Carlo calculations have been performed to study 4He adsorption on a single α-graphyne sheet that is a hexagonal network of sp2- and sp3-bonded carbon atoms. Using the 4He-substrate interaction described by a pairwise sum of the helium-carbon inter-atomic potentials, we have found that each hexagon of a graphyne can accommodate one 4He atom at its in-plane center. The first layer of 4He atoms adsorbed on this 4He-attached graphyne sheet with a composite of C16H16 exhibits various quantum phases depending on the helium coverage. It is found to be in a Mott insulating state at a coverage of 0.0706 Å⁻² with three 4He atoms occupying each unit cell while the helium atoms form a commensurate triangular solid at 0.0941 Å⁻². With the introduction of Ising pseudospins for two degenerate configurations of three 4He atoms in a hexagonal cell, the transition from the Mott insulator to the triangular solid can be interpreted as a ferromagnetic transition. In addition we find stable formation of zero-point vacancies in the commensurate triangular solid and their roles in possible realization of supersolidity are under investigation.

1supported by the Basic Science Research Program (2012006887) and the WCU Program (R31-2008-000-10057-0) through the National Research Foundation of Korea funded by the Ministry of Education, Science and Technology.

10:00AM Y22.00011 Pursuit of the Elusive Supersolid1, XIAO MI, JOHN D. REPPY, Cornell University — The excitement following the initial report of supersolid behavior for 4He embedded in porous Vycor glass has been tempered by the realization that many of the early supersolid observations were contaminated by effects arising from an anomaly in the elastic properties of solid 4He. In an attempt to separate dynamic elastic effects from a true supersolid signal, we employed a torsional oscillator with two eigen frequencies to study the 4He-vycor system. We found that frequency dependent elastic signals can entirely account for the observed period shift signals. Although, we conclude that supersolid does not exist for the 4He-Vycor case, the question of its presence in bulk samples remains open. In our current experiments we apply the two-frequency test to bulk samples of solid 4He. Again we find a frequency dependent contribution arising from elastic effects. However, in some cases we also find a small frequency independent contribution, which may indicate the existence of a remnant supersolid phase. Given the history of this subject such results must be treated with caution.

1This work is supported by the National Science Foundation through Grant DMR-060586, DMR-0965698 and CCMR Grant DMR-050404.

10:12AM Y22.00012 An Ordered State of Dislocations in Solid Helium, HANS JOCHEN LAUTER, Oak Ridge National Laboratory, ECKHARD KROTSCHECK, University at Buffalo-SUNY, EFIM KATS, Landau Institute for Theoretical Physics, KENNETH HERWIG, ANDREY PODLESNYAK, DIALLO SOULEYMANE, Oak Ridge National Laboratory, GLYDE HENRY, University of Delaware, ANDREII SAVICI, Oak Ridge National Laboratory — An ordered state of dislocations, see e.g. [1], is disclosed from neutron inelastic scattering data taken from solid helium at 40mK and a pressure of about 30bar. A characteristic feature is the phonon gap at the origin of about 0.15 meV, which reveals the non-equilibrium state of stressed helium created by rapid cooling with the blocked-capillary method. Energy gain scattering starts to appear at a temperature of 0.5 K that underlines the non-equilibrium state of stressed helium and the non-applicability of the detailed balance. The increasing thermal occupation of phonon-states observed as increasing intensity in energy gain scattering builds to a phase transition close to 1.4K. The creation of a helium single crystal with hcp-structure in thermal equilibrium [2] is observed at this temperature. This phase transition is in agreement with the vanishing quasi two-dimensional superfluid helium in solid helium confined in aerogel around 1.3K [3]. The event of the “supersolid” transition around 100mK is not observed in the two neutron scattering experiments.

2E. Blackburn, et. al., PRAMANA 71, 673 (2008)

10:24AM Y22.00013 Stability limit of a metastable state of hcp solid helium-4, FABIEN SOURIS, JULES GRUCKER, JACQUES DUPONT-ROC, PHILIPPE JACQUIER, Laboratoire Kastler Brossel, ENS/CNRS/Université Paris 6, 24 rue Lhomond, Paris 75005, France, ATOMES DANS MONOCRISTAUX TEAM — Solid helium has the unique feature of having an horizontal melting curve in the P,T plane. This offers novel opportunities to study the stability limits of a metastable solid, by using the pressure as a control parameter of the metastability. The metastable state is obtained by focusing a 1 MHz ultrasonic sound wave inside an helium-4 crystal. Around 4 bar below the melting pressure, the metastable crystal becomes unstable. Different configurations with one or two ultrasonic emitters have been used and lead to the same stability limit. This happens at much lower depression than predicted by nucleation theory or by quantum Monte Carlo simulations. Repeated experiments show that the instability initially appears as a small defect (~0.2 mm) located at the maximum isotropic strain. Further studies are performed to understand the underlying mechanism of the instability. Possible scenarios accounting for this unexpected observation are discussed.

10:36AM Y22.00014 Path-Integral Monte Carlo Simulations of Ideal Strength and Peierls Stress in HCP 4He, EDGAR JOSUE LANDINEZ BORDA, MAURICE DE KONING, Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas, UNICAMP — The ideal strength of a crystal is defined as the stress required to induce plastic deformation in a defect-free crystal. It is a theoretical upper bound to the strength of real crystals. The Peierls stress, on the other hand, is the minimum stress required to move a lattice dislocation and produce defect-mediated deformation. Here we present results for both quantities in HCP 4He as obtained from a series of Path-integral Monte Carlo simulations and discuss them in terms of its deformation behavior.
10:48AM Y22.00015 Superfluid transition in a correlated dislocation network¹ HANNES MEIER, MATS WALLIN, KTH, Stockholm, Sweden, STEPHEN TEITEL, University of Rochester — The search for a supersolid state in He-4 solids has motivated theoretical investigations of 3D connected superfluid dislocation networks. It has usually been assumed that a 3DXY universality class controls the superfluid transition in such systems since the random distance between intersections of the dislocation lines carrying superfluidity appears as uncorrelated disorder which is irrelevant at the 3DXY transition. We consider the possibility that the random disorder instead has long range correlations, and investigate several different models of correlated defects. Analytic arguments and extensive Monte Carlo simulations demonstrate new disordered universality classes for the superfluid transition with a smooth temperature dependence at the transition of the superfluid density and heat capacity.

¹Work supported by NSF Grant No. DMR-1205800 and Swedish Research Council Grant No. 2009-3656. Simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at PDC.

Friday, March 22, 2013 8:00AM - 11:00AM —
Session Y36 DCMP: Novel Superconductors III 344 - N. Peter Armitage, Johns Hopkins University

8:00AM Y36.00001 Spin incommensurability varies linearly with hole content in single-layer Bi2201 cuprate¹. JOHN TRANQUADA, Brookhaven National Lab, M. ENOKI, M. FUJITA, T. NISHIZAKI, K. YAMADA, Tohoku U., S. IIKUBO, Kyushu Inst. Tech., D.K. SINGH, S. CHANG, NCNR — We have performed inelastic neutron scattering measurements on the single-layer cuprate Bi2201 cuprate approach to determine its detailed behavior seems to exist. The resonance mode does seem to be a reliable fingerprint for an unconventional, sign-changing order parameter, it is a strong coupling phenomenon and no reliable doesn’t change sign remains if one includes higher order vertex corrections, ii) vertex corrections are of order unity and cannot be ignored. Thus, while the spectrum. In this work we analyze such vertex correction and show that: i) the qualitative difference in the behavior between a gap that changes sign and that antiferromagnetic fluctuations. In this theory, a resonance occurs in case of a sign change of the superconducting gap function for momenta on the Fermi surface and energy. A promising theory for the resonance is based on the analysis of the particle-hole spectrum in the superconducting state and in the presence of antiferromagnetic fluctuations. In this theory, a resonance occurs in case of a sign change of the superconducting gap function for momenta on the Fermi surface that are coupled by the antiferromagnetic ordering vector. So far, the theory was analyzed without including higher order vertex corrections of the particle-hole spectrum. In this work we analyze such vertex correction and show that: i) the qualitative difference in the behavior between a gap that changes sign and that doesn’t change sign remains if one includes higher order vertex corrections, ii) vertex corrections are of order unity and cannot be ignored. Thus, while the resonance mode does seem to be a reliable fingerprint for an unconventional, sign-changing order parameter, it is a strong coupling phenomenon and no reliable approach to determine its detailed behavior seems to exist.

8:12AM Y36.00002 Strong coupling behavior of the neutron resonance mode in unconventional superconductors , PATRIK HLOBL, BORIS NAROZHNY, JOERG SCHMALIAN, Karlsruhe Institute of Technology, INSTITUTE FOR THEORY OF CONDENSED MATTER COLLABORATION — A number of unconventional superconductors are characterized by a resonance mode in the spin excitation spectrum, measured via inelastic neutron scattering, which emerges below the superconducting transition temperature and is sharp as function of momentum and energy. A promising theory for the resonance is based on the analysis of the particle-hole spectrum in the superconducting state and in the presence of antiferromagnetic fluctuations. In this theory, a resonance occurs in case of a sign change of the superconducting gap function for momenta on the Fermi surface that are coupled by the antiferromagnetic ordering vector. So far, the theory was analyzed without including higher order vertex corrections of the particle-hole spectrum. In this work we analyze such vertex correction and show that: i) the qualitative difference in the behavior between a gap that changes sign and that doesn’t change sign remains if one includes higher order vertex corrections, ii) vertex corrections are of order unity and cannot be ignored. Thus, while the resonance mode does seem to be a reliable fingerprint for an unconventional, sign-changing order parameter, it is a strong coupling phenomenon and no reliable approach to determine its detailed behavior seems to exist.

8:24AM Y36.00003 Distinct Fe-induced magnetic states in the underdoped and overdoped regimes of La2−xSrCu1−yFeO4 revealed by muon spin relaxation. KENSUKE SUZUKI, TADASHI ADACHI, YOUICHI TANABE, HIDETAKA SATO, Department of Applied Physics, Tohoku University, RISDY RISDIANA, YASUYUKI ISHII, TAKAO SUZUKI, ISAO WATANABE, Advanced Meson Science Laboratory, Nishina Center for Accelerator-Based Science, RIKEN, YOJI KOIKE, Department of Applied Physics, Tohoku University — Zero-field muon-spin-relaxation measurements have been performed in partially Fe-substituted La2−xSrCu1−yFeO4 (Bi2201) with x = 0.2, 0.3, 0.4 and 0.5, a doping range that spans the spin-glass (SG) to superconducting (SC) phase boundary [1]. The doping evolution of low energy spin fluctuations (≤ 11 meV) was found to be characterized by a change of incommensurate modulation wave vector from the tetragonal [110] to [100]/[010] directions, while maintaining a linear relation between the incommensurability and the hole concentration, δ ≈ p. In the SC regime, the spectral weight is strongly suppressed below ~ 4 meV. Similarities and differences in the spin correlations between Bi2201 and the prototypical single-layer system La2−xSrCuO4 will be discussed.


8:48AM Y36.00005 Understanding of Nuclear Quadrupole Interaction of $^{19}\text{F}^*$ and Binding Mechanism in Solid Fluorine at First-Principles Level. D.R. MISHRA, M.M. ARYAL, N.P. ADHIKARI, Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal, R.H. PINK, T.P. DAS, Department of Physics, University at Albany, SUNY — We have carried out a theoretical study of the nuclear quadrupole interaction (NQI) parameters of $^{19}\text{F}^*$ excited nuclear state in solid fluorine as well as the intermolecular binding of fluorine molecules in the solid. This is in continuation of our investigation [1] of the properties of solid halogens using the first-principles Hartree-Fock (HF) cluster procedure combined with many-body perturbation theory (MBPT), implemented by the Gaussian 03 set of programs. For the NQI parameters, the value of $(e^2QQ/h)$ obtained from our investigation for the $^{19}\text{F}^*$ excited nuclear state in solid fluorine is 120.9 MHz, which agrees with the experimental value 127.2 MHz, quoted in [2], within 5% and the asymmetry parameter, $\eta$ is essentially zero. For obtaining $(e^2QQ/h)$ the value of the quadrupole moment, $Q$ for $^{19}\text{F}^*$ is taken from [3] as 0.072 x $10^{-26}$ m$^2$. As regards the binding of fluorine molecules in solid fluorine, our quantitative binding energy results show that the binding arises mainly from the van der Waals interaction obtained from intermolecular-body effects with the one electron HF contribution being weak and repulsive in nature.


9:00AM Y36.00006 Enhanced charge stripe order in superconducting La$_{2-x}$Ba$_x$CuO$_4$ in high magnetic fields, M. HUECKER, Brookhaven National Laboratory, M. V. ZIMMERMANN, Deutsches Elektronen-Synchrotron DESY, Z.J. XU, J.S. WEN, G.D. GU, J.M. TRANQUADA, Brookhaven National Laboratory — There is mounting evidence for a proximity of the superconducting ground state in the cuprates to competing states with static spin and/or charge density modulations. One such competing state is the spin and charge stripe order in La$_{2-x}$Ba$_x$CuO$_4$. By means of high energy (100 keV) x-ray diffraction we have studied the effect of a high magnetic field (H=(c)) on the charge stripe order in a broad range of doping (0.095 $\leq x \leq 0.155$). We find that the field can significantly enhance the charge stripe order, but only at temperatures and dopings where it coexists with bulk superconductivity at zero field. The field also increases stripe correlations between the planes, which can result in an enhanced frustration of the interlayer Josephson coupling. Close to the famous $x=1/8$ compound, where zero field stripe order is pronounced and bulk superconductivity is suppressed, charge stripe order is independent of the field. The results imply that static stripe order and three-dimensionally coherent superconductivity are competing ground states.

1The work at Brookhaven was supported by the Office of Basic Energy Sciences, Division of Materials Science and Engineering, U.S. Department of Energy (DOE), under Contract No. DE-AC02-98CH10886.

9:12AM Y36.00007 Lifetime of Skyrmions in Cuprates and Other Layered Materials, LIUEFI CAI, EUGENE CHUDNOVSKY, DMITRY GARANIN, CUNY Lehman College, CUNY Lehman COLLEGE TEAM — Collapse of a skyrmion due to the discreteness of a crystal lattice in isotropic two-dimensional ferro- and antiferromagnets has been studied analytically and by numerical solution of equations of motion for up to 2000 x 2000 classical spins on a square lattice coupled via Heisenberg exchange interaction. Excellent agreement between analytical and numerical results has been achieved. The lifetime of the skyrmion scales with its initial size, $\lambda_0$, as $(\lambda_0/a)^{1.7}$ in ferromagnets and as $(\lambda_0/a)^{2.17}$ in antiferromagnets, with $a$ being the lattice parameter. This makes antiferromagnetic skyrmions significantly shorter lived than ferromagnetic skyrmions.

1Research supported by DOE grant DE-FG02-93ER45487.

9:24AM Y36.00008 Fractional Flux Quantization in Loops of Unconventional Superconductors, FLORIAN LODER, ARNO KAMPF, THILO KOPP, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — The magnetic flux threading a conventional superconducting ring is typically quantized in units of $\Phi_0 = hc/2e$. The factor 2 in the denominator of $\Phi_0$ originates from the existence of two different types of pairing states with minima of the free energy at even and odd multiples of $\Phi_0$. Here we show that spatially modulated pairing states exist with energy minima at fractional flux values, in particular at multiples of $\Phi_0/2$. In such states condensates with different center-of-mass momenta of the Cooper pairs coexist. The proposed mechanism for fractional flux quantization is discussed in the context of cuprate superconductors, where $hc/4e$ flux periodicities as well as uniaxially modulated superconducting states were observed.

9:36AM Y36.00009 Magnetic structures in YBCO single crystals under tilted magnetic fields, VITALII VLASKO-VLASOV, ULRICH WELP, ALEXEI KOSHELEV, WAI KWOK, Argonne National Laboratory — We study magnetic flux distributions in YBCO single crystals remagnetized by magnetic fields of different orientations using the magneto-optic indicator technique. Application of the perpendicular field to the crystals cooled in the in-plane magnetic field, application of the in-plane field to the crystals cooled in the normal magnetic field, and remagnetization by magnetic field tilted to the sample surface result in unusual quasi-periodic vortex structures. These strongly inhomogeneous vortex patterns can be associated with the flux cutting and strong anisotropy of the vortex kink motion depending on the trapped flux and external field orientations. We discuss the effect of resulting inhomogeneous current distributions on the current carrying ability of the YBCO coated conductors. Work supported by the US DOE-BES funded Energy Frontier Research Center and by Department of Energy, Office of Science, Office of Basic Energy Sciences under Contract No. DE-AC02-06CH11357.

9:48AM Y36.00010 Vortex lock-in transition coinciding with the 3D to 2D crossover in YBa$_2$Cu$_3$O$_y$. SASKIA BOSMA, STEPHEN WEYENETH, Physics Institute - University of Zurich, ROMAN PUZNIAK, Institute of Physics - Polish Academy of Sciences, ANDREAS ERB, Wälther Meissner Institute - Bavarian Academy of Sciences, HUGO KELLER, Physics Institute - University of Zurich — Dimensionality is essential to understand the behavior of vortices in layered cuprate superconductors. A 3D (three-dimensional) to 2D (two-dimensional) crossover takes place when the out-of-plane coherence length becomes smaller than the interplane distance. We directly detected a vortex lock-in transition by torque magnetometry in an overdoped YBa$_2$Cu$_3$O$_{7-\delta}$ single crystal of low anisotropy. The locked-in state was observed below the 3D to 2D crossover temperature, independently of extrinsic pinning effects thanks to a high quality clean crystal and the use of a vortex shaking technique. The lock-in is enhanced by decreasing temperature and increasing magnetic field. The shape of the torque signal is in very good agreement with the model developed by Feinberg and Etoh in [Int. J. Mod. Phys. B 7, 2085 (1993)] for quasi-2D superconductors, despite the low anisotropy of the material. Additionally, we present a new torque magnetometer design featuring vortex shaking, and compatible with the Quantum Design PPMS system.
10:00AM Y36.00011 Investigating the low-field vortex lattice phase diagram in CeCoIn$_5$ with $H \parallel c^*$, P. DAS, Los Alamos National Laboratory, NM, USA, M. R. ESKILDSEN, University of Notre Dame, IN, USA, E. M. FORGAN, University of Birmingham, UK, H. KAWANO-FURUKAWA, Ochanomizu University, Japan, C. PETROVIC, Brookhaven Natl. Lab., NY, USA — Here we present small angle neutron scattering studies of the vortex lattice (VL) phase diagram in CeCoIn$_5$ in the low-field high-temperature regime with $H \parallel c^*$ which remained unexplored. While previous studies [A. D. Bianchi et al. Science 319, 177 (2008)] reported the phase boundary between the high-field square $\rightarrow$ rhombic $\rightarrow$ hexagonal VLs, the lower boundary between hexagonal $\rightarrow$ rhombic $\rightarrow$ square remained unexplored at higher temperatures where only estimates were provided. We have investigated this regime and mapped out these VL transitions. Interestingly, at the base temperature, no rhombic phase is observed but a direct transition from hexagonal to square phase. A possible explanation for this deviation from earlier reports may be that the current measurements were done following a field-ramp at the temperature rather than field-cool used in previous measurements. This indicates a slight hysteresis associated with this transition. While the measured hexagonal to rhombic phase transition agrees with the earlier estimates, the square VL phase occupies a larger region at higher temperatures than previously estimated.

1Supported by NSF award no. DMR-0804887 (Notre Dame). Work at LANL under the auspicious of the US DOE.

10:12AM Y36.00012 Vortices in superconducting MoGe pentagon, TAKEKAZU ISHIDA, HO THANH HUY, MASARU KATO, Osaka Prefecture University, MASAHIKO HAYASHII, Akita University — Vortices in bulk prefer to form a triangular lattice while a mesoscopic superconductor with a size comparable to coherence length $\xi$ or the magnetic penetration depth $\lambda$ is quite different so as to create particular configuration of vortices. The behavior of such structures in an external magnetic field is strongly influenced by the boundary conditions. Vortex states in superconducting disk, triangle and square pattern have been extensively studied both theoretically and experimentally [B. J. Baelus et al., Phys. Rev. B 69, 064506 (2004)]. We present vortex structures in MoGe pentagon disks imaged by means of a scanning quantum interference device (SQUID) microscopy [Ho Thanh Huy et al., Physica C, in press; DOI 10.1016/j.physc.2012.03.037]. Systematic measurements allow us to reveal how vortex arrangement evolves with the applied magnetic field. Moreover, we found that shell filling rule is subjected to change when a pinning center is introduced. Numerical calculations of vortex structure in pentagon disks on the basis of the nonlinear Ginzburg-Landau theory reveal that there are good agreement between experimental data and theoretical calculations.

10:24AM Y36.00013 Unconventional Vortex States in Nanoscale Superconductors Due to Shape-Induced Resonances in the Inhomogeneous Cooper-pair Condensate, LING-FENG ZHANG, LUCIAN COVACI, MILORAD MILOSEVIC, GOLIJON BERDIYOROV, FRANCOIS PEETERS, University of Antwerp — Vortex matter in mesoscopic superconductors is known to be strongly affected by the geometry of the sample. Here we show that in nanoscale superconductors with coherence length comparable to the Fermi wavelength the shape resonances of the order parameter results in an additional contribution to the quantum topological confinement leading to unconventional vortex configurations. Our Bogoliubov de Gennes calculations in a square geometry reveal a plethora of asymmetric giant multivortex, and vortex antivortex structures. Stability with respect to vortex dynamics is given by the size of the system and the Fermi energy we show that ground states with different symmetries can be obtained. By increasing the temperature we observe first-order transitions from multivortex to giant vortex states. These unconventional states are relevant for high Tc nanograins, confined Bose Einstein condensates, and graphene flakes with proximity induced superconductivity.

10:36AM Y36.00014 Competition between covalent bonding and charge transfer tendencies at complex-oxides interfaces, J. SALAFRANCA, J. TORNOS, J. GARCÍA-BARRIOCANAL, C. LÉON, J. SANTAMARIA, Universidad Complutense de Madrid, J. RINCÓN, G. ÁLVAREZ, S.J. PENNYCOOK, Oak Ridge National Laboratory, E. DAGOTTO, Oak Ridge National Laboratory and University of Tennessee, M. VARELA, Oak Ridge National Laboratory and U. Complutense de Madrid — Interfaces alter the subtle balance among different degrees of freedom responsible for exotic phenomena in complex oxides, such as cuprate-manganite interfaces. We study these interfaces by means of scanning transmission electron microscopy and theoretical calculations. Microscopy and EEL spectroscopy indicate that the interfaces are sharp, and the chemical profile is symmetric with two equivalent interfaces. Spectroscopy also allows us to establish an oxidation state profile with sub-nanometer resolution. We find an anomalous charge redistribution: a non-monotonic behavior of the occupancy of d orbitals in the manganite layers as a function of distance to the interface. This is important for graphene based spintronics devices as dielectric layers between the ferromagnetic electrode and graphene have been shown to increase the spin relaxation time measured utilizing non-local detection and spin precession measurements. However, simply depositing metal oxide layers such as aluminum oxide on graphene results in non-uniform film lowering the quality of the interface barrier. We will present a systematic study of aluminum oxide layers grown on CVD (chemical vapor deposition) graphene under ultra-high vacuum conditions with and without titanium seed layers. The aluminum oxide layers with the titanium seed layers showed reduced surface roughness. The chemical and structural composition determined by XPS (X-ray photoelectron spectroscopy) will be also presented that shows full oxidation of the aluminum and partial oxidation of the titanium. Our previous work which demonstrated that introducing HfO$_2$ barrier layer in the epitaxial graphene devices on SiC wafer improves the measured lifetime and spin injection efficiency will be briefly presented as well.
8:12AM Y40.00002 Atomically Resolved Surface of Laser-MBE Grown SrRuO$_3$ Thin Films$^1$
A. TSILEV, P. GANESH, A.P. BADDORF, S.V. KALININ, Oak Ridge National Laboratory, Oak Ridge, TN — Surface of SrRuO$_3$ (SRO) thin films is of high interest since SRO layers are used as bottom electrodes in oxide heterostructures demanding sharp interfaces. Here we studied SRO films in-situ using STM with atomic resolution. Films were grown on undoped, SrTiO$_3$ substrates by laser-MBE. Depending on preparation conditions, the film surfaces exhibited varying reconstructions. Films deposited at 650°C and annealed at deposition conditions for 15 min, revealed surfaces with double-row 1D-structures along $\langle 110 \rangle$. Aoms in the 1D-structures are packed in square or zigzag arrangements. The surface in-between the structures appeared poorly ordered. Similar patterns were observed on surfaces of films deposited at 700°C without anneal. In turn, deposition at 700°C with post-anneal resulted in well-ordered surfaces covered by double-ruled structures with square atomic arrangement. Ab initio DFT calculations show a high local DOS from oxygen adatoms with zigzag and square patterns contributing to STM images. Oxygen atoms have high adsorption energies and will be present at our growth conditions. Surface O-adatoms show AFM coupling to the film, with possible ramifications to understand interfacial bonding/magnetism between SRO and oxide-insulators.

$^1$Research was supported by MSED, BES, U.S. DOE, and conducted at ORNL's CNMS, which is sponsored by the Scientific User Facilities Division, BES, U.S. DOE.

8:24AM Y40.00003 Transport phenomena in SrVO$_3$ thin films$^1$, MAN GU, STUART WOLF, JIWEI LU, University of Virginia, UNIVERSITY OF VIRGINIA TEAM — Bulk SrVO$_3$ (SVO) with a 3d$^1$ electronic configuration has been found to exhibit metallic and Pauli paramagnetic behavior. We have obtained epitaxial SVO films grown on various substrates (STO, SLAO, LSAT and LAO) using a pulsed electron-beam deposition (PED) technique. The film transport properties were found to be strongly dependent on the substrate. A 40 nm SVO film deposited on an STO substrate exhibited metallic behavior with the electrical resistivity following a $T^2$ law that corresponds to a Fermi liquid system, the resistance ratio R(300K)/R(2K) was ~1.6. Hall measurements showed that the mobility increased slightly as the temperature was decreased. A small positive out-of-plane magnetoresistance was observed, it was only 0.045% at 5 K and 7 Tesla. SVO films with the same thickness grown on SLAO, LSAT and LAO showed semiconducting behavior, the different transport properties in the SVO films could be attributed to the compressive film strain or the different film-substrate interfaces.

8:36AM Y40.00004 High quality, hybrid-MBE growth of SrVO$_3$ thin films$^1$, JARRETT MOYER, Department of Physics, Department of Materials Science and Engineering, Pennsylvania State University, CRAG EATON, Department of Materials Science and Engineering, Pennsylvania State University, ROMAN ENGEL-HERBERT, Department of Materials Science and Engineering, Pennsylvania State University — Vanadium-based transition metal oxides are an intriguing class of materials to study due to the metal-to-insulator (MIT) transitions that arise in many of the binary oxides (i.e. VO$_2$, V$_2$O$_3$, V$_2$O$_5$). The perovskite SrVO$_3$ is metallic in bulk; however, it is possible to induce an MIT by modulating the bandwidth through strain or dimensional confinement. A mandatory requirement for controlling the electronic phase transition properties in material systems with strong correlation is the growth of high quality, stoichiometric thin films. This is demonstrated here with the growth of SrVO$_3$ on LSAT (001) substrates using a hybrid-MBE technique, where the Sr is evaporated from an effusion cell and the V is provided through the metal-organic precursor vanadium oxo-tri-isopropoxide (VTIP). The structural properties of films with varying VTIP:Sr ratios are characterized by RHEED, XRD, AFM and TEM. These measurements demonstrate that SrVO$_3$ can be grown with excellent structural quality, atomically flat surfaces and rocking curves of the same width as the substrate, accomplishing a necessary first step in controlling the MIT in SrVO$_3$.

$^1$This research is primarily supported by ONR Grant N00014-11-1-0665

8:48AM Y40.00005 Optimizing Pt/TiO$_2$ templates for textured PZT growth and MEMS devices, DANIEL DOTIREPAK, U.S. Army Research Laboratory, Adelphi, MD 20783, USA, GLENN FOX, Fox Materials Consulting LLC, Colorado Springs, CO 80908, USA, LUZ SANCHEZ$^1$, Department of Materials Science & Engineering, University of Maryland, College Park, MD 20742, USA, RONALD POL-CAWICH, U.S. Army Research Laboratory, Adelphi, MD 20783, USA — Crystallographic texture of lead zirconate titanate (PZT) thin films strongly influences piezoelectric properties used in MEMS applications. Textured growth can be achieved by relying on crystal growth habit and can also be initiated by the use of surface templates for textured PZT growth and MEMS de-

9:00AM Y40.00006 First-principles calculations of water-based surfactant-assisted growth of polar CaO(111) oxide film, XIN TAN, PETER ZAPOL, Materials Science Division, Argonne National Laboratory, USA — Despite many attempts to grow rocksalt (111) oxide surfaces, the growth of an atomically flat polar oxide film with an arbitrary thickness still remains challenging because of surface roughening during the growth process, such as faceting into neutral (100) surface planes. This seemingly unavoidable behavior leads to a grainy morphology and diminished functionality. Here, we present a first-principles investigation of the surfactant-assisted growth of polar CaO(111) film in the presence of a water-based surfactant, both from thermodynamic and kinetic points of view. We show that water molecules not only supply a surfactant by depositing hydrogen on the surface throughout the growth process, but also supply oxygen atoms as an elemental constituent in the film growth, i.e. water oxygen atoms are easily inserted into the top surface layer of the growing film. We suggest that adding water surfactants to conventional synthesis techniques leads to the continuous presence of hydrogen atoms in the surface region during the growth process, which efficiently quenches polarity and dynamically stabilizes the growth of the polar surface, and thus facilitates the growth of CaO(111) films with arbitrary thickness.

9:12AM Y40.00007 The Electronic Structure of Nonpolar Surfaces in Insulating Metal Oxides, DANYLO ZHEREBEDSKYY, LIN-WANG WANG, Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — Understanding the electronic and geometric structures of metal oxide surfaces has a key interest in many technological areas. A randomly chosen crystal surface has a high probability of being polar, unstable and containing in-gap states due to surface dangling bonds. As a result, the surface should be stabilized by passivation or reconstruction. However, do the nonpolar surfaces of ionic crystals of insulating metal oxides need the passivation or reconstruction similar to covalent crystals? We address this question by analyzing the nonpolar surfaces and their electronic structure for the common crystal structures of metal oxides. The study using first-principles DFT calculations is performed for following representatives: Cu$_2$O, ZnO, Al$_2$O$_3$, TiO$_2$, V$_2$O$_5$, WO$_3$, CaTiO$_3$, Mg$_2$SiO$_4$. It has been shown that the nonpolar surface can be constructed out of dipole-free, charge-neutral and stoichiometric unit cells for each crystal. We demonstrate that all constructed and relaxed nonpolar surfaces of the metal oxides show a clear band gap. It should be emphasized that the constructed surfaces are neither reconstructed nor passivated. Additionally, we show a correlation between the electronic structure of the relaxed surfaces and Ewald energies calculated for the surface ions.
9:24AM Y40.00008 In-situ study of Nb oxide and hydride for SRF cavity applications using aberration-corrected STEM and electron energy loss spectroscopy

RUNZHE TAO, ROBERT Klie, University of Illinois at Chicago, YOONJUN KIM, DAVID SEIDMAN, Northwestern University, LANCE COOLEY, ALEXANDER ROMANENKO, Fermi Lab, UNIVERSITY OF ILLINOIS AT CHICAGO COLLABORATION, NORTHWESTERN UNIVERSITY COLLABORATION, FERMI LAB COLLABORATION — We present an atomic-resolution study of the effects that a 48 hour bake at 120 °C in vacuum has on the high-field properties of Nb-based SRF cavities. This bake results a significant increase in the high-field quality factor Q, reversely, 800 °C bake for 2 hour reduces the H_{c2}/H_{c1} ratio of cavities. Several mechanisms have been proposed, including an increased NbO_x surface layer thickness and the precipitation of NbH_y. Using a combination of atomic-resolution Z-contrast imaging and electron energy-loss spectroscopy with in-situ heating and cooling experiments, we examine the atomic and electronic structures of Nb and related oxides/hydrdes near the cavity surface. We quantify the oxygen diffusion on surface during bake by measuring the local Nb valence using EEL spectra. Also, we demonstrate that hydrogen atoms incorporated into the Nb crystal, forming β-NbH precipitates, can be directly visualized using annular bright field imaging in our aberration-corrected JEOL ARM-200CF. Finally, the effects of the 800 °C baking process on the local hydrogen and other impurity will be examined by in-situ heating and cooling experiments. Our results will be combined with atom-probe tomography to develop a 3-D impurity and phase profile of Nb near the SRF cavity surface.

9:36AM Y40.00009 Incorporation of Non-metal Impurities at the Anatase TiO_2(001)-(1×4) Surface

JUN HEE LEE, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA, DANIEL FERNANDEZ HEVIA, Universidad de Las Palmas de Gran Canaria, Campus de Tafira, 35017 Las Palmas de Gran Canaria, Spain, ANNABELLA SELLONI, Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — Surface doping of TiO_2 is of special interest because the distribution of impurities at or near the surface can have a significant influence on the photocatalytic properties of TiO_2. We have used first-principles density functional theory (DFT) calculations to determine the incorporation mechanisms of nitrogen (N) and carbon (C), two widely used p-type dopants, at the reconstructed (001) surface of anatase, the TiO_2 polymorph most relevant for photocatalysis. Starting from adsorbed impurities, we identify various incorporation pathways and show that the non-exposed oxygen sites just below the surface play a crucial role in accommodating non-metal impurities at the TiO_2(001) surface. Based on the obtained results, we propose strategies which could help to increase the doping concentration and the photocatalytic activity at the TiO_2 surface by exploiting the morphology of the reconstructed surface [1].


9:48AM Y40.00010 TiO_2 Surface Defects with the Tetrahedral Cationic Coordination

KEN PARK, Department of Physics, Baylor University, VINCENT MEUNIER, Department of Physics, Applied Physics, & Astronomy, Rensselaer Polytechnic Institute, NAN HSIN YU, Department of Physics, Baylor University, WARD PLUMMER, Department of Physics & Astronomy, Louisiana State University — Titanium dioxide is one of the most extensively investigated transition metal oxide. It has well-known applications in catalytically converting toxic organic and inorganic materials to benign products, as well as turning solar energy into a chemical. In these processes, it is believed that surface defects with lower coordination and/or stoichiometry play crucial roles. Our study of a (2×2 ×2) R45 reconstructed TiO_2(001) using scanning tunneling microscopy and density functional theory reveals that the basic building blocks of the reconstruction can be modeled as fully stoichiometric nanocluster defects. As in the bulk-terminated (001) surface, the atoms in the nanocluster are under-coordinated, for example, 4-coordinated Ti, 1-coordinated, and 2-coordinated O atoms. However, the absence of neighboring atoms drives the nanocluster to relax into a structure, which possesses tetrahedrally coordinated Ti atoms. This result will be compared and discussed with the reported nanocluster defects on TiO_2(110).

10:00AM Y40.00011 Increase of Structural Phase Transition Temperature with Cr doping in Cr:VO_2 Thin Films

B.L. BROWN, MARK LEE, University of Texas at Dallas, P. CLEM, C.D. NORDQUIST, T.S. JORDAN, S.L. WOLFLEY, D. LEONHARDT, Sandia, J.A. CUSTER, SSA — Bulk crystal VO_2 has a well-known structural phase transition near T_c = 68 °C that separates a low-temperature insulating phase from a high-temperature metallic phase with several orders-of-magnitude resistance contrast between the two phases. We report electrical and optical studies of the effect of Cr doping on the T_c in Cr:VO_2 thin films. Resistivity, Hall effect, and infrared reflectivity all show that Cr doping systematically increases T_c from 50 °C up to ~ 75 °C at 11% Cr with similar transition width and hysteresis from DC to infrared, but the effect appears to saturate. At the same time, there is a modest decrease in resistance contrast. We will discuss the possible effects of both carrier density and scattering changes across T_c. Our results will be combined with atom-probe tomography to develop a 3-D impurity and phase profile of Nb near the TiO_2(001) surface.

4) Surface, arXiv:1209.1602

10:12AM Y40.00012 Non-Destructive Element Specific Depth Profiling by Resonant Soft X-ray Reflectometry

SEBASTIAN MACKE, ADRIANO VERNA, MAURITS HAVERKORT, Max Planck - UBC Centre for Quantum Materials, Canada, ABDULLAH RADI, Department of Chemistry, University of British Columbia, Canada, RONNY SUTARTO, Canadian Light Source, Canada, GEORG CHRISTIANI, GENNADY LOGVENOV, BERNHARD KEIMER, Max-Planck Institute for Solid State Research, Germany, GEORGE SAWATZKY, Quantum Matter Institute, University of British Columbia, Canada, VLADIMIR HINKOV, Max Planck - UBC Centre for Quantum Materials, Canada — X-ray resonant reflectometry (XRR) is the ideal tool to study the depth resolved and element-specific electronic structure of multilayer films. By changing angle, energy and polarization of the incoming beam complete reflectivity maps can be measured leading in principle to an accurate picture of the depth resolved electronic states of thin films. The standard model used in reflectometry is based on compound layers with a defined thickness, roughness and dielectric tensor. But such a simple model is usually not capable to reproduce a full measured reflectivity map. The main reasons are especially contaminations, additional oxide layers and interdiffusion between layers. However, introducing a layer system based on the element specific atomic density and scattering factors instead of dielectrics allows to remove the effects of film thickness, roughness and dielectric tensor. The new model can be used to reproduce the reflectivity maps. Thereby the advanced model is capable to retrieve the element specific density profiles of thin films. The method is introduced by analyzing a simple film of PrNio3 grown on an

10:24AM Y40.00013 Investigation of electronic and magnetic properties of wurtzite NiO thin films

BRIAN BUSEMEYER, Department of Physics, University of California, Davis, CA 95616-8677 USA, MICHAEL SHAUGHNESSY, Sandia National Laboratories at Livermore, Livermore, CA 94551 USA, LIAM DAMEWOOD, C.Y. FONG, Department of Physics, University of California, Davis, CA 95616-8677 USA — We study the electronic and magnetic properties of wurtzite (B4) NiO thin films grown epitaxially on wide gap semiconductors to understand factors affecting their half-metallic properties, in particular, the effect of film thickness, interface geometry, and dangling bonds. One, two, and four consecutive layers of NiO are considered, both buried within bulk ZnO, and as thin surface films on bulk ZnO. We perform GGA+U calculations, with the U value determined via a self consistent linear response approach. We find that the interface generates small s-p hybridized states at the Fermi energy, which can possibly destroy the half metallicity; these states are likely due to effects from strain at the interface. We also find that the interface can influence the Ni d states markedly different ways, depending on the presence of dangling bonds. These factors can determine whether the interface Ni d states resemble those from Ni in bulk wurtzite NiO, or demonstrate semiconductivity, more akin to d states of Zn atoms within bulk ZnO.

3Work at UC Davis was supported in part by the National Science Foundation Grant No. ECCS-1232275.
10:36 AM Y40.00014 Structure of Oxide Surfaces, RONG YU, Tsinghua University — Surfaces of metal oxides are of crucial importance for a variety of technological applications such as heterogeneous catalysis, thin film growth, gas sensing, and corrosion prevention. Due to the complexities of oxides in crystal structure and electronic structure, however, the surface science of oxides lags far behind that of metals or semiconductors. Conventional surface-science techniques are usually limited to surfaces of single crystals of conductors. Metal oxides are usually good insulators, making them difficult for conventional surface science techniques. On the other hand, the complex atomic structures of oxides results in too many structural parameters to be determined by spectroscopy or diffraction methods. We will show that the surface structure of oxides can be directly imaged and measured at the sub-angstrom scale using aberration-corrected transmission electron microscopy. The atomic positions of oxide surfaces can be measured to an accuracy of picometers, comparable to that obtained by conventional surface science techniques on single crystals.


11:15 AM Z1.00001 Ultrafast Optical Excitation of a Persistent Surface-State Population in the Topological Insulator Bi₂Se₃, JONATHAN SOBOTA, Stanford University — Bi₂Se₃ is a material which has gained great attention since it was recognized to be a topological insulator. Due to their topologically-protected spin-textured Dirac surface states, topological insulators have been recognized for their potential in device applications, particularly for spintronics. Thus, much of the experimental focus has been on ways to electronically or optically couple to the surface spin-texture. Using time- and angle- resolved photoemission spectroscopy (TR-ARPES), we optically excite p-type Bi₂Se₃ and study the dynamical response of its electronic structure on a femtosecond timescale. The strength of this technique is that its energy- and angle- resolution allows us to study these dynamics directly within the electronic band structure, so that surface and bulk contributions can be separately resolved. We find that optical excitation produces a metastable population of bulk carriers due to the presence of the bandgap. We discuss the coupling of these carriers to the Dirac surface state, which results in a long-lived nonequilibrium surface carrier distribution. This spin-textured population may present a channel in which to drive transient spin-polarized currents.

11:51 AM Z1.00002 Ultrafast momentum-dependent quasiparticle dynamics in high-\(T_c\) superconductors, UWE BOVENSIEPEN, University Duisburg-Essen — Femtosecond time- and angle-resolved photoelectron spectroscopy trARPES facilitates insight into electronic relaxation and electronic structure of non-equilibrium states of matter [1]. Hot electrons and holes relax in metals on ultrafast time scales due to the screened Coulomb interaction [2]. In superconductors the relaxation rates of quasiparticles at energies close to the superconducting gap edge are reduced because of the loss of quasiparticle states near \(E_F\). Since in the superconducting state the relaxation of optically excited carriers proceeds partly by Cooper pair reformation, the study of the quasiparticle dynamics becomes the potential to analyze the interaction responsible for Cooper pair formation. Results of trARPES will be discussed for optimally doped Bi₂Sr₂CaCu₂O_{8+\delta} in the superconducting state [2] and on EuFe₂As₂ in the antiferromagnetic state [3]. In the cuprate system we find a predominant excitation of quasiparticles at momenta near the antinode. We show furthermore, that at excitation densities of several 10^{10} \text{cm}^{-2} quasiparticle relaxation is dominated by Cooper pair reformation, which again proceeds near the antinode. In the Fe-pnictide material we monitor a difference in the relaxation rate for electrons and holes near the Fermi momentum, which disappears above the Neel temperature. We conclude that this anisotropic relaxation of electrons and holes is a consequence of the optical modification of the antiferromagnetic order. Analysis of energy transfer from electrons to phonons allows to determine the momentum averaged electron-phonon coupling constant \(\lambda\). We find values below 0.25 for Bi₂Sr₂CaCu₂O_{8+\delta} [5] and below 0.15 for EuFe₂As₂ [4].


12:27 PM Z1.00003 Measurement of intrinsic Dirac fermion cooling of a topological insulator with time- and angle- resolved photoemission spectroscopy, YIHUA WANG, MIT — Three-dimensional topological insulator (TI) is a new phase of matter with exotic surface electronic properties. Even though the bulk states have a bandgap, the surface electrons possess a linear energy-momentum dispersion that is protected by the nontrivial topology of TI to cross the Fermi level. These properties provide a promising platform for new physics and applications in future electronics and computers including high-speed quantum information processing, whose performance depends critically on the dynamics of hot carriers. Unlike the case in graphene, helical Dirac fermions in a TI interact not only with phonons but also with an underlying bulk reservoir of electrons. In this talk, we will present our recent results of time- and angle-resolved photoemission spectroscopy (TR-ARPES) study of a prototypical TI Bi₂Se₃. We show that TR-ARPES is a powerful tool to distinguish the coupled dynamics between these different degrees of freedom. With the combined sub-picosecond time resolution and energy-momentum resolution, we have directly visualized the coupling between surface and bulk electrons through phonons. At low temperature, such coupling is suppressed and the unique cooling of surface Dirac fermions by acoustic phonons is revealed through the power law cooling rate dependence on doping level. The effect on the TR-ARPES spectra from varying excitation photon energy will also be discussed.
1:03PM Z1.00004 Time-resolved ARPES and f-electron coherence1, TOMASZ DURAKIEWICZ, Los Alamos National Laboratory, MPA-CMMS Group, Los Alamos, NM 87544, USA — The coherence temperature, $T^*$, sets an important energy scale in correlated f-electrons. In this scale the hybridization gap opens at or in the vicinity of the Fermi level and the gap magnitude scales with effective quasiparticle mass. The new quasiparticle bands are heavy, as demonstrated by their small dispersion, and the quasiparticle lifetime is long, as seen by the narrow width of the peaks. Unless magnetic ordering suppresses the gap or mass enhancement is observed due to, e.g., magnetic excitations, the gap scales with effective mass in a universal manner across the heavy fermion systems. Possible deviations from this pattern, e.g., a small finite gap persisting at high temperatures above $T^*$ require models beyond a mean-field approach, and may be understood within e.g. the model of periodic array of Anderson impurities with correlations described by coupling to specific boson modes.

Self-energy approach is commonly used in ARPES of correlated systems. The coherent part of the self-energy corresponding to the gap formation is reduced at high temperatures, and the incoherent part corresponds to quasiparticle scattering. The coherent term in the self-energy expresses the mixing of f and d bands and is directly responsible for repulsion, producing the hybridization gap. This theoretical framework provides a direction towards understanding quasiparticle dynamics in correlated electron systems through ultrafast self-energy measurements and modeling. Here we show examples of time-resolved ARPES measurements of f-electron systems, providing valuable information about the evolution of coherence and the dynamics of the related quasiparticle states.

References

1Supported by the U.S. DOE through the LANL LDLD Program and the Office of Basic Energy Sciences, Division of Materials Sciences and Engineering.

1:39PM Z1.00005 Ultrafast quasiparticle dynamics and pair recombination in cuprate high-temperature superconductors , CHRIS JOZWIAK, Lawrence Berkeley National Lab — Understanding how superconductivity emerges from other competing phases and how this balance evolves through the phase diagram is one of the biggest challenges in the field of high-$T_c$ superconductors. By using high resolution time- and angle-resolved photoemission spectroscopy (tr-ARPES) we are able to directly probe the effects of optical excitation on the electronic structure of cuprate superconductors, and study the resulting quasiparticle, superconducting gap, and Cooper pair formation dynamics near their natural time scales. In particular, we observed a pump-induced meltdown of quasiparticles, which occurs only within the energy scale defined by a particular boson mode. This meltdown was observed only below $T_c$, suggesting a link between superconductivity and quasiparticles in momentum space where the superconducting gap is zero. We observed that the excited quasiparticle decay dynamics were strongly pump-fluence dependent and consistent with the picture that the observed dynamics reflect actual Cooper pair formation. Further, these quasiparticle recombination dynamics were strongly momentum dependent, increasing away from the superconducting nodes. Direct measurements of momentum dependent superconducting gap dynamics and the evolution of other non-equilibrium spectral phenomena through the phase diagram further illustrate the power of this unique time- and momentum-resolved spectroscopy. These results reveal new windows into the nature of the pairing interaction in high-$T_c$ superconductors.

Friday, March 22, 2013 11:15AM - 2:15PM –
Session Z2 DCMP GSNP: Invited Session: Jamming and Rheology of Disordered Systems
Ballroom II - Bulbul Chakraborty, Brandeis University

11:15AM Z2.00001 Impact-activated solidification of dense suspensions , SCOTT WAITUKAITIS, The James Franck Institute at The University of Chicago — Shear-thickening, non-Newtonian fluids have typically been investigated under steady-state conditions. This approach has produced two pictures for suspension response to imposed forcing. In the weak shear-thickening picture, the response is typically attributed to the hydrodynamic force generating rise of hydroclusters, small groups of particles interacting through lubrication forces. At the other end of the spectrum, in the discontinuous shear-thickening regime, the response can be seen as a system-wide jamming that is ultimately limited in strength by the system boundaries. While these steady-state pictures have proven extremely useful, some of the most interesting phenomena associated with dense suspensions is transient and local in character. A prototypical example is the extraordinarily large impact resistance of dense suspensions such as cornstarch and water. When pointed lightly these materials respond like a fluid, but when punched or kicked they seem to temporarily “solidify” and provide enormous resistance to the motion of the impacting object. Using an array of experimental techniques, including high-speed video, embedded force and acceleration sensing, and x-ray imaging, we are able to investigate the dynamic details this process as it unfolds. We find that an impacting object drives the rapid growth of a jammed, solid-like region directly below the impact site. Being coupled to the surrounding fluid by grain-mediated lubrication forces, this creates substantial peripheral flow and ultimately leads to the sudden extraction of the impactor’s momentum. With a simple jamming picture to describe the solidification and an added mass model to explain the force on the rod, we are able to predict the forces on the impactor quantitatively. These findings highlight the importance of the non-equilibrium character of dense suspensions near jamming and might serve as a bridge between the weak and discontinuous shear-thickening pictures.

11:51AM Z2.00002 Dilatancy and shear thickening of particle suspensions , DANIEL BONN, Institute of Physics, University of Amsterdam — Shear thickening is a fascinating subject, as 99.9% of complex fluids are thinning; thickening systems thus are the “exception to the rule” that needs to be understood. Moreover, such tunable systems show very promising applications, e.g. to block large underground pores in oil recovery to maintain a constant oil flow by plugging water filled pores (an approach used in oil recovery by e.g. Shell), or to manufacture bulletproof vests that are comfortable to wear, but stop bullets nonetheless. We study the rheology of non-Brownian particle suspensions (notably, cornstarch) that exhibit shear thickening. By using magnetic resonance imaging (MRI), the local properties of the flow are obtained by the determination of local velocity profiles and concentrations in a Couette cell. We also perform macroscopic rheology experiments in different geometries. The results suggest that the shear thickening is a consequence of dilatancy: the system under flow attempts to dilate but instead undergoes a jamming transition, because it is confined. This proposition is confirmed by an independent measurement of the dilation of the suspension as a function of the shear rate.

12:27PM Z2.00003 Simulations of shear-induced jamming in athermal particulate systems1, COREY O’HERN, Yale University — We perform simulations of athermal particulate systems that are prepared in unjammed states with zero static shear modulus and then subjected to successive pure or simple quasistatic shear strains at either fixed packing fraction or fixed pressure. In response to applied shear, these systems jam forming anisotropic networks of interparticle contacts. We determine the onset of shear-induced jamming as a function of the amplitude of the shear strain, packing fraction, pressure, and system size. We find that the parameter space for shear-induced jamming expands for particles with frictional interactions and nonspherical shapes.

1NSF DMR-1006537
1:39PM Z2.00005 Rigidity of Dry Granular Solids. DAPENG BI, Syracuse University — Solids are distinguished from fluids by their ability to resist shear. In traditional solids, the resistance to shear comes as an energy cost of straining, which works to distort density modulations that exists in both crystalline or amorphous structures. In our recent work, we focus on the emergence of shear-rigidity in a special class of solids: dry (non-cohesive) granular materials which have no energetically preferred density modulations. In contrast to traditional solids, the emergence of mechanical rigidity in these marginal granular solids is a collective process, which is controlled solely by boundary forces, the constraints of force and torque balance, and the positivity of the contact forces. We develop a theoretical framework based on these constraints, and show that these solids can be characterized by topological invariants and that, in two dimensions, they have internal patterns that are most naturally represented in the space of gauge field of the stress. Broken translational invariance in this gauge space is a necessary condition for rigidity in granular solids. We apply our theory to experimentally shear-jammed states as well as numerically generated jammed force networks to show that the statistics of stress fluctuations, and the ability of jammed configurations to resist deformations can be understood within this theoretical framework.

Friday, March 22, 2013 11:15AM - 2:15PM —
Session Z5 DCMP: Focus Session: Graphene: Transport and Optical Phenomena: Hot Electrons and Photocurrents 301 - Alex Holleitner, Technische Universitaet Muenchen

11:15AM Z5.00001 Hot carriers, phonons and electron-phonon decoupling in graphite1. TUNG-WU HSIEH, CHIH-WEI LAI, Michigan State University — Visible and near-IR radiation and hot phonons are observed in HOPG graphite following the excitation of picosecond laser pulses at 1.58 eV of fluences exceeding 1000 J/m$^2$. The optically generated electron-hole carriers lead to non-thermal radiation ranging from 1.2 to 2.8 eV, including black-body-like emissions above the excitation and a broad spectral peak near 1.4 eV. We determine an effective electronic temperature $T_e$ of $10^5$ K. The electronic and lattice degrees of freedom are strongly correlated via electron-phonon coupling. At a fluence below 10$^5$ J/m$^2$, followed by a slower decay of $\sim 10^4$ K over several picoseconds. The dynamics depend sensitively on the doping level. We will present our analysis of the results in terms of the transient density matrix formalism.

11:27AM Z5.00002 Doping dependence of the ultrafast relaxation dynamics of hot electrons in graphene. LIANG ZHAO, JIE SHAN, Case Western Reserve University, KIN FAI MAK, TONY HEINZ, Columbia University — The ultrafast relaxation dynamics of highly excited electrons in graphene has attracted much attention due to both its fundamental interest and its practical importance in relation to optoelectronic devices. Several mechanisms including electron-optical phonon scattering and disorder assisted electron-phonon scattering have been proposed to be responsible for electron cooling on the picosecond time scale. In this work, we apply the technique of two-color femtosecond pump-probe spectroscopy to investigate the electron relaxation dynamics as a function of doping. The photo-induced absorption in graphene is seen to vary rapidly in the first a few 100’s fs, followed by a slower decay of $\sim$ ps. The dynamics depend sensitively on the doping level. We will present our analysis of the results in terms of the transient electron chemical potential and temperature and discuss the role of different doping mechanisms, in particular, in the regime where the Fermi energy approaches half of the probe photon energy.

11:39AM Z5.00003 Hot Carrier Transport at the Graphene-Metal Interface Induced by Strong Lateral Photo-Dember Effect1. CHANG-HUA LIU, YOU-CHIA CHANG, NANDITHA DISSANAYAKE, YAOZHONG ZHANG, ZHAOHUI ZHONG, University of Michigan — Ultrastart photo-excitation in a semiconductor can lead to transient spatial charge gradient if electrons and holes have different drift velocities. The charge gradient builds up the transient electric field and causes the subsequent terahertz emission. This phenomenon, known as the photo-Dember effect, was typically considered insignificant in graphene due to its similar electron and hole mobilities. Here, we observe hot carrier transport at the graphene-metal interface driven by the photo-Dember electric field under femtosecond pulse laser excitation. The polarity of hot carrier transport is determined by the asymmetry of electron and hole mobilities of the graphene device and cannot be flipped sign by tuning graphene doping level. This indicates the formation of strong photo-Dember field, dominating over the graphene/metal built-in electric field or thermal electric field. We further analyze the spatial distribution and temporal evolution of the transient electric field near the contact edge by using the drift-diffusion model. The modeling results suggest that strong photo-Dember effect is caused by the low electronic specific heat of graphene and a huge charge gradient near the graphene-metal interface under pulse laser excitation.

11:51AM Z5.00004 Giant Nonlocal Photocurrent at the Charge Neutrality Point in Graphene1. QIONG MA, NATHAN GABOR, NITIYAN NAIR. Department of Physics, MIT, WENJING FANG, JING KONG, Department of Electrical Engineering and Computer Science, MIT, PABLO JARILLO-HERRERO, Department of Physics, MIT — Graphene based photodetectors have attracted considerable attention due to monolayer graphene's broadband optical absorption and gate tunable capacities. As the quality of graphene increases, emergent phenomena are being observed in both transport and optical measurements. Here we report measurements of giant nonlocal photocurrent that emerges at the charge neutrality point in graphene transistor devices. Scanning photocurrent imaging of uniformly undoped monolayer graphene transistors reveals highly ordered spatial patterns with alternating photocurrent signs as a function of laser position. The charge density dependence of the photocurrent, combined with in-situ improvement of device mobility, reveals a strong correlation between the nonlocal photocurrent and the derivative of the thermopower as a function of charge density. Photocurrent enhancement is pronounced in high-mobility devices and at intermediate temperatures. Such behaviors are suggestive of phonon drag effects that emerge at the charge neutrality point under photoexcitation.

1Supported by NSF DMR-0955944.

2This work was supported by the Donors of the American Chemical Society Petroleum Research Fund and the U-M/SJTU Collaborative Research Program in Renewable Energy Science and Technology.

3Air Force Office of Scientific Research, a NSF Early Career Award (P.J.H.), and the Packard Foundation
previously presented charge current injection [J. Rioux et al., PRB 83, 195406 (2011)], the effect presented here relies on a single monochromatic beam. The resulting implications for the spin current injection are presented. Unlike the effect on the polarization dependence of the spin current injection. In combination with interlayer coupling, which induces trigonal warping of the electronic bands, the bias voltage allows to control the warping at the Fermi surface. The geometry and the thermal coupling of the devices to the environment [2]. We acknowledge the very fruitful cooperation with L. Prechtel, S. Manus, D. Schuh, W. Wegscheider, L. Song, and P. Ajayan.

We verify that both built-in electric fields, similar to those in semiconductor-metal interfaces, and a photo-thermoelectric effect give rise to the photocurrent measurements in a dual-gated bilayer graphene FET under continuous-wave and pulsed laser excitation. We find that photocurrent generation in native bilayer graphene is dominated by hot carriers, as is the case in monolayer graphene, but it behaves very differently from monolayer graphene once a bandgap has been opened.

work supported by the NSF Early Career Grant and DARPA N66001-11-1-4124.

12:27PM Z5.00007 Focused Laser Induced Spatially Controllable p-n junction in Graphene Field-Effect Transistor, YOUNG DUCK KIM, Department of Physics and Astronomy, Seoul National University, MYUNG-HO BAE, Korea Research Institute of Standards and of Materials Science, JUNG-TAK SHU, Department of Physics, Sungkyunkwan University, YOUNG SEUNG KIM, Department of Physics, Graphene Research Institute, Jeongseon, JOUNG REAL AHN, Department of Physics, Sungkyunkwan University, SEUNG-HYUN CHUN, Department of Physics, Graphene Research Institute, Jeongseon, W. FANG, J. KONG, P. JARILLO-HERRERO, N. GEDIK, MIT — Energy relaxation and cooling of photoexcited charge carriers in graphene has recently attracted significant attention due to possible hot carrier effects, large quantum efficiencies, and photovoltaic applications. However, the details of these processes remain poorly understood, with many conflicting interpretations reported. Here we use time-resolved terahertz spectroscopy to explore multiple relaxation and cooling regimes in graphene in order to elucidate the fundamental physical processes which occur upon photoexcitation of charge carriers. We observe a novel negative terahertz photoconductivity that results from the unique linear dispersion and allows us to measure the electron temperature with ultrafast time resolution. Additionally, we present measurements of the relaxation dynamics over a wide range of excitation fluences. By varying the pump photon energy, we demonstrate that cooling dynamics of photoexcited carriers depend on the amount of energy deposited in the graphene system by the pump pulse, not the number of absorbed photons. The data suggest that fundamentally different regimes are encountered for different excitation fluences. These results may provide a unifying framework for reconciling various measurements of energy relaxation and cooling in graphene.

1Korea Research Institute of Standards and Science

12:39PM Z5.00008 Multiple regimes of carrier cooling in photoexcited graphene probed by time-resolved terahertz spectroscopy, A.J. FRENZEL, MIT / Harvard University, N.M. GABOR, MIT, P.K. HERRING, MIT / Harvard University, W. FANG, J. KONG, P. JARILLO-HERRERO, N. GEDIK, MIT — Energy relaxation and cooling of photoexcited charge carriers in graphene has recently attracted significant attention due to possible hot carrier effects, large quantum efficiencies, and photovoltaic applications. However, the details of these processes remain poorly understood, with many conflicting interpretations reported. Here we use time-resolved terahertz spectroscopy to explore multiple relaxation and cooling regimes in graphene in order to elucidate the fundamental physical processes which occur upon photoexcitation of charge carriers. We observe a novel negative terahertz photoconductivity that results from the unique linear dispersion and allows us to measure the electron temperature with ultrafast time resolution. Additionally, we present measurements of the relaxation dynamics over a wide range of excitation fluences. By varying the pump photon energy, we demonstrate that cooling dynamics of photoexcited carriers depend on the amount of energy deposited in the graphene system by the pump pulse, not the number of absorbed photons. The data suggest that fundamentally different regimes are encountered for different excitation fluences. These results may provide a unifying framework for reconciling various measurements of energy relaxation and cooling in graphene.

12:51PM Z5.00009 Terahertz generation and picosecond photo-thermoelectric currents in graphene, ALEXANDER HOLLEITNER, Technical University Munich, Walter Schottky Institut and Physics Department — We demonstrate that THz radiation is generated in optically pumped bilayer graphene. The electro-magnetic radiation is detected via a time-domain THz spectroscopy utilizing coplanar metal stripine circuits in combination with an on-chip pump/probe scheme [1]. The striplines act as highly sensitive near-field antennae with a bandwidth of up to 1 THz. Our ultrafast experiments further clarify the optoelectronic mechanisms contributing to the photocurrent generation at graphene-metal interfaces. We verify that both built-in electric fields, similar to those in semiconductor-metal interfaces, and a photo-thermoelectric effect give rise to the photocurrent at graphene-metal interfaces at different time scales. We particularly discuss how the picosecond photocurrents in monolayer graphene depend on the geometry and the thermal coupling of the devices to the environment [2]. We acknowledge the very fruitful cooperation with L. Prechtel, S. Manus, D. Schuh, W. Wegscheider, L. Song, and P. Ajayan.

We acknowledge the very fruitful cooperation with L. Prechtel, S. Manus, D. Schuh, W. Wegscheider, L. Song, and P. Ajayan.

2A. Brenneis et al. (2013).
3Financial support by the ERC grant NanoREAL is acknowledged.

1:03PM Z5.00010 Optical pure spin current injection in graphene, JULIEN RIOUX, GUIDO BURKARD, Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — Pure spin current injection by optical methods is investigated in single-layer and bilayer graphene within the tight-binding model, including bias and interlayer coupling effects. Interlayer coupling in bilayer graphene has a distinct qualitative effect on the polarization dependence of the spin current injection. In combination with interlayer coupling, which induces trigonal warping of the electronic bands, the bias voltage allows to control the warping at the Fermi surface. The resulting implications for the spin current injection are presented. Unlike the previously presented charge current injection [J. Rioux et al., PRB 83, 195406 (2011)], the effect presented here relies on a single monochromatic beam.
1:15PM Z5.00011 Probing the Optoelectronic Response of a Monolayer MoS₂ Field-Effect Transistor. KATHRYN L. MCGILL, Laboratory of Atomic and Solid State Physics, Cornell University; KIN FAI MAK, Kavli Institute at Cornell for Nanoscale Science, JOSHUA W. KEVER, Laboratory of Atomic and Solid State Physics, Cornell University, JIWOONG PARK, Department of Chemistry and Chemical Biology, Cornell University; Kavli Institute at Cornell for Nanoscale Science, PAUL L. MCEUEN, Laboratory of Atomic and Solid State Physics, Cornell University; Kavli Institute at Cornell for Nanoscale Science — Two-dimensional materials contain a wealth of interesting optoelectronic properties. Single-layer molybdenum disulfide (MoS₂), with its broken inversion symmetry, is of particular interest. This broken symmetry results in the formation of direct band gaps at the K and K' valleys in its band structure, allowing long-lived optical excitations. Furthermore, monolayer MoS₂ has valley-dependent electronic properties allowing confinement of charge carriers to a single valley by optical pumping [1]. We have fabricated two- and four-terminal devices based on single layers of MoS₂. We observe an efficient photocurrent response at the two-dimensional semiconductor-metal interface displaying Shottky diode behavior, in which an interfacial field splits excitons at the contacts to produce current. We also find that the photocurrent drastically increases under reverse biasing of the diode. Additionally we are exploring the dependence of this photocurrent response on the polarization state of incident light.


1:27PM Z5.00012 Photoresponse of Quasi-One Dimensional Graphene Nanostructures. TU HONG, ZEYNAB JARRAH, YUNHAO CAO, ALEX HÜFFSTUTTER, YAQIONG XU, Vanderbilt University — Here, we perform simultaneous photocurrent and photoluminescence measurements of free-standing graphene nanostructures. Their photocurrent intensities show a linear relationship with the incident laser power, whereas their photoluminescence intensities increase non-linearly when the incident power rises. The photoluminescence may result from the thermal radiation generated during hot carrier relaxation. The power dependences of their photoluminescence reveal that these graphene nanostructures are quasi-one dimensional materials.

1:39PM Z5.00013 Hybrid graphene-organic molecule transistors with large photoresponse. SHAO-YU CHEN, Institute of Atomic and Molecular Sciences, Academia Sinica, YI-YING LU, Department of Chemistry, National Taiwan University, FU-YU SHIH, Institute of Atomic and Molecular Sciences, Academia Sinica, PO-HSUN HO, CHUN-WEI CHEN, Department of Materials Science and Engineering, National Taiwan University, YANG-FANG CHEN, Department of Physics, National Taiwan University, YIT-TSONG CHEN, Department of Chemistry, National Taiwan University, WEI-HUA WANG, Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan — We present large photoresponse in hybrid graphene-organic molecule transistors, which exhibit high gain and large responsivity. High-quality graphene phototransistors are achieved via resist-free fabrication and noncovalent bonding of the organic molecules. The photocurrent of the devices is tunable with back gate which enables high controllability by electrical means. The strong photoresponse can also be attributed to charge transfer and photogating effect in the layer of organic molecules. High photo-sensitivity in the hybrid graphene-organic molecule transistors is promising for the future development of graphene-based optoelectronic applications.

1:51PM Z5.00014 Photocurrent Response of Graphene Heterostructures. JOAQUIN RODRIGUEZ-NIEVA, MILDRED S. DRESSELHAUS, MIT — One of the obstacles to the use of graphene as an alternative to silicon electronics has been the absence of a band gap. One solution to some of the limitations of this obstacle introduces is to integrate graphene into a heterostructure such as a field-effect tunneling transistor that uses an atomically thin dielectric [1]. We explore theoretically some of the interesting properties of optically excited graphene heterostructures, where novel behaviors can appear due to the tunability of the Fermi level and thus, of the charge carrier densities and intrinsic electronic cooling mechanisms. We also discuss possible applications of such types of optically activated heterostructures in different areas of science and engineering. References: [1] L. Britnell, R. V. Gorbachev, R. Jalil, et al., Science, 335, 947-950 (2012)

2:03PM Z5.00015 Near-field spectroscopy of graphene during ultrafast photoexcitation. MARTIN WAGNER, ZHE FEI, ALEXANDER MCLEOD, ALEKSANDR RODIN, University of California San Diego, WENZHONG BAO, University of California Riverside, LINGFENG ZHANG, Boston University, ZENG ZHAO, University of California Riverside, ERIC IWINSKI, MARK THIEMENS, MICHAEL FOGLER, University of California San Diego, ANTONIO CASTRO-NETO, National University of Singapore, CHUNNING LAU, University of California Riverside, FRITZ KEILMANN, Max Planck Institute of Quantum Optics, DIMITRI BASOV, University of California San Diego — Recently, impressive progress in nanomaterials of graphene using near-field spectroscopy and imaging has been reported [Z. Fei et al., Nano Lett. 11, 4701 (2011), Z. Fei et al., Nature 487, 82 (2012)]. However, these studies of the interaction of the graphene plasmon with the SiO₂ substrate surface phonon were time-independent. Here we combine imaging and material characterization on the nano scale with ultrafast sub-picosecond time resolution and present optical pump broadband mid-infrared probe spectroscopy of graphene. We discuss the optical pump induced changes of the coupled plasmon-phonon modes with respect to carrier density and time-dependence. The difference between ultrafast photoexcitation and conventional electrostatic doping via the field effect is analyzed and compared with modeling.

Friday, March 22, 2013 11:15AM - 2:03PM — Session Z6 DCMP: Nanotubes and Nanowires (non-carbon): Other Phenomena 302 - Yanjie Zhou, Purdue University

11:15AM Z6.00001 Thin-Film Nanowire Networks for Transparent Conductor Applications: Simulations of Sheet Resistance and Percolation Thresholds. KAREN I. WINEY, ROSE M. MUTISO, MICHELLE C. SHERROTT, Department of Materials Science and Engineering, University of Pennsylvania, AARON R. RATHMELL, BENJAMIN J. WILEY, Department of Chemistry, Duke University — Thin-film metal nanowire networks are being pursued as a viable alternative to the expensive and brittle indium tin oxide (ITO) for transparent conductors. For high performance thin films, we have performed numerical modeling of the electrical conductivity of three-dimensional rod-networks in bulk polymer nanocomposites. We adapted our 3D simulation approach and analytical percolation used complimentary experimental, simulation and theoretical techniques to explore the effects of filler aspect ratio (L/D), orientation, and size-dispersion on the electrical conductivity of three-dimensional rod-networks in thin-film networks and provide an analytical expression for the critical area fraction as a function of L/D.
11:27AM Z6.00002 A simple method to make an electrical connection between ZnO microwire and substrate through nanoscale metal evaporation1. HAKSEONG KIM, JINKYUNG LEE, HOYEOL YUN, SANG WOOK LEE, Division of Quantum Phases and Devices, School of Physics, Konkuk University, 143-701, Seoul, Korea, NANO ELECTRONICS & NANO MECHANICS TEAM — We developed a simple method to make an electrical connection with nanoscale electrodes on microscale wire using suspended Poly(methyl methacrylate) (PMMA) strings. Less than 90 nm height of Ti/Au made a complete electrical connection on the ZnO microwires of which diameter is around 2 μm. A cross linked PMMA string was bridged between ZnO microwire and substrate for making good electrical connection. The contact resistance of ZnO microwire fabricated by this method was much lower than that of device fabricated by standard E-beam lithography and evaporation. This fabrication method is readily extendible to prepare nano scale electrodes on various micro sized materials and serves as a pathway for studying their mesoscopic transport phenomena.

1This work is supported by WCU, BK21 and NRF.

11:39AM Z6.00003 High-performance Flexible Photodetectors based on Aligned Cadmium Sulfide Nanowire Networks. DONG-GUK CHO, Department of Physics and Astronomy, Seoul National University, KWANG HEO, HYUNG-WOO LEE, YONGJU PARK, JINHOO PARK, Seoul National University, HYUN-JIN LIM, DUHEE YOON, Sogang University, CHANGHEE LEE, MIYOUNG KIM, Seoul National University, HYEVERI CHEONG, Sogang University, JONGHYURK PARK, Electronics and Telecommunications Research Institute, JIKANG JIN, Xianju National, SEUNGJUN HONG, Seoul National University — We developed a method to mass-produce aligned cadmium sulfide (CdS) nanowire (NW) network channels for highly flexible and high-performance photodetectors. In this method, CdS NWs were aligned along the molecular patterns on flexible substrates by a directed assembly strategy. The aligned CdS NW patterns were utilized as the channel of flexible photodetectors. The photodetectors based on aligned CdS NWs showed ~10 times higher photosensitivity and ~100 times faster photoresponse than those based on randomly-oriented CdS NW networks.

11:51AM Z6.00004 Growth of aligned Mo6S6 nanowires on a Cu(111)1, MARAL AMINPOUR, DUY LE, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA, DEZHENG SUN, Pierce Hall, University of California, Riverside, CA 92521, USA; Department of Physics, Columbia University, New York, NY 10027, USA, WENHAO LU, CHEN WANG, QUAN MA, LUDWIG BARTELS, Pierce Hall, University of California, Riverside, CA 92521, USA, TALAT S. RAHMAN, University of Central Florida, Department of Physics, Orlando FL 32816-2385, USA — We report the possibility of using the Cu(111) surface for growing molybdenum sulfide nanowire (Mo6S6) based on density functional theory and scanning tunneling microscopy investigations [1]. A small lattice mismatch between the nanowires and strong substrate interactions lead to epitaxial growth of the nanowires at alignment with the substrate crystallographic axes and at a preferred inter-wire separation.

[1] Duy Le, Dezheng Sun, Wen Hao Lu, Maral Aminpour, Chen Wang, Quan Ma, Talat S. Rahman, Ludwig Bartsels

1This work was supported in part by DOE grant DE-FG02-07ER15842.

12:03PM Z6.00005 Structural Characterization and Transport Properties of GaN nanowires in non-serrated and newly discovered serrated morphologies1. ZHENG MA, Department of Physics, Northeastern University, ADAM FRIEDMAN, Materials Science and Technology Division, Code 6361, US Naval Research Laboratory, LATIKA MENON, Department of Physics, Northeastern University — We present results on the synthesis, structural characterization and transport properties of single crystal GaN nanowires in two different morphologies (non-serrated and serrated nanowires). The synthesis of these two types of nanowires is carried out in chemical vapor deposition with Au catalysts. Different from the regularly non-serrated GaN nanowires, the GaN nanowires in “serrated” morphology have been newly discovered by our group. By controlling the growth conditions, it has been demonstrated that GaN nanowires with regular periodic serrations along the surface of the nanowire can be produced under specific conditions as for large-sized Au catalysts and excess concentration of gallium oxide. Detailed structural and morphological characterization studies reveal interesting features for these two growth modes. In an attempt to understand how these structural and morphological variations impact the electrical properties, transport studies on single GaN nanowires (both serrated and non-serrated) are currently underway. The transport properties, namely current versus voltage will be obtained for such nanowires which in turn will reveal important information on the potential applications of such wires in optoelectronic devices.

1Acknowledgement to NSF ECCS Grant # 0925285.

12:15PM Z6.00006 On/off-current Ratio and Ambipolar Behavior of Narrow Bandgap III-V Nanowire FETs. YANJIE ZHAO, Department of Physics, Purdue University, DREW CANDEBAT, COLLIN DELKER, School of Electrical and Computer Engineering, Purdue University, YUNLONG ZI, Department of Physics, Purdue University, DAVID JANES, JOERG APPENZELLER, School of Electrical and Computer Engineering, Purdue University, CHEN YANG, Department of Physics, Purdue University — III-V nanowires (NW) are promising linked to some form of electromigration of Ag electrodes. Additional ex- and in-situ characterization studies to elucidate observed trends are in progress.

12:27PM Z6.00007 Resistive Switching in Metal-Nanowire/Polymer Nano-Gap Devices. ROSE M. MUTISO, Department of Materials Science and Engineering, University of Pennsylvania, JAMES K. KIKKAWA, Department of Physics and Astronomy, University of Pennsylvania, KAREN I. WINEY, Department of Materials Science and Engineering, University of Pennsylvania — We recently presented the first examples of reversible resistive switching in bulk, glassy polymer nanocomposites. At compositions near the percolation threshold, Ag nanowire-polystyrene composites exhibit reversible resistive switching upon increase voltage at room temperature. We proposed that switching in these materials is the result of the field-induced formation of Ag filaments that bridge adjacent nanowire clusters, extending the percolation network and decreasing the sample’s bulk resistivity. To further understand the switching mechanism and explore possible applications, we have designed and fabricated single-gap nano-gap devices comprised of lithographically-defined metal lines separated by polymer-filled nano-gaps. We have successfully demonstrated reversible resistive switching in our nano-gap Ag/PS devices when the gap size is 20 - 100nm, observing highly reversible switching behaviors in some samples with high on/off ratios for over 50 cycles. Preliminary ex-situ high resolution imaging of the devices shows significant gap remodeling after a switching event, implying that the switching mechanism is linked to some form of electromigration of Ag electrodes. Additional ex- and in-situ characterization studies to elucidate observed trends are in progress.
12:39PM Z6.00008 Nonlocal Response of Plasmonic Nanowire Metamaterials in the ENZ Regime. BRIAN WELLS, University of Massachusetts Lowell, ANATOLY ZAYATS, Kings College London. VIKTOR PODOLSKIY, University of Massachusetts Lowell — Nanowire metamaterials are a class of materials formed by an array of aligned plasmonic nanowires embedded in a dielectric host which exhibit strongly anisotropic behavior. For a wide range of excitation frequencies, the optical properties of these systems are dominated by two waves with different polarizations. In contrast to this behavior, in the epsilon-near-zero (ENZ) frequency range, excitation of additional wave mode has been observed. In this frequency range the contribution of spatial dispersion becomes increasingly important and a modified dispersion relationship for the anisotropic metamaterials must be used. The properties of the additional wave need to be taken into consideration during design and analysis of the properties of nanowire-based systems. Here we present analytical and computational studies of the nonlocal optical response of plasmonic nanowire metamaterials. Dispersion of photonic modes of plasmonic metamaterials have been studied as a function of wavelength, geometry, and material parameters. A new analytical description of the optical properties of nonlocal nanowire systems has been developed. It is shown that the optical response of the system results from the coupling of conventional effective-medium-dominated oscillations with plasmon-polariton-type oscillations. The presented model is in agreement with numerical solutions of Maxwell’s equations.

12:51PM Z6.00009 ABSTRACT WITHDRAWN —

1:03PM Z6.00010 First-principles study of bio-conjugated ultra-thin silicon nanowires: Interaction with a PNA-RNA double helix. XIAOLIANG ZHONG, WILLIAM SLOUGH, RAVIDRA PANDEY, CRAIG FRIEDRICH, Michigan Technological University — We present the results of a first-principles study based on density functional theory of peptide nucleic acid (PNA) - ribonucleic acid (RNA) double helix conjugated silicon nanowires (SiNWs). The effects of a hexane linker functionalization, probe PNA strand immobilization, and target RNA strand hybridization on the electronic states of the ultra-thin SiNWs in a dry condition are investigated. All of these effects appear to marginally modify the core silicon states of the nanowires, manifested by a low level of p-doping in SiNWs. The intrinsic energy gap of the SiNWs is essentially unchanged, though there exist mid-gap states contributed by the PNA/RNA molecules which tend to localize near the Fermi energy. Overall, the bio-conjugation considered does not appear to significantly affect the intrinsic electronic and transmission states of the ultra-thin SiNWs.

1:15PM Z6.00011 Wide bandwidth nanowire electromechanics on insulating substrates at room temperature. ABDHILAS SEBASTIAN, JOHN MATHEW, SHAMASHIS SENGUPTA, MAHESHWAR GOKHALE, ARNAB BHATTACHARYA, MAN-DAR DESHMUKH, Tata Institute of Fundamental Research, Mumbai, India — We present a simple fabrication scheme for nano-scale devices on insulating substrates. Doubly clamped InAs nanowire resonators with local gate configuration are fabricated on sapphire substrates. Parasitic capacitance is reduced on insulating substrates thus enabling measurements at all temperatures and particularly above room temperature, an essential requirement for NEMS sensors. Mechanical motion of the nanowire is capacitatively actuated and detected using a network analyzer. This technique provides wide bandwidth radio frequency transduction and allows the nanowire oscillations to be probed at a much faster rate compared to mixing techniques. Both in-plane and out-of-plane vibrational modes of the nanowire are observed and the non-linear response of the resonators is studied. Quality factor of the resonator increases at low temperatures. We also study the relation between mechanical motion and thermal strains in the nanowire. This opens up a new approach in studying thermal properties of nanostructures. Our method of fabrication can be extended to NEMS devices on flexible substrates and other nanostructures.

1:27PM Z6.00012 Enhanced Performance in Flexible Binder-free SWCNT Membrane EDLC. DANHAO MA, PRAHAL SHETTY, The Pennsylvania State University, KOFI ADU, The Pennsylvania State University, Altoona College, RAMAKRISHNAN RAJAGOPALAN, The Pennsylvania State University — We present results on an aqueous symmetric double layer electrochemical capacitor (EDLC) constructed with flexible binder-free single wall carbon (SWCNTs) membrane as electrodes. The capacitors were cycled from 0 to 1V @ 10 A/g for 10,000 cycles with 99.9% coulombic efficiency and 94% energy efficiency, and 100% depth of discharge. The power performance of the aqueous symmetric SWCNTs membrane capacitor is almost 100 ~1000 times better than commercial non-aqueous EDLC capacitors.

1:39PM Z6.00013 Synthesis and HRTEM Electron Diffraction Characterization of Monocrystalline V_{2}O_{5}. LUISA TAFOYA, LUIS RENDON, PATRICIA SANTIAGO, Instituto de Física, Universidad Nacional Autónoma de México, 04510 México D. F., México, ELIZABETH CHAVIRA, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, 04510 México D. F., México, ERNESTO E. MARINERO, HGST San José Research Center, 3404 Yerba Buena Rd., San Jose, CA 95135, USA, VICENTE GARIHAY, Instituto Mexicano del Petroleo, de Física, Eje Lázaro Cárdenas Norte 152, Col. San Bartolo Atepehuacan, 07730; México D.F., México, LEOANDRO GONZALEZ, Universidad Autónoma Metropolitana, Azcapotzalco, Av. San Pablo 180, Col. Reynosa, 02200; México D.F., México — We have synthesized V_{2}O_{5} nanorods via solvothermal synthesis. By controlling the synthesis conditions, unidirectional crystalline growth is achieved. HRTEM and XRD studies reveal that the resulting nanorods are monocrystalline and are on average 80 nm in width and readily grow to a few microns in length. Utilizing electron diffraction we investigate the growth of these nanostructures along preferential crystalline planes. XRD confirms also that the crystalline phase of the nanorods is orthorhombic.

1:51PM Z6.00014 Narrow peaks in the current power spectra of nanomechanical resonators. . DONG LIU, Michigan State University, ADRIAN BACHTOLD, JOEL MOSE, Institut Catala de Nanotecnologia, ALEX LEVCHENKO, MARK I. DYKMAN, Michigan State University — We show that the power spectrum of current through a nanomechanical resonator has narrow peaks at the frequencies of mechanical modes. These peaks can be selectively downshifted to low frequencies by applying almost resonant ac source-drain or gate voltage. Our analysis refers to the Coulomb blockade regime, where the current is limited by tunneling through the contacts. Where the tunneling rate largely exceeds the vibration frequency, the analysis can be done in terms of the conductance that analytically depends on the displacement of the nanoresonator. In a more general case the current power spectrum near the narrow vibration-induced peaks is related to the vertex correction for the corresponding Green function. The spectral peak at low frequencies can result also from the vibration nonlinearity in the absence of inversion symmetry. We note that measuring the power spectra of the current noise provides an alternative to the often complicated direct measurements of the absorption spectrum of coupled electron-vibrational systems.

Friday, March 22, 2013 11:15AM - 2:15PM –
Session Z8 DCMP: Topological Insulators: Transport and interfaces 307 - Rolando Valdes Aguilar, Los Alamos National Laboratory
11:15AM Z9.00001 Time-reversal anomaly and Josephson effect in time-reversal invariant topological superconductors. SUK BUM CHUNG, University of California Los Angeles, JOSHUA HOROWITZ, XIAO-LIANG QI, Stanford University — Topological superconductors are gapped superconductors with protected Majorana surface/edge states on the boundary. In this paper, we study the Josephson coupling between time-reversal invariant topological superconductors and s-wave superconductors. The Majorana edge/surface states of time-reversal invariant topological superconductors in all physical dimensions 1, 2, 3 have a generic topological property which we named as time-reversal anomaly. Due to the time-reversal anomaly, the Josephson coupling prefers a nonzero phase difference between topological and trivial superconductors. The nontrivial Josephson coupling leads to a current-flux relation with a half period in a SQUID geometry, and also a half period Fraunhofer effect in dimension higher than one. We also show that an in-plane magnetic field restores the ordinary Josephson coupling, as a sharp signature that the proposed effect is a consequence of the unique time-reversal property of the topological edge/surface states. Our proposal provides a general approach to experimentally verify whether a superconductor is topological or not.

Supported by the Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under contract DE-AC02-76SF00515.

11:27AM Z9.00002 Symmetry Protected Josephson Superconductors in Three-Dimensional Topological Insulators. SUNGJAE CHU, BENJAMIN M. FREGOSO, HOI-YIN HUI, ALEJANDRO M. LOBOS, SANKAR DAS SARMA, The University of Maryland College Park, THE JOINT QUANTUM INSTITUTE TEAM — We theoretically consider the mysterious topic of the topological edge/surface states of time-reversal invariant topological superconductors (TI) coupled to an s-wave superconductor, and show that the Majorana edge/surface states of TI are protected by a symmetry which we term the “Josephson symmetry”. Our results suggest a new class of topological materials which could be used to realize Majorana fermions in a clean and experimentally accessible manner.

TAKEI, EDSON VERNEK, Federal University of Uberlândia, ANTONITIO C.F. SERIDÔNIO. Universidade Estadual Paulista Júlio de Mesquita Filho, JOSÉ C. E.GUES, Instituto de Física de São Carlos - USP — We study the appearance of Majorana fermions in a quantum wire connected to a normal lead. We employ a Kitaev model for the wire with induced superconductivity with a full coupling with a normal wire. In comparison with previous study of this problem, our approach has the advantage of allowing us to fine tune the Kitaev Hamiltonian model all the way from its normal to its superconducting topological phase. By developing an exact Green’s function calculation scheme, we are able to explore the full parameter space of the model via analysis of the electron and the Majorana density of states. Our results show clearly that the main effect of a particle-hole symmetric lead is the broadening of the Majorana density of states at the end of the wire, while particle-hole asymmetric leads are detrimental to the Majorana bound states. We also study the transmission through a quantum dot connected to two normal leads and to a superconducting wire. We show that by driving the wire from its normal to its topological phase, a great change in the transmission function through the dot is observed, clearly indicating the emergence of a Majorana mode in the wire. Although such a signature has already been predicted in recent works, our model leads to substantially different results.

We thank support from FAPESP, FAPEMIG and CNPq.

11:39AM Z9.00003 Majorana fermions in a quantum wire connected to normal leads. MING GONG, LI MAO, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 USA, SUMANTA TEWARI, Department of Physics and Astronomy, Clemson University, Clemson, SC, 29634 USA, CHUANWEI ZHANG, Department of Physics, The University of Texas at Dallas, Richardson, TX, 75080 USA, CHUANWEI ZHANG TEAM, SUMANTA TEWARI TEAM — Spin-orbit coupled semiconductor nanowires with Zeeman splitting in proximity contact with bulk s-wave superconductivity have recently been proposed as a platform for realizing Majorana fermions. However, in this setup the chemical potential of the nanowire is generally pinned by the Fermi surface of the superconductor. This makes the tuning of the chemical potential by external electrical gates, a crucial requirement for unambiguous detection of Majorana fermions, very challenging in experiments. Here, we show that tunable topological superconducting regime supporting Majorana fermions in a quantum wire connected to normal leads.

We study the appearance of Majorana fermions in a quantum wire connected to a normal lead. We employ a Kitaev model for the wire with induced superconductivity with a full coupling with a normal wire. In comparison with previous study of this problem, our approach has the advantage of allowing us to fine tune the Kitaev Hamiltonian model all the way from its normal to its superconducting topological phase. By developing an exact Green’s function calculation scheme, we are able to explore the full parameter space of the model via analysis of the electron and the Majorana density of states. Our results show clearly that the main effect of a particle-hole symmetric lead is the broadening of the Majorana density of states at the end of the wire, while particle-hole asymmetric leads are detrimental to the Majorana bound states. We also study the transmission through a quantum dot connected to two normal leads and to a superconducting wire. We show that by driving the wire from its normal to its topological phase, a great change in the transmission function through the dot is observed, clearly indicating the emergence of a Majorana mode in the wire. Although such a signature has already been predicted in recent works, our model leads to substantially different results.

We thank support from FAPESP, FAPEMIG and CNPq.

12:03PM Z9.00005 The soft superconducting gap in semiconductor Majorana nanowires. SO TAKEI, BENJAMIN M. FREGOSO, HOI-YIN HUI, ALEJANDRO M. LOBOS, SANKAR DAS SARMA, The University of Maryland College Park, THE CONDENSED MATTER THEORY CENTER AND THE JOINT QUANTUM INSTITUTE TEAM — We theoretically consider the mysterious topic of the soft gap in the tunneling conductance of the proximity-induced superconductivity in a semiconductor-superconductor hybrid structure, where the observation of a zero-bias conductance peak has created considerable excitement because of its possible connection with the elusive zero-energy Majorana mode. The observed experimental superconducting tunneling gap in the semiconductor nanowire looks v-shaped with considerable subgap conductance even at very low temperatures in sharp contrast to the theoretically expected hard BCS gap with exponentially suppressed subgap conductance. We systematically study, by solving the appropriate BdG equations both numerically and analytically, a number of physical mechanisms (e.g. magnetic and non-magnetic disorder, finite temperature, dissipative Cooper pair breaking, interface fluctuations), which could, in principle, lead to a soft gap, finding that only the interface fluctuation moves through the true topological regime characterized by the presence of only surface currents. We compare our results to 3D quantum transport simulations, and determine the effects of bulk/surface mixing, disorder, and magnetic field; in particular, we show that the supercurrent is largely carried by surface states, due to the inherent topology of the bands, and that it is robust against disorder. Our results thus clarify key open issues regarding the nature of supercurrents in TIs.

12:15PM Z9.00006 ABSTRACT WITHDRAWN —

12:27PM Z9.00007 Majorana edge modes of topological exciton condensate with superconductors. BABAK SERADJEH, Indiana University, Bloomington — I study the edge states of the topological exciton condensate formed by a Coulomb interaction between two parallel surfaces of a strong topological insulator. When the condensate is contacted by superconductors with a π phase shift across the two surfaces, a pair of counterpropagating Majorana modes close the gap at the boundary. I propose a nanostructured system of topological insulators and superconductors that hosts unpaired Majorana fermions when and only when the exciton condensate forms. Therefore, measuring the Majorana signal in this structure provides a way of detecting the topological exciton condensate that is uniquely related to its topological nature. The relevant experimental signatures as well as implications for related systems are discussed.

Sergey S. Pershoguba and Victor M. Yakovenko, Phys. Rev. B

observed in an experiment [2], until it drops down abruptly to zero at the critical magnetic field $B_c$. (2)


sin with magnetic field deviates from the usual Fraunhofer diffraction pattern, suggesting modifications to a sinusoidal CPR consistent with a $\sin(2\phi)$ component. We are corroborating those results with direct measurements of the CPR using a phase-sensitive SQUID interferometry technique.

1:03PM Z8.00010 Current-phase relationship of planar Josephson junctions mediated by the surface states of a topological insulator. C. KURTER, A.D.K. FINCK, C.D. ENGLISH, University of Illinois at Urbana Champaign, Y.S. HOR, Missouri University of Science and Technology, D.J. VAN HARLINGEN, University of Illinois at Urbana Champaign — It is predicted that the presence of Majorana fermions manifests itself with a $4\pi$ periodic current-phase relation (CPR) in planar Josephson junctions formed with topological weak links. To test this proposal, we have fabricated planar junctions by depositing Nb leads on exfoliated Bi$_2$Se$_3$ single crystals. The temperature and magnetic field dependence of the proximity-induced supercurrent have been examined in various doping regimes accessed via top gating. The critical current modulation conductance $\sigma$ of the two surfaces states. An overlap between the shifted Fermi circles and spinor wave functions result in unusual non-monotonic dependence of the tunneling effect between conventional superconductors such as Sn, Pb and the strong spin-orbit coupling materials Bi$_2$Te$_3$ and Bi$_2$Se$_3$. The most prominent proposal involves a 1D semiconducting quantum wire in proximity to a bulk s-wave superconductor, where in addition a Zeeman field is applied. Here we investigate the Josephson effect in TNT and TNTN junctions, consisting of topological (T) and non-topological (N) phases of semiconductor-superconductor 1D heterostructures in the presence of a Zeeman field [1]. A key feature of our setup is that, in addition to the variation of the phase of the superconducting order parameter, we allow the orientation of the magnetic field to change along the junction. We find a novel magnetic contribution to the Majorana Josephson coupling that permits the Josephson current to be tuned by changing the orientation of the magnetic field along the junction. We also predict that a spin current can be generated and additionally controlled by a finite superconducting phase difference. This new type of coupling not only constitutes a unique fingerprint of Majorana fermions but also provides an alternative pathway for manipulating and braiding topological qubits.

1:15PM Z8.00011 Signatures of Majorana Fermions in Topological Insulator Josephson Junction Devices. BENJAMIN WIEDER, FAN ZHANG, CHARLES KANE, University of Pennsylvania Department of Physics and Astronomy — We study theoretically the electrical current and low-frequency noise for a linear Josephson junction structure on a topological insulator, in which the superconductor forms a closed ring, and currents are injected from normal regions inside and outside the ring. We find that this geometry offers a unique signature for the presence of gapless 1D Majorana fermion modes that are predicted to exist in the channel when the phase difference $\phi$, controlled by the magnetic flux through the ring, is $\pi$. We show that for low temperature, the linear conductance jumps by $2e^2/h$ when $\phi$ passes through $\pi$, accompanied by non-local correlations between the currents from the leads inside and outside of the ring. We compute the dependence of these features on temperature, voltage, and linear dimensions, and discuss the implications for experiments.

1:27PM Z8.00012 Spinful Majorana fermions and magnetoelectricity in junctions of semiconductor / superconductor heterostructures$.^1$ PANAGIOTIS KOTETES, ALEXANDER SHNIRMAN, GERD SCHÖEN, Karlsruhe Institute of Technology — Recently, the interest in topological quantum computing has grown due to the appearance of promising platforms for realizing Majorana fermions. The most prominent proposal involves a 1D semiconducting quantum wire in proximity to a bulk s-wave superconductor, where in addition a Zeeman field is applied. Here we investigate the Josephson effect in TNT and TNTN junctions, consisting of topological (T) and non-topological (N) phases of semiconductor-superconductor 1D heterostructures in the presence of a Zeeman field [1]. A key feature of our setup is that, in addition to the variation of the phase of the superconducting order parameter, we allow the orientation of the magnetic field to change along the junction. We find a novel magnetic contribution to the Majorana Josephson coupling that permits the Josephson current to be tuned by changing the orientation of the magnetic field along the junction. We also predict that a spin current can be generated and additionally controlled by a finite superconducting phase difference. This new type of coupling not only constitutes a unique fingerprint of Majorana fermions but also provides an alternative pathway for manipulating and braiding topological qubits.

$^1$We acknowledge funding from the EU projects NanoCTM, SOLID and GEOMDISS.

1:39PM Z8.00013 Proximity-effect-induced superconductivity in Bi$_2$Se$_3$ and Bi$_2$Te$_3$. LI LUI, JIE SHEN, YUE DING, FANMING QU, FAN YANG, JUN CHEN, ZHONGQING JI, JIE FAN, XIUJIAN JING, CHANGLI YANG, Daniel Chee Tsui Laboratory, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — In this talk I will present our experimental investigations on the proximity effect between conventional superconductors such as Sn, Pb and the strong spin-orbit coupling materials Bi$_2$Se$_3$ or Bi$_2$Te$_3$ [1-3]. Several types of hybrid devices were fabricated, and their electron transport properties were measured down to ~10 milli-Kelvin temperatures. The results show that a superconducting phase can be easily induced in Bi$_2$Se$_3$ and Bi$_2$Te$_3$ single crystals by superconducting Pb electrodes that are deposited on the surface of the former. The induced superconducting phase can be regarded as a true superconducting phase, i.e., it has an energy gap of the order of 0.1 meV, and carries a Josephson supercurrent over a distance as far as several microns. The conductance spectrum of the interface between the induced superconducting phase and the normal phase of Bi$_2$Se$_3$ or Bi$_2$Te$_3$ exhibits a zero-bias peak. Based on the induced superconducting phase, single Josephson junction devices and superconducting quantum interference devices (SQUIDs) were constructed, and their critical current were investigated as a function of applied magnetic flux. We will discuss the implication of the results in terms of the pairing symmetry of the induced superconducting phase.


1:51PM Z8.00014 Spin-polarized tunneling current through a thin film of a topological insulator in a parallel magnetic field. VICTOR YAKOVENKO, SERGEY PERSHOGUBA, Condensed Matter Theory Center, Department of Physics, University of Maryland, College Park, Maryland 20742-4111, USA — We calculate the tunneling conductance between the surface states on the opposite sides of an ultra-thin film of a topological insulator in a parallel magnetic field $B$. The parallel magnetic field produces a relative shift of the in-plane moments of the two surfaces states. An overlap between the shifted Fermi circles and spinor wave functions result in unusual non-monotonic dependence of the tunneling conductance $\sigma$ on the magnetic field $B$. The conductance $\sigma(B)$ grows with the magnetic field $B$, which corresponds to a negative magnetoresistance observed in an experiment [2], until it drops down abruptly to zero at the critical magnetic field $B_{c1}$. Because spin orientation of the electronic surface states in topological insulators is locked to momentum, spin polarization of the tunneling current can be controlled by the magnetic field.

Polarization selective micro-Raman spectroscopy of gated 3D topological insulators\textsuperscript{1}.  
JEFF SECOR, MILAN BEGLJARBEKOV, LUKAS ZHAO, HAIMING DENG, LIA KRUSIN-ELBAUM, Physics Department, City College of New York. One of the major challenges to understanding the behavior of the quantum states in 3D topological insulators (TIs) is a significant carrier conduction in the bulk. Understanding phonons and electron-phonon interactions can shed light on the link between surfaces and the bulk and are critical in potential applications based on TIs. Raman scattering is a fast nondestructive technique used to analyze electron lattice interactions. In this work we study micro-Raman scattering of few quintuple layer thin 2nd generation excellent crystalline quality 3D TIs, such as Sb\textsubscript{2}Te\textsubscript{3}, Be\textsubscript{2}Te\textsubscript{3}, and Bi\textsubscript{2}Se\textsubscript{3} in the 15-300 K temperature range in order to probe the interaction of circularly polarized light between the lattice phonon modes and helical surface states of TIs. Circularly and linearly polarized light combined with an applied gate bias and the temperature dependence is used to examine the helicity dependence of Raman scatter to analyze the strength of electron-phonon coupling in these systems.

\textsuperscript{1}Supported in part by NSF-DMR-1122594.

Friday, March 22, 2013 11:15AM - 12:39PM –  
Session Z19 DCMP: f-Electron System Properties - Theory & Experiment 321 - Ryan Baumbach, Los Alamos National Laboratory

**11:15AM Z19.00001** Tuning thermoelectric power factor by crystal-field and spin-orbit couplings in Kondo lattice materials\textsuperscript{1}.  
SEUNGMIN HONG, POUYAN GAHEMI, University of Illinois at Urbana-Champaign, JOEL MOORE, University of California, Berkeley, and Lawrence Berkeley National Laboratory, PHILIP PHILLIPS, University of Illinois at Urbana-Champaign — We study thermoelectric transport at low temperatures in correlated electron materials, motivated by the recent observation of a high thermoelectric figure of merit (ZT) in Fe\textsubscript{2}Sb\textsubscript{2} at T \sim 10 K. Even at room temperature, correlations have the potential to lead to high ZT, as in Yb\textsubscript{2}Al\textsubscript{3}, one of the most widely used thermoelectric metals. At low temperature correlation effects are especially worthy of study because fixed band structures are unlikely to give rise to the very small energy gaps E\textsubscript{g} \sim 1 K necessary for a weakly correlated material to function efficiently at low temperature. We explore the possibility of improving the thermoelectric properties of correlated Kondo insulators through tuning of crystal field and spin-orbit coupling and present a model for design more efficient low-temperature thermoelectric materials.

\textsuperscript{1}This work is supported by NSF-DMR-1104909 (S.H. and P.W.P.) and DE-AC02-05CH11231 (P.G. and J.E.M.). P.G. also acknowledge support from NSF DMR-1064319.

**11:27AM Z19.00002** Quantum Oscillations of Nitrogen Atoms in Uranium Nitride\textsuperscript{1}.  
S.E. NAGLER, A.A. ACZEL, G.E. GRANROTH, D.L. ABERNATHY, Quantum Condensed Matter Division, Oak Ridge National Laboratory, W.J.L. BUYERS, Canadian Neutron Beam Center, National Research Council, G.J. MACDOUGALL, Department of Physics, University of Illinois, G.D. SAMOLYUK, G.M. STOCKS, Materials Science and Technology Division, Oak Ridge National Laboratory — The quantum harmonic oscillator is among the very few soluble fundamental models in quantum mechanics and the foundation for understanding phonons in crystalline solids. Inelastic neutron scattering typically reveals acoustic and optic phonon modes at low energies, and as energy increases a complex continuum of many-phonon excitations. In contrast, measurements using chopper spectrometers at the SNS have shown that for the binary crystal uranium nitride, where the nitrogen atoms are very light compared to the uranium atoms, the response above the optic phonon modes exhibits a remarkable spectrum of well-defined local levels that are equally spaced by 50 meV intervals and that extend to the tenth order 500 meV. The levels are attributed to nearly isotropic, quantum harmonic oscillator behavior of the nitrogen atoms vibrating within a largely static uranium cage. See Nature Communications 3, 1124 (2012).

\textsuperscript{1}Work at SNS supported by the US Department of Energy, Office of Basic Energy Sciences, Scientific User Facilities Division and

**11:39AM Z19.00003** First-principles study of the Kondo physics of a Pu impurity in a Th host\textsuperscript{1}.  
JIAN-XIN ZHU, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, K. HAULE, Rutgers University, Piscataway, New Jersey 08854, R.C. ALBERS, J.M. WILLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545 — From the viewpoint of condensed matter physics properties, crystal structure, and metallurgy, plutonium is the most complicated element in the Periodic Table, including a phase diagram with six allotropic phases. Its anomalous properties are related to the special position of Pu in the Periodic Table, which is at the boundary of the light actinides with localized 5f electrons and the heavy actinides with localized 5f electrons, indicative of a very strongly correlated state. To reveal the role of electronic correlations in Pu, we investigate the electronic structure of a Pu atom embedded in a Th host by combining density functional theory within the local density approximation with the continuous-time quantum Monte Carlo simulation of a Pu impurity. As a hallmark of electronic correlations, the Kondo resonance peak around the Fermi energy is obtained in the local density of states on the Pu impurity. Furthermore, we show that the resonance peak width is narrower for Pu atoms that are at the surface of Th when compared to those in the bulk, due to a weakened Pu 5f-ligand hybridization in the former geometry.

\textsuperscript{1}This work was performed at Los Alamos National Laboratory under the auspices of the U.S. Department of Energy and the LANL LDRD Program.

**11:51AM Z19.00004** Electron Spin Resonance in Antiferro-Quadrupolar Ordered CeB\textsubscript{6}\textsuperscript{1}.  
PEDRO SCHLOTTMANN, Florida State University — CeB\textsubscript{6} is a cubic heavy fermion compound with a Γ\textsubscript{8} ground-quartet with antiferro-quadrupolar (AFQ) order below 4 K. An ESR signal was observed \textsuperscript{1} in the AFQ phase. Single ions with a Γ\textsubscript{8} ground-multiplet should display four transitions, but only one resonance was observed. Several fundamental questions arise: (1) why is only one transition seen, (2) why was this transition observed if the Kondo temperature is larger than the linewidth of the resonance, and (3) can the resonance be explained with localized moments or is an itinerant picture of heavy electron spins necessary? The interplay of AFQ and ferromagnetic correlations on the phase diagram, the magnetization and the ESR linewidth are discussed \textsuperscript{2}. In contrast to other Yb and Ce heavy fermion systems displaying an ESR signal, CeB\textsubscript{6} does not have strong magnetic anisotropy with ferromagnetic correlations, rendering an observable narrow resonance \textsuperscript{3,4}. The AFQ state is necessary for an ESR signal in the present case \textsuperscript{2}.


\textsuperscript{1}Work supported by the Department of Energy under grant No. DE-FG02-98ER45707.
12:03PM Z19.00005 Heavy antiferromagnetic phases in Kondo lattices, ILYA VEKHTER, LEONID ISAEV, Louisiana State University — We propose a microscopic physical mechanism that stabilizes coexistence of the Kondo effect and antiferromagnetism in heavy-fermion systems. We consider a two-dimensional quantum Kondo-Heisenberg lattice model and show that long-range electron hopping leads to a robust antiferromagnetic Kondo state. By using a modified slave-boson mean-field approach we analyze the stability of the heavy antiferromagnetic phase across a range or parameters, and discuss transitions between different phases. We also address connection to experiments on heavy fermion compounds.

12:27PM Z19.00007 Possible Itinerant Moment Contributions to the Magnetic Excitations in Gd, Studied by Neutron Spectroscopy1, G.E. GRANROTH, A.A. ACZEL, J.A. FERNANDEZ-BACA, S.E. NAGLER, Oak Ridge National Laboratory — Many experimental features in magnetic superconductors are also present when these complex materials are in the normal state. Therefore studies of simpler itinerant magnets may help provide understanding of these phenomena. We chose to study Gd as it is has an

1Supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

Friday, March 22, 2013 11:15AM - 2:27PM
Session Z22 DCMP: He3 - He4 Quantum Fluids 324 - Benjamin Hunt, Massachusetts Institute of Technology

11:15AM Z22.00001 Chiral Phases of Superfluid $^3$He in an Anisotropic Medium1, JAMES SAULS, Northwestern University — I report theoretical results for the phases of superfluid $^3$He infused into homogeneous uniaxial aerogel. Ginzburg-Landau (GL) theory for a class of equal-spin-pairing (ESP) states in a medium with uniaxial anisotropy is developed and used to analyze recent experiments on uniaxially strained aerogels. For $^3$He in an axially “stretched” aerogel GL theory predicts a transition from normal liquid into a chiral ABM phase in which the chirality axis is aligned along the strain axis. This state is protected from random fluctuations in the anisotropy direction, has a positive NMR shift, a sharp NMR resonance line and is in quantitative agreement with NMR in the high-temperature ESP-1 phase of superfluid $^3$He in axially stretched aerogel. A second transition into a bi-axial phase is predicted to onset at a slightly lower temperature. This phase is an ESP state, breaks time-reversal symmetry, and is defined by an order parameter that spontaneously breaks axial rotation symmetry. The bi-axial phase has a continuous degeneracy associated with broken axial symmetry. Theoretical predictions for the NMR frequency shifts provide an identification of the ESP-2 phase as the bi-axial state, partially disordered by random anisotropy (Larkin-Imry-Ma effect).

1Supported by National Science Foundation Grant DMR-1106315.

11:27AM Z22.00002 Topological current at an interface between superfluid $^3$He A- and B-phases, YASUMASA TSUTSUMI, Condensed Matter Theory Laboratory, RIKEN — At a surface of the superfluid $^3$He, the surface Andreev bound state accompanied with edge current emerges due to a topological phase transition. The topological phase transition at the surface is occurred because the superfluid gap of the superfluid $^3$He among topological superfluids is closed at the interface of a topologically trivial vacuum. Since the paring symmetries are different between the superfluid $^3$He A- and B-phases, topological features are quite different and modified as needed to alter the transport characteristics of the confined $^3$He. The cells are suitable for NMR and Torsion Oscillator measurements on the superfluid phases of $^3$He.

11:39AM Z22.00003 Nanofabricated cells for confined $^3$He, NIKOLAY ZHELEV, ROBERT BENNETT, ROB ILIC, JEEVAK PARPIA, Cornell University, LEV LEVITIN, ANDREW CASEY, JOHN SAUNDERS, Royal Holloway University London — We describe methods for fabrication of Silicon-Glass and all-silicon cells with a height specified to be between 100nm and 1100nm, and with areas on the order of cm x cm. These cells need to meet different requirements, including pressure capability to 30 bar with minimal distortion, and surface roughness which can be characterized and modified as needed to alter the transport characteristics of the confined $^3$He. The cells are suitable for NMR and Torsion Oscillator measurements on the superfluid phases of $^3$He.

11:51AM Z22.00004 Study of Liquid $^3$He Films with MEMS Devices1, PAN ZHENG, MIGUEL GONZALEZ, YOONSEOK LEE, Department of Physics, University of Florida, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology — Liquid $^3$He films with thicknesses of 0.75 and 1.25 µm were established and probed by micro-electro-mechanical (MEMS) resonators each of which consists of a pair of parallel plates with a well defined separation. The mechanical resonances of the devices immersed in liquid $^3$He were studied in a wide range of temperatures from 10 to 800 mK and at sample pressures of 3, 21, and 29 bar. A crossover from Fermi liquid to classical fluid was observed on warming. In the Fermi liquid regime, the damping coefficient associated with the film exhibits an unexpected temperature dependence below 100 mK. This work demonstrates the capacity of MEMS devices as sensitive probes suitable for the study of quantum fluids in a micrometer scale.

1This work is supported by NSF through DMR-1205891 (YL).
12:03PM Z22.00005 Spin and mass currents on the surface of the topological superfluid, $^3$He-B\(^1\), HAO WU, JAMES SAULS, Northwestern University — The surface excitation spectrum of superfluid $^3$He-B is discussed for a translationally invariant interface (specular surface). We report calculations of surface spectral spin-current and mass current densities originating from the Andreev bound state and the continuum response. Two branches of gapless Fermions, bound to the surface, disperse linearly with momentum $\vec{p}$ along the surface. These states are spin polarized transverse to their direction of propagation, $j_{\vec{p}}$. The spectral functions reveal the subtle role of the spin-polarized surface states in relation to the ground-state spin current. By contrast, these states do not contribute to the ground-state mass current density. However, the surface states do give rise to a power law suppression of the superfluid mass current for $0 \ll T < T_c$, providing a direct signature of the Majorana branches of surface excitations in the fully gapped 3D topological superfluid, $^3$He-B.

\(^1\)Supported by National Science Foundation Grant DMR-1106315.

12:15PM Z22.00006 Observation of the Larkin-Imry-Ma Effect in Superfluid $^3$He-A in Aerogel\(^1\), J.J.A. LI, Northwestern University, J. POLLANEN, California Institute of Technology, A.M. ZIMMERMAN, C.A. COLLETT, W.J. GANNON, W.P. HALPERIN, Northwestern University — It was proposed by Volovik that $^4$He-A in aerogel will be a superfluid glass owing to the Larkin-Imry-Ma (LIM) effect where arbitrarily small amounts of disorder can disrupt long range directional coherence of a vector order parameter in a condensed system. Several reports of NMR experiments in $^4$He-A have been interpreted as evidence for this phenomenon. However it is not trivial to distinguish the LIM effect induced from disorder on a microscopic scale from macroscopic non-uniformity or anisotropy in the aerogel sample. Order parameter disorder from these two possible mechanisms have very different distributions of order parameter orientations directly observable in the width of the NMR spectrum. If a complete LIM effect is operative there should be no contribution to the line width, contrary to previous reports. On warming from the low temperature isotropic state, we find NMR spectrum shifts characteristic of the dipole-locked axial state, i.e. no sign of a LIM superfluid glass. However, on cooling from the normal state this same phase is fully disordered in a LIM state. We will discuss the origin of the different order parameter structures in superfluid $^4$He-A that result when prepared from the normal state, as compared with warming from the B-phase.

\(^1\)This work was supported by the National Science Foundation, DMR-1103625.

12:27PM Z22.00007 Phase transitions and critical currents in superfluid $^3$He films\(^1\), ANTON VORONTSOV, Montana State University, JAMES SAULS, Northwestern University — Using the quasiclassical theory of superfluidity we investigate thermodynamic and transport properties of superfluid $^3$He in confined geometries. Classic flow experiments, as well as more recent NMR and flow experiments on superfluidity in slab and film geometries, exhibit inconsistencies between experimental results and existing theoretical models of confinement effects. In order to explain the origin of some of these inconsistencies we describe a theoretical model for confinement effects based on scattering of quasiparticles from rough surfaces that is more general than the `specular’ and `diffusive’ scattering models. Using this more general boundary scattering model we report theoretical results for (a) the suppression of the superfluid critical temperature $T^{c}_{\text{film}}$ (b) the confinement-driven transition between A and B phases, $T_{c,\text{AB}}$, and (c) effects of the surface roughness on the critical current. The new scattering model should provide a more complete framework for analysis of the properties of confined superfluid $^3$He.

\(^1\)Supported by NSF Grants: DMR-0954342 and 1106315.

12:39PM Z22.00008 Unusual Behavior of a MEMS Resonator in Superfluid $^4$He\(^1\), MIGUEL GONZALEZ, PAN ZHENG, BYOUNG HEE MOON, ERIK GARCELL, YOONSEOK LEE, Department of Physics, University of Florida, HO BUN CHAN, Department of Physics, The Hong Kong University of Science and Technology — Mechanical resonators based on micro-electro-mechanical systems (MEMS) technology were developed for the study of superfluid $^4$He [1]. The MEMS device is composed of a movable plate ($200 \times 200 \mu m^2$) suspended above the substrate by four serpentine springs. The suspended plate moves parallel to the substrate while maintaining a uniform gap between them. A specific device with a 1.25 $\mu m$ gap was tested in the superfluid phase of $^4$He down to 100 mK. The device exhibits an extreme sensitivity to the excitation level below 400 mK, displaying a nonlinear and hysteretic behavior accompanied by switching. This phenomenon might be related to quantum turbulence generated by a rather simple oscillating plate.


\(^1\)This work is supported by NSF (YL) under DMR-0803516 and DMR-1205891.

12:51PM Z22.00009 Superfluid helium-4 in one dimensional channel\(^1\), DUK Y. KIM, SAMHITA BANAVAR, MOSES H. CHAN, Department of Physics, Pennsylvania State University, University Park, PA 16802, USA, JOHN HAYES, PIER SAZIO, Optoelectronics Research Centre, University of Southampton, Highfield, Southampton SO17 1BJ, United Kingdom — Superfluidity, as superconductivity, cannot exist in a strict one-dimensional system. However, the experiments employing porous media showed that superfluid helium can flow through the pores of nanometer size. Here we report a study of the flow of liquid helium through a single hollow glass fiber of 4 cm in length with an open id of 150 nm between 1.6 and 2.3 K. We found the superfluid transition temperature was suppressed in the hollow cylinder and that there is no flow above the transition. Critical velocity at temperature below the transition temperature was determined. Our results bear some similarity to that found by Savard et. al. [1] studying the flow of helium through a nanohole in a silicon nitride membrane.


\(^1\)Experimental study at Penn State is supported by NSF Grants No. DMR 1103159.

1:03PM Z22.00010 Effect of Helium on Vycor Glass: Anomalous Thermal Conductivity Reduction\(^1\), ZHIGANG CHENG, SAMHITA BANAVAR, MOSES H. CHAN, The Pennsylvania State University — There is a long history of studying helium adsorbed in Vycor. In this talk we present the results showing that helium can have a profound effect on the thermal conductivity property of Vycor glass. Although the thermal conductivity of liquid $^4$He is four orders of magnitude higher than that of Vycor, the filling of liquid $^4$He inside the Vycor pores brings about a three-fold reduction of the thermal conductivity as compared with empty Vycor between 0.06 and 0.5 K. By comparing these results with that of superfluid films, liquid $^4$He and solid helium in the Vycor pores, we found that heat is conducted primarily through the silica network even when the pores are filled with solid or liquid helium. The dramatic reduction is brought about by the presence of slow sound mode in liquid $^4$He that greatly facilitates the quantum tunneling of the two level systems (TLS) in the silica which enhances the scattering of the thermal phonons.

\(^1\)This research was supported by NSF Grant No. DMR1103159.
1:15PM Z22.00011 Observation of a New Casimir Effect in Saturated Superfluid $^4$He Films¹
JOHN ABRAHAM, GARY WILLIAMS, UCLA, KONSTANTIN PENANEN, Jet Propulsion Lab — We report the results of experiments on saturated superfluid $^4$He films in the vicinity of the bulk superfluid transition temperature $T_\lambda$, measuring the film thickness with a capacitance technique and the superfluid density with third sound. For moderately slow temperature sweep rates (0.5 mK/hr) we measure the critical Casimir film-thinning effect with good resolution, and find that the Kosterlitz-Thouless superfluid onset in the film occurs just at the start of the dip in film thickness. When warming through $T_\lambda$ at extremely slow rates (a few μK/hr), however, we have observed a sudden large increase in the film thickness (nearly 25 Å in a film initially 480 Å thick) within microkelvins of $T_\lambda$. We propose that this is a new type of Casimir effect arising from the viscous suppression of second sound modes in the film, leading to a large free energy difference in the superfluid state that disappears abruptly when second sound ceases to propagate in the bulk helium at $T_\lambda$.

¹Work supported in part by NASA, and in part by the NSF, Grant DMR 09-06467

1:27PM Z22.00012 Cubic interactions in superfluid $^4$He. BJORN FÅK, CEA, Grenoble, THOMAS KELLER, MPI, Stuttgart, MICHAEL ZHITOMIRSKY, CEA, Grenoble, ALEXANDER CHERNYSHEV, University of California, Irvine — High-resolution neutron resonance spin-echo measurements of superfluid $^4$He show that the roton energy does not have the same temperature dependence as the inverse lifetime, in contrast to the Landau-Khalatnikov theory. We present a diagrammatic analysis that attributes this effect to the interaction of rotons with thermally excited phonons via both four- and three-particle processes, the latter being allowed by the broken gauge symmetry of the Bose condensate.

1:39PM Z22.00013 Photon-Roton Modes in Liquid $^4$He coexist with Bose-Einstein Condensation. HENRY R. GLYDE, Department of Physics and Astronomy, University of Delaware, JACQUES BOSSY, Institut Neel, CNRS-UJF, BP 166, 38042 Grenoble Cedex 9, France, JACQUES OLLIVIER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, HELMUT SCHOBER, Institut Laue-Langevin, BP 156, 38042 Grenoble, France, Universite Joseph Fourier, UFR de Physique, F38041 Grenoble Cedex 9, France — We present neutron scattering measurements of the phonon-roton (P-R) and layer modes of liquid $^4$He confined in MCM-41 under pressure up to 38 bar. The data shows unambiguously that the P-R mode exists at low temperature only. As temperature is increased there is a gradual transfer of intensity from the P-R mode to the normal liquid response, which lies at a lower energy at higher pressure. The transfer takes place with no observable mode broadening. The loss of P-R modes is identified with the loss of Bose-Einstein condensation (BEC). The mode giving rise to the specific heat, $c_V$, of liquid $^4$He in porous media (e.g. gelsil) at higher temperature is the layer mode since the energy of the mode extracted from $c_V$ and the layer mode energy are the same.

1:51PM Z22.00014 Helium-4 crossover from a 3d superfluid to a 1d Luttinger liquid in a nanopore¹. BOHDAN KULCHYTSKYY, Mcgill University, ADRIAN DEL MAESTRO, University of Vermont, GUILLAUME GERVAIS, Mcgill University — Quantum Monte Carlo studies of helium-4 below the bulk superfluid transition temperature show that when it is confined to flow in narrow cylindrical pores with nanometer radii, it tends to form concentric shells around a possible inner core. The latter potentially represents an experimental playground for exploring the implications of Luttinger liquid theory for one dimensional quantum fluids. We have performed large scale numerical simulations investigating the crossover from a bulk three dimensional superfluid to a one dimensional Luttinger liquid as the nanopore radius is reduced at low temperature. Measurements of the superfluid density employing both stiffness and angular momentum estimators provide new insights into confinement induced fluctuation effects in strongly interacting quantum fluids.

¹Computa Canada

2:03PM Z22.00015 Metastable pin sites for a superfluid vortex. RENA ZIEVE, INGRID NEUMANN, University of California, Davis — Circulation trapped around a straight, fine wire can be detected through its effect on the wire’s vibration. Here we use such a wire in a cylindrical cell to examine pinning of a superfluid helium vortex line at a macroscopic bump. Hydrodynamic considerations imply that, as long as the fluid velocity is fixed and not too large, a vortex can pin at a unique place on the bump. However, for two separate geometries we find that the vortex has metastable locations both at the apex of the bump and near its edge. In one case, the vortex is trapped around the wire, which terminates in the center of a bump on the cylindrical endcap. We find that the vortex can follow the entire length of the wire to the bump apex, or it can leave the wire and make its way through the fluid to the edge of the bump. The former situation is more stable, but the latter can also persist for long times. The second geometry involves a free vortex that extends from the wire to a bump on the cylindrical wall of the container. Again our measurements show pinning at multiple sites on the bump. Interaction of the vortex with the surface curvature may produce the unexpected additional pin sites.

2:15PM Z22.00016 Recent Progress in Low-Temperature Research from the Davis Lab at the University of Alberta¹. JOHN P. DAVIS, XAVIER ROJAS, YIKAI YANG, ANDREJ DUH, GREG POPOWICH, University of Alberta, Department of Physics — In this talk I will briefly describe our recent progress towards new low-temperature experiments at the University of Alberta in the Davis Lab. We are currently setting up two nuclear demagnetization fridges - one new cryostat that has two independent $9$ T magnets (the second magnet being useful for a double demag stage or combined high field and low temperature experiments). The other fridge is an older unit that is extensively refurbished, with all new pumping systems. We are planning numerous experiments at the intersection of low-temperature physics and nanoscience, including quantum properties of nanomechanical resonators and quantum fluids in confined geometries. Concerning the latter, we have fabricated high quality microfluidic devices suitable for low-temperature research. We will discuss our progress towards quantum fluids measurements using these devices.

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