Multi-Valley Superconductivity in Ion-Gated MoS2 Layers

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Session T60: Poster Session III

Poster

Room: *LACC West Hall A*

T60.00001: INSULATORS AND DIELECTRICS

T60.00002: Multiferroic properties in chloromenite $Cu_9O_2(SeO_3)_4Cl_6$

DONGJIE HSIEH, Hung-Cheng Wu, D Chandrasekhar Kakarla, Chung-Kai Chang, Yu-Chun Chuang, Helmuth Berger, Hung-Duen Yang

For a sake of searching potential candidate for new multiferroic materials in CuO–SeO_2–$CuCl_2$ composite, $Cu_9O_2(SeO_3)_4Cl_6$ single crystal was synthesized using a standard vapor-phase method. Magnetic, electrical, and low-temperature synchrotron X-ray diffraction measurements were performed on $Cu_9O_2(SeO_3)_4Cl_6$. The DC magnetization measurements showed the antiferromagnetic ordering (AFM) of $Cu_9O_2(SeO_3)_4Cl_6$ near 16 K (T_N) and T_N is decreased with magnetic fields. In addition, the dielectric anomaly near 267 K (T_E) was observed, while no transition in pyroelectric current and polarization-electric field hysteresis-loop could be detected below T_E. The results support that T_E is related to antiferroelectric ordering. However, temperature dependent high-resolution synchrotron X-ray diffractions of $Cu_9O_2(SeO_3)_4Cl_6$ reveal a structural distortion near T_E. Thus, the comprehensive studies suggest that $Cu_9O_2(SeO_3)_4Cl_6$ could be a new type-I multiferroic material.

T60.00003: Plasmonic Excitations in Nanoscale Clusters

Zhihao Jiang, Malte Rösner, Stephan Haas

In this poster, we discuss the plasmonic excitations in nanoscale clusters in the presence of an applied external electromagnetic field. The nonlocal dielectric function is calculated in real space within the random phase approximation, with the electronic energy levels and wavefunctions determined from tight-binding models. The resonant frequencies of plasmons are then identified using a self-consistent field approach. Our aim is to understand the effects of quantum tunneling and Coulomb interactions on the plasmonic excitations in nanoscale clusters. By changing the separation between clusters and embedding them into tunable dielectric backgrounds, we are able to control these two effects.

T60.00004: Electrical Characterization of GaAs, Si and SrTiO3 Semiconductor Nanostructure Based Capacitors

Masoud Kaveh-Baghbadorani, W Hughes, Maeven Luedke, Nikolas Roeske, Hoe Tan, Mykhaylo Lysevych, Chennupati Jagadish

We design and fabricate different capacitors with SrTiO3 nanopowder and GaAs and Si nanowires (NW) as dielectric materials. The effect of geometry and the type of semiconductor nanostructure on the total capacitance are investigated using electrical measurements. The vertically aligned 50 nm diameter GaAs NWs were grown using the Au catalyzed vapor-liquid-solid method. The Si NWs are randomly oriented with an average diameter of 70 nm. The SrTiO3 nano-particles are cubical with a width of around 30 nm. The capacitor Au plates are 300 nm thick and are fabricated using an electron beam deposition system on both solid glass and flexible poly(methyl methacrylate) (PMMA) substrate. The semiconductor based capacitors are composed of parallel arrays of GaAs NWs, as well as a random distribution of Si NWs and micrometer chunks of SrTiO3, lying on an Au coated substrate. Capacitance measurements on the Au plates with air as the dielectric spacer, reveal capacitance in the pF order. Capacitor structures with semiconductor dielectrics however show an enhancement of the total capacitance, mainly explained by the semiconductor spacer weakening the effective internal electric field and thus accumulating more charges on the capacitor plates.

T60.00005: Microwave absorption properties of graphene composite with magnetite multi-granular nanoclusters in X-band

Boo Hyun An, Bum Chul Park, Ji Sung Lee, Lijun Pan, Hamad Al Yassi, Mariam Mansouri, Hamda Al Shibli, Tawaddod Alkindi, Jung-Rae Park, Young Keun Kim, Daniel Choi

Ferrite materials are generally used for microwave absorbing materials due to their permeability and dielectric property. Carbon-based materials, e.g., single or multiwall carbon nanotubes, graphene, carbon fiber, and carbon black can also be used as alternative conducting materials for the EMI shielding applications. We prepared nanocomposites composed of magnetite multi-granular nanocluster (MGNC), conductive graphene sheet and carbon nanotube sheet. The graphene sheets were efficiently decorated with MGNCs by spray coating to prepare novel nanocomposites which can exhibit the microwave-absorbing performance. Effects of the various size and volume percentages of MGNC in the nanocomposites with two different matrix materials such as graphene sheet and carbon nanotube sheet on the radar absorbing performance were studied. The structural properties of the composites with varied granule size and cluster size were characterized. The behavior of microwave absorption of the composites was investigated by free space measurements in the range of 8.2 GHz — 12.4 GHz. Materials characterization was conducted by TEM, SEM and Raman spectroscopy.

T60.00006: Investigating Resistive Switching Mechanism in Niobium oxide Thin Film based Resistive Switches

Sweety Deswal, Ashok Kumar, Ajeet Kumar

There is large interest in exploring various transition metal oxides for their potential applications in resistive random access memories (RRAM) with emphasis on understanding the switching mechanism. Niobium oxide as resistive switching device is believed to be valence change memory (VCM) mechanism, where oxygen vacancies are responsible for formation of conducting filament. However, in Nb-oxide based VCM devices, we observe metallic nature of conducting filament, made of Nb atoms, which is similar to redox based electrochemical metallization memory (ECM) mechanism. By tuning the current compliance, we are able to make point contact filament resulting in quantization of conductance which can be useful in multilevel storage applications. We correlate atomic structure, conductance and mechanism of formation of conducting filament which provides new insights in understanding the resistive switching mechanism.

T60.00007: Low ferroelectric hysteresis by strain and polarization gradients

Arnoud Everhardt, Thibaud Denneulin, Anna Grünebohm, Yu-Tsun Shao, Sylvia Matzen, Petr Ondrejkovič, Fedir Borodavka, Silang Zhou, Neus Domingo, Gustau Catalan, Jiri Hlinka, Jian-Min Zuo, Etienne Snoeck, Martin Hÿtch, Beatriz Noheda

Phase transitions are among the most interesting and ubiquitous phenomena in nature. In materials science, they are responsible for the technological impact of ferromagnets, ferroelectrics, shape-memory alloys or memristors. First order phase transitions are associated to desirably large, nonlinear changes in the order parameters (polarization, magnetization, resistance, etc) and susceptibilities, but at the same time they are often coupled to the presence of hysteresis, which is related to energy losses. Here local inhomogeneous strain and polarization gradients are found in $BaTiO_3$ thin films, connecting a tetragonal to an orthorhombic phase through a bridging monoclinic phase. The associated gradual polarization rotation gives bulk-like values for the coercive field and fully reversible low hysteresis ferroelectric switching. An essentially temperature-independent huge dielectric constant (~4000) is found, together with a rather large d_{33} of 100 pm/V and the ability to create a strain diode with a five-fold increase of the piezoresponse by asymmetric electrodes. This low hysteresis direction enables energy-efficient electromechanical functionalities and can aid in the search for new ferroelectrics, piezoelectrics and ferromagnets.

T60.00008: Measuring the Permittivity of Barium Titanate Nanoparticles in an Epoxy Composite

Alejando Baptista, Andrew Bishop, Charles Dawson, Richard Liu, Lupe Macintosh, Albert Dato, Peter Saeta, Todd Monson

Barium titanate (BTO) is used as a dielectric material due to its high dielectric constant, which ranges from 1500 to 2000 in bulk [1]. Literature remains unclear on how BTO nanoparticle size impacts the dielectric constant, particularly for non-sintered, discrete nanoparticles. Studies have reported nanoparticle dielectric constants ranging from 135 [2] to 5000 [3].

We developed a procedure for fabricating BTO-epoxy nanocomposite materials, using ball-milling steps alongside surfactants to reduce nanoparticle agglomeration. We compare observed composite dielectric constants to finite-element models at various levels of agglomeration to determine the nanoparticle dielectric constant for nanoparticles with diameters between 50 and 500 nm.

[1] Arlt et al. Journal of Applied Physics 58 (1985): 1619.
[2] Siddabattuni et al. Journal of the American Ceramic Society 96.5 (2013): 1490.
[3] Wada et al. Japanese Journal of Applied Physics 42 Part 1, No. 9B (2003): 6188.

T60.00009: Surface Engineering for Improved Stability of $CH_3NH_3PbBr_3$ Perovskite Nanocrystals

Artavazd Kirakosyan, Seokjin Yun, Deul Kim, Jihoon Choi

Organohalide perovskite nanocrystals (NCs) with a variety of nano-scale structure and morphology have shown a promising potential owing to their size- and composition-dependent optoelectronic properties. (e.g. solar energy harvesting, piezoelectric energy generator, lighting, sensor for gas and chemical substances, polarity chemosensor, photodetectors, etc.). Despite extensive studies on their size dependent optical properties, a lack of understanding on their morphological transformation and the relevant stability issues limits a wide range of applications. Herein we hypothesize a mechanism on the morphological transformation of perovskite NCs, which leads to dissolving NCs and forming microscale rectangular grains, resulting in a reduction of photoluminescence. We found that the

morphological transformation from nanocrystal solids to microscale rectangular solids occurs via Ostwald ripening. A surface treatment with the identical surfactant suppresses the transformation, resulting in nearly monodisperse NCs with a square shape, and thus improves the stability of NC solution as well as their photoluminescence performance and quantum yield.

T60.00010: Ultrasound Pulse-Echo Setup for Studying Elastic Properties of the Electric Field Induced Phase Transitions in Ferroelectric Materials

Betzaida Berrios, Peter Crossman, Grace Yong, Lynn Boatner, Oleksiy Svitelski

Not long ago, we proposed a new design for ultrasonic measurements based on commercially available, mass-produced microchips [1]. Thanks to the high-linearity of the amplitude and phase characteristics of the design and to its broad dynamic range, the test measurements demonstrated superior performance of the instrument, achieving phase sensitivity of ~0.06 deg and amplitude sensitivity of ~0.05 dB with an input S/N ratio of 3. However, the pulse-forming and -receiving circuitry is vulnerable to electric discharge. To enable measurements in the presence of high electric fields, we designed and built special protective stages. Performance of the modified instrument has been tested on the example of electric field induced phase transitions in ferroelectric $KTaNbO_3$ crystal.

1. J. Grossmann, A. Suslov, G. Yong, L. Boatner, O. Svitelskiy, Rev. Sci. Instr., v. 87, 044901 (2016).

T60.00011: Characterizing Magnetism in Magnetically Doped Topological Insulators

Raina Crawford, Susan Kempinger, Nitin Samarth

Topological insulators are materials with non-trivial topological order, which behave as conductors on the surface but insulators in their interiors. Some previous studies on magnetically doped topological insulators have observes ferromagnetic behavior while others have observed superparamagnetic behavior. This study was conducted to characterize the magnetic behavior of V-$(Bi,Sb)_2Te_3$ and V-Sb_2Te_3 and determine how this varies with thickness, method of doping, and the addition of bismuth. A superconducting quantum interference device magnetometer was used to measure the magnetic moment of V-$(Bi,Sb)_2Te_3$ and V-Sb_2Te_3 as a function of temperature and field. From the temperature-dependent data, the samples of V-$(Bi,Sb)_2Te_3$ had lower Curie temperatures than those of V-Sb_2Te_3, with the thin samples of V-$(Bi,Sb)_2Te_3$ also having somewhat lower Curie temperatures than the thicker samples of V-$(Bi,Sb)_2Te_3$. From the field-dependent data, two-phase switching behavior was observed below the Curie temperatures of the samples of V-Sb_2Te_3 and delta-doped V-$(Bi,Sb)_2Te_3$. It is apparent that there are multiple factors that influence the magnetic behavior of topological insulators.

T60.00012: Topological classification of solids with momentum-nonsymmorphic symmetries

Arpit Dua, Ching-Kai Chiu, Aris Alexandradinata

Conventionally studied symmetries such as time-reversal or particle-hole symmetries map the Brillouin wavevector k to -k. Here we study a class of symmetries that map k to k+2pi/n, with n an integer and 2pi the Brillouin period. These so-called projective symmetries may be found in quasimomentum sub-manifolds of the Brillouin zones of Bravais lattices as projective mirror lines and planes as well as projective rotation lines. We classify such quasi-momentum submanifolds for the tenfold symmetry classes as well as identify the lines and planes in the Brillouin zones of Bravais lattices which have such symmetries. For Chern insulators, for quasimomentum sub-manifolds invariant under projective mirror, a topological invariant can be seen in the form of twists in the eigen-spectrum of Wilson loops. We discuss the properties and robustness of these twists.

T60.00013: Size-driven ferroelectrics in 2D pseudo-spin Ising model

Se-Hun Kim

We performed Monte Carlo simulation of the pseudo-spin Ising model in a two-dimensional ferroelectric system. The Metropolis method was employed by studying the size dependence of dielectric properties along the electric-field direction and the internal energy of the two-dimensional ferroelectric system. The critical phenomena in the vicinity of the phase transition temperature were considered by the scaling function obeying the values of critical exponents in view of the large-scale lattice.

T60.00014: Exploring Defects in Topological Insulators Using X-ray Diffraction and Atomic Force Microscopy

Maeve O'Brien, Anthony Richardella, Nitin Samarth

Topological insulators such as the Bi- and Sb- chalcogenides are of great interest to because they have unusual metallic surface states that allow the spin of electrons moving through them to be controlled and used for spintronic devices. Much progress has been made in the epitaxial growth of thin films of these materials. However, the common defects present need to be better characterized so that higher quality materials can be synthesized. Our aim was to better understand the structural defects present within the various topological insulators synthesized via molecular beam epitaxy. The methods used were primarily high-resolution x-ray diffraction and atomic force microscopy. These two techniques were used in conjunction in order to better understand both the surface defects and the defects present within the crystalline structure. The quality of the thin films is known to depend on the type of substrate the films are deposited upon. We report detailed characterization of Bi_2Se_3 grown on sapphire substrates and compare our results with those reported for growth on other substrates such as InP and $SrTiO_3$.

T60.00015: The Magnetocaloric Effect in Magnetic Topological Insulators

Shu-Wei Wang, Ziwei Dou, Stephen Fleming, Cui-Zu Chang, Charles Smith, Malcolm Connolly

Ferromagnetic exchange in magnetically-doped topological insulators (TIs) can break time-reversal symmetry and open a gap in the quasiparticle Dirac spectrum of the two-dimensional surface states[1-2]. Tuning the Fermi level out of the exchange gap repopulates the surfaces, resulting in changes in temperature with magnetization that can be considerable at millikelvin temperatures[3]. We study this magnetocaloric effect by performing magnetization loops while simultaneously monitoring the resistance and temperature of $(Bi_{0.29}Sb_{0.71})_{1.89}V_{0.11}Te_3$ films. We find that sweeping the external magnetic field beyond the coercive field and back to zero field lowers the sample temperature, while magnetization reversal around zero field results in a prominent heating effect. We rule out the influence of eddy current heating and show that the possible origin of the heating and cooling is the magnetocaloric effect from the film. In the demagnetization process we demonstrate that the film can reach a temperature below the base temperature of the dilution refrigerator.

T60.00016: Direct evidence of the antiparallel magnetization alignment in a quantum anomalous Hall heterostructure for realizing axion insulator state

Wenbo Wang, Di Xiao, Jue Jiang, Jae-Ho Shin, Yi-Fan Zhao, Chaoxing Liu, Moses Chan, Nitin Samarth, Cui-zu Chang, Weida Wu

Quantum anomalous Hall (QAH) sandwich with antiparallel magnetization alignment was proposed to realize the axion insulator state, and was reported to be realized in two recent experimental works. [3,4] The observed zero Hall conductance (σ_{xy}) plateau these heterostructures was interpreted as an evidence of antiparallel magnetization alignment between the top and bottom magnetic TI layers. However, no direct evidence of this antiparallel magnetization alignment was presented. Herein, we will present cryogenic magnetic force microscopy (MFM) studies of magnetic domain behavior in QAH sandwich heterostructures in which two compositionally different magnetic TI layers are separated by an undoped TI layer. [5] Our MFM results reveal sequential magnetization reversals of the top and bottom layers at different coercive fields, providing a direct evidence of the antiparallel magnetization alignment that is necessary for realizing axion insulator states.

[1] M. Mogi *et al.*, *Nat. Mater.* **16**, 516 (2017).
[2] M. Mogi *et al.*, *Sci. Adv.* , **3**, eaao1669 (2017).
[3] D. Xiao *et al.*, arXiv 1710.00471 (2017).

T60.00017: Quantum ratchet effect in periodically driven dimer chain

Jin-yu Zou, Bang-Gui Liu

In condensed matter physics, one of the major topics is to find out and classify interesting novel topological matters and phenomena. Topologically nontrivial systems can also be achieved by using periodical driving fields. On the other hand, ratchet effect can be used to realize directed transport in symmetrically-driven systems. Here, we promote a dimer chain by applying two mutually-parallel ac electric fields, and obtain an effective two-dimensional Hamiltonian in the low-frequency regime. We thereby derive Floquet quantum anomalous Hall conductance and then find a quantized ratchet effect in the resulting current along the chain. Our further analysis shows that these are originated from the electric fields only. This lengthwise quantized ratchet effect without magnetic field should be useful to designing novel high-performance electronic applications.

T60.00018: Black Hole Horizon in a Type-III Dirac Semimetal $Zn_2In_2S_5$

Huaqing Huang, Kyung-Hwan Jin, Feng Liu

Recently, realizing new fermions, such as type-I and type-II Dirac/Weyl fermions in condensed matter systems, has attracted considerable attention. Here we show that the transition state from type-I to type-II Dirac fermions can be viewed as a type-III Dirac fermion, which exhibits unique characteristics, including a Dirac-line Fermi surface with nontrivial topological invariant and critical chiral anomaly effect, distinct from previously known Dirac semimetals. Most importantly, we discover $Zn_2In_2S_5$ is a type-III Dirac semimetal material, characterized with a pair of Dirac points in the bulk and Fermi arcs on the surface. We further propose a solid-state realization of the black-hole-horizon analogue in inhomogeneous $Zn_2In_2S_5$ to simulate black hole evaporation with high Hawking temperature. We envision that our findings will stimulate researchers to study novel physics of type-III Dirac fermions, as well as astronomical problems in a condensed matter analogue.

T60.00019: Dirac-like dispersion in nearly compensated Dirac semimetal $ZrAs_2$

Firoza Kabir, Md Mofazzel Hosen, Gyanendra Dhakal, Klauss Dimitri, Tay-Rong Chang, Christopher Sims, Hsin Lin, Tomasz Durakiewicz, Dariusz Kaczorowski, Madhab Neupane

Recently, the transition metal dipnictide family with a monoclinic crystal structure is predicted as a potential candidate for supporting this compensated Dirac like electronic structure. Here we report an angle-resolved photoemission spectroscopy (ARPES) study of $ZrAs_2$, a transition metal dipnictide with an orthorhombic crystal structure exhibiting large MR properties and nearly electron-hole compensation mechanisms. Our studies reveal multiple Fermi surface pockets such as the 6-fold petal-like Fermi pockets around the center (Γ point) and ellipsoidal shaped Fermi pockets at the corner (X point) of the Brillouin zone (BZ). Interestingly, Dirac like linearly dispersive states are observed at the zone corner of the BZ. Moreover, our magnetoresistance measurements and the occupied Fermi surface area calculations reveal the nearly compensated semimetallic characteristics of $ZrAs_2$. Our findings suggest that type 12 system $ZrAs_2$, with an orthorhombic crystal structure, is a new platform for unveiling interesting physics beyond Weyl semimetal and topological insulator systems.

T60.00020: Dynamic Terahertz Response in the Three-Dimensional Dirac Semimetal Cd_3As_2 by Ultrafast Optical Excitation

Wei Lu, Jiwei Ling, Faxian Xiu, Dong Sun

Three-dimensional (3D) Dirac semimetal, as 3D analogues of graphene, has great potential toward electronic and optoelectronic device applications with extreme performance benefiting from its topological protected state of Dirac Fermions. It is crucial to understand the behaviors of excited Dirac Fermions. Here, by using the low-photon-energy terahertz (THz) probe, we have measured the transient transmission spectra and dynamics of the photoexcited carriers that are Dirac-Fermi-like approaching the Dirac point, on a nano-film sample of 3D Dirac semimetal Cd_3As_2. Negative pump induced transmission is observed which is mainly attributed to pump excited photocarrier absorption of THz. This response is very sensitive and nonlinear increasing with the pump power. The relaxation dynamics can be illustrated by two time constants both of which are in picosecond time scale, and increasing with the pump power and lattice temperature, while the characteristics of THz transmission are decreasing with the temperature. This can be explained by two-temperature model. The Drude model has been used to get the kinetic parameters of Dirac Fermions in Cd_3As_2.

T60.00021: Magnetotransport Features of Bulk and Surface States in Weyl Semimetals

Pablo Perez-Piskunow, Nicandro Bovenzi

We study the conductivity of a Weyl slab, where the number of bulk states is much larger than of surface states. If the dominant scattering mechanism is forward long-range scattering, the surface conductivity can overcome the bulk conductivity.

When transport is dominated by surface states, the system can show a large magnetoresistance with a magnetic field perpendicular to the surface. This marks a clear contrast with what is expected if transport is dominated by bulk states. Thus, simulating the conductivity by solving the Boltzmann equation for a Weyl slab allow us to predict the magnetoresistance for magnetic field in different directions.

Our results are obtained by solving the Boltzmann equation in two dimension with gaussian scatterers. Previous studies show that the method reproduces the magnetoresistance features of complex systems such as oxide interfaces [1, 2]. The results for a Weyl slab are further compared to the magnetotransport numerical calculations of the 3D Boltzmann equation for a bulk Weyl system.

[1] N. Bovenzi and M. Diez, Phys. Rev. B 95, 205430 (2017).
[2] N. Bovenzi et al., arxiv:1707.01038 (2017).

T60.00022: Prediction of Dirac semimetal phase with layer-resolved orbital texture in ternary tantalum nitrides

QuanSheng Wu, Christophe Piveteau, Zhida Song, Matthias Troyer, Oleg Yazyev

Three-dimensional topological Dirac semimetals are materials constituting a novel state of quantum matter which has attracted a lot of interest. Dirac semimetals are characterized by topologically protected double-degenerate band crossings with linear dispersion near the Fermi energy, giving rise to quasiparticles that behave like Dirac fermions. By means of first-principles calculations, we discover the Dirac semimetal phase in ternary tantalum nitrides Mg1 – x Ta2+x N3 and Li1–xTa3+xN4. The electron charge densities of the two crossing band pairs which form the Dirac nodes are located in different crystal layers in real space, thus realizing a layer-resolved orbital texture. The band inversion which leads to the Dirac points happens from the dz2 orbital from one Ta layer and dx2-y2 orbitals from another Ta layer.

T60.00023: Quantum Transport Study of the Type-II Dirac Semimetal VAl_3

Linshu Wang, Yeyu Huang, Yunjie Yu, Jiamin Ni, Chuanying Xi, Li Pi, TayRong chang, ChinShan Lue, Shiyan Li

The transition-metal icosagenides VAl_3 was predicted to be a Lorentz-violating type-II Dirac semimetal. We report the quantum transport study of VAl_3 single crystals in magnetic fields up to 38 T. The Shubnikov-de Hass (SdH) oscillations of the longitudinal resistance are clearly observed at low temperatures. By analyzing the SdH oscillations, we obtain the Fermi surface area and compare it with the band structure calculations. We further discuss its topological property.

T60.00024: Nanoconfinement to Reveal Structural Evolution of Solution-Processed $MAPbI_3$ Crystals

Sangchul Lee, Joshua Feldman, Stephanie Lee

We demonstrate the use nanoconfinement as a strategy to reveal structural evolution in solution-processed methylammonium lead triiodide ($MAPbI_3$) systems. MAI and PbI_2 precursors were co-deposited from organic solvents into anodized aluminum oxide (AAO) templates comprising uniaxially aligned nanopores. 2D x-ray diffraction patterns revealed the formation of an intermediate crystalline phase in as-spun samples. Interestingly, this phase adopted a preferential orientation in the AAO templates, allowing for prediction of the unit cell dimensions based on the observed diffraction pattern. We identified the intermediate phase as a PbI_2:solvent complex with sheets of PbI_2 running parallel to the long axes of the pores. Upon thermal annealing, the PbI_2:solvent complex converted to $MAPbI_3$, accompanied by a complete loss of preferential crystal orientation. Critically, nanoconfined $MAPbI_3$ crystals displayed significantly longer stability compared to unconfined $MAPbI_3$ crystals during exposure to humidity. Such extended stability is critical to progressing solution-processed metal-halide perovskite solar cells towards commercialization.

T60.00025: Raman Temperature Coefficients and Thermal Conductivity of Methylammonium Lead Bromide Perovskite Materials

Jacob Lewis, Fariborz Kargar, Hong-Hua Fang, Maria Antonietta Loi, Alexander Balandin

Interest in the organic-inorganic hybrid perovskite materials has exploded in recent years due to the dramatic increase in the perovskite solar cells' solar power conversion efficiency and the potential for low manufacturing costs of such devices. Unfortunately, these materials and the solar cells based upon them suffer from instability due to environmental factors such as humidity, ultraviolet light, and heat. This motivates the investigation of the thermal conductivity and thermal diffusivity of these materials. The first experimental and theoretical studies found that the thermal conductivity of perovskites is rather low, i.e., below 1 W/mK at room temperature. We used the Raman optothermal technique, previously developed for graphene [1], in order to study in-plane and cross-plane thermal properties of perovskites and their dependence on temperature and defects. The temperature-dependent Raman spectra were obtained under 633-nm laser excitation. The thermal conductivity data obtained by the optothermal Raman technique will be compared with that of other methods. [1] A. A. Balandin, "Thermal properties of graphene and nanostructured carbon materials," Nature Mater., 10, 569 (2011).

T60.00026: Measuring Phonon Lifetimes and Lattice Dynamics of Single-Crystal Methylammonium Lead Iodide with Neutron Triple-Axis Spectroscopy

Michael Toney, Aryeh Gold-Parker, Peter Gehring, Ian Smith, Daniel Parshall, Jarvist Frost, Aron Walsh, Hemamala Karunadasa

There is growing interest in the fundamental physical properties of the photovoltaic absorber methylammonium lead iodide ($CH_3NH_3PbI_3$). In particular, the phonons provide information about the dynamical coupling of electronic states to the lattice and the vibrational coupling between PbI_6 octahedra and the MA^+ cations, both of which may influence the opto-electronic properties. We report results from neutron inelastic scattering measurements on fully-deuterated single crystals of $CD_3ND_3PbI_3$ to characterize the low-energy lattice dynamics.

We have measured the momentum-resolved transverse acoustic (TA) phonon dispersion and lifetimes in the orthorhombic, tetragonal, and cubic phases. The TA phonon becomes strongly damped with increasing wave vector, and on heating into the tetragonal phase the TA phonon lifetimes decrease by roughly a factor of two for wave vectors near the Brillouin zone boundary. This has major implications for the carrier scattering and cooling processes.

In addition, we observe quasi-elastic scattering (QES) that increases in intensity upon heating into the tetragonal phase. This QES varies strongly with reduced wave vector and corresponds to the coupled dynamics of the MA^+ cation and PbI_6 octahedral distortions over nm-scale domains and a few-ps timescale.

T60.00027: Controlled Growth of Perovskite Single Crystal for High Mobility Field-Effect Transistors

Junzhan Wang

The organolead halide perovskites have recently garnered tremendous research efforts in a broad range of photovoltaic and optoelectronic applications, despite of which a comprehensive physical picture of the intrinsic charge transport remains elusive and only rare example of perovskite field-effect transistors can be found. In this work, we have achieved controlled growth of the perovskite single crystal for field-effect transistor applications and investigated the electrochemical mechanism behind electrode degradation of perovskite field-effect transistors. By chemical modification of electrodes, field-effect transistors exhibit clear p-type nature of charge transport in CH3NH3PbBr3 and highly hole carrier mobilities could further reach up to ~20cm2/Vs, which is also the highest values reported so far.

T60.00028: Scalable Synthesis of Exfoliated Organometal Halide Perovskite Nanocrystals by Ligand-Assisted Ball Milling

Seokjin Yun, Artavazd Kirakosyan, Deul Kim, jihoon choi

Organometal halide perovskite materials have attracted much attention in the photovoltaic and light emitting devices due to the compositional flexibility with ABX_3 formula (A is an organic amine cation; B is a metal ion; X is a halogen atom). Recently, several approaches have been proposed to synthesize organometal halide perovskite nanocrystals (NCs) with a size-tunability of their bandgaps. However, despite successful synthetic methods of the perovskite NCs based on the precipitation of precursors in a poor solvent, a high-yield production of perovskite NCs still remains a key challenge. In this work, we show a new scalable method for exfoliated perovskite NCs by a ligand-assisted ball-milling process that combines chemical and mechanical exfoliating process. In particular, when the ligands such as octylamine and stearylamine were employed during ball-milling, the size of perovskite NCs was significantly decreased, and their photoluminescence quantum yield (PLQY) was increased, compared to the case without ligands. Moreover, it also exhibits compositional bandgap engineering that can broaden its optoelectronic applications.

T60.00029: Electronic transport in thin crystals of ruthenium chloride

Amirari Diego, Josue Rodriguez, Drew Latzke, Nicholas Breznay, Robert Kealhofer, Gilbert Lopez, Christopher Kim, Samantha Crouch, Alessandra Lanzara, James Analytis, Claudia Ojeda-Aristizabal

Ruthenium chloride ($RuCl_3$) is a layered material where crystal field effects, electronic correlations and spin-orbit coupling give rise to a Mott insulator with spin-orbit coupled moments arranged in a honeycomb lattice with bond-directional interactions. The ensemble of these features makes this material a very close experimental realization of the Kitaev-Heisenberg model. Exciting ground states have been predicted for this system, such as quantum spin liquids, consistent with recent

inelastic neutron scattering experiments [1] as well as long ranged magnetic ordered states [2]. Here we present preliminary electronic transport experiments on thin crystals of $RuCl_3$ as well as the band structure of this material through Angle resolved Photoemission Spectroscopy ARPES measurements and the effects of electrostatic doping.

[1] A. Banergee, et al. Science **356**, 1055-1059 (2017).
[2] J. A. Sears, M. Songvilay, K. W. Plumb, J. P. Clancy, Y. Qiu, Y. Zhao, D. Parshall and Young-June Kim, Phys. Rev. B **91,** 144420 (2015).

T60.00030: Electronic devices of thin crystals of sodium iridate

Josue Rodriguez, David Rosser, Amirari Diego, Drew Latzke, Nicholas Breznay, Robert Kealhofer, Gilbert Lopez, Samantha Crouch, Alessandra Lanzara, James Analytis, Claudia Ojeda-Aristizabal

Sodium iridate (Na_2IrO_3) is predicted to present exciting phenomena thanks to the honeycomb arrangement of its iridium ions and the interplay of electronic correlations and spin-orbit coupling, making it a close experimental incarnation of the Kitaev-Heisenberg model. Magnetic susceptibility and heat capacity measurements in this material have shown signature of magnetic ordered states [1]. Our Angle Resolved Photoemission Spectroscopy (ARPES) experiments have shown additionally the presence of a metallic feature near the Fermi energy, consistent with other experiments [2] identified as a surface state. Here we present electronic transport measurements on thin crystals of Na_2IrO_3 that aim to address and control magnetic ordered ground states in this material.

[1] Y. Singh and P. Gegenwart, Phys Rev B **82**, 6 (2010).
[2] N. Alidoust, C. Liu, S. Xu, I. Belopolski, T. Qi, M. Zeng, D. S. Sanchez, H. Zheng, G. Bian, M. Neupane, Y. Liu, S. D. Wilson, H. Lin, A. Bansil, G. Cao, and Z. M. Hasan, Phys Rev B, **93**, 245132 (2016).

T60.00031: Phase evolution of perovskite PZT nanotubes caused by metal ion diffusion

Sang Don Bu, Sam Yeon Cho, Jin Woo Kim, Eun Young Kim, Seon Yong Kim

We report the phase evolution of $Pb(Zr_{0.52}Ti_{0.48})O_3$ nanotubes (PZT-NTs) caused by ion diffusion. The PZT-NTs were fabricated in pores of porous anodic alumina membrane (PAAM) using a spin coating of PZT sol-gel solution and subsequent thermal annealing under oxygen atmosphere. The surface morphology and composition of PZT-NTs were examined as a function of the annealing temperature, and the diffusion of elements over nanometer length scales was investigated based on analyses using field emission transmission electron microscopy (FETEM), scanning transmission electron microscopy (STEM), and energy dispersive X-ray spectroscopy (EDX). STEM analyses with EDX line profiles provide a characterization of the interface between PZT-NT and PAAM, suggesting that Pb, Zr, and Ti diffused into the PAAM. The diffusion results in the secondary phase in the PZT-NTs, such as the pyrochlore phase of Pb-deficient. TEM analyses suggest that the interface was mostly lead aluminate, such as $Pb_2Al_2O_5$ or $PbAl_{12}O_{19}$, or aluminum titanate like Al_2TiO_5. These results indicate that considerable diffusion of metal ions occur, and furthermore such diffusion brings great difficulties in the phase control of metal oxides.

T60.00032: Enhanced piezoelectric response of AlN via CrN alloying

Sukriti Manna, Kevin Talley, Prashun Gorai, John Mangum, Andriy Zakutayev, Geoff Brennecka, Vladan Stevanovic, Cristian Ciobanu

We report density functional theory calculations of structure and properties of the Cr-AlN system for Cr concentrations ranging past the wurtzite-rocksalt transition point. By studying the different contributions to the longitudinal piezoelectric coefficient, we propose that the physical origin of the enhanced piezoelectricity in $Cr_xAl_{(1-x)}N$ alloys is the increase of the internal parameter u of the wurtzite structure upon substitution of Al with the larger Cr ions. Among a set of wurtzite-structured materials, we have found that Cr-AlN has the most sensitive piezoelectric coefficient with respect to alloying concentration. Based on these results, we propose that Cr-AlN is a viable piezoelectric material whose properties can be tuned via Cr composition; we support this proposal by combinatorial synthesis experiments, which show that Cr can be incorporated in the AlN lattice up to 30% before a detectable transition to rocksalt occurs. At this Cr content, the piezoelectric modulus d_{33} is approximately four times larger than that of pure AlN. This finding, combined with the relative ease of synthesis, may propel Cr-AlN as the prime piezoelectric material for applications such as resonators and acoustic wave generators.

T60.00033: Clean Flipping of the Electric Dipole Moment in Pd-doped BiFeO3 Film Along [111] Direction

PO-YU CHEN, WEI-ZHEN QIU, Shih-Jye Sun, Hsiung Chou

Multiferroic materials involve multiple couplings between electricity and magnetism, especially for magnetoelectric multiferroic materials. This shows inherent coupling between magnetic and ferromagnetic materials that could be used as a mechanism to switch magnetic moment of an adjacent magnetic layer by applying an external electric field and vice-versa. The pseudocubic structure of BiFeO3, which is a multiferroic layer on a SrTiO3 (100) substrate, provides eight degenerate electric polarization directions. In addition, the leakage problem at domain walls causes great difficulty in control and application. This research aims to solve these problems by growing Pd-doped BiFeO3 and $SrRuO_3$ bilayers along [111] direction on atomically flat $SrTiO_3$ (111) substrates. The Pb doping will stop the electric leakage and the [111] orientation will simplify the polarization orientation switch states. By using a Piezoresponse Force Microscopy (PFM), we observed a very clean switch of electric polarization along [111] direction with no response on the in-plane direction to the swiped electric field. A charge accumulation phenomenon is observed that shifts the hysteresis loop similar to the exchange bias effect.

T60.00034: Why is $NaNbO_3$ the most complicated perovskite structure?

Yali Yang, laurent bellaiche, Wei Ren

Sodium niobate ($NaNbO_3$) is known to have unusual complex sequences of phase transitions when varying temperature and pressure. Such sequences result in the formation of various and rather different phases, including ferroelectric states, nanotwins and purely antiferrodistortive phases. The motivation of our work is to explain the microscopic origins of such complexity, by performing and analyzing first principles simulations (with different functionals) as well as effective Hamiltonian simulations. As we will see, very subtle and field-controllable competitions are in play in $NaNbO_3$, which is promising to design new functionalities.

T60.00035: TiO_2 doped with different atoms to modify its catalytic characteristics

Pablo De la Mora, Gustavo Tavizon, Faustino Aguilera Granja

TiO_2 has photocatalytic capabilities with a 2.9eV band gap. The gap is quite large and can only be used in very specific situations. By introducing different elements, the gap can be modified, it can introduce states in different positions of the gap, depending on the nature of the impurity. In this way, the photocatalytic characteristics of TiO_2 can be modified.

With electronic structure calculations based on Density Functional Theory the gap is underestimated. This can be solved by using the GW approximation, but this is quite computationally demanding. Recently Becke and Johnson proposed a potential to do these calculations, Tran and Blaha found a modification that reproduce the band gap with great accuracy and the computational cost is low, but the process is clumsy and it needs many iterations to converge. In this work, with the introduction of several cations in the TiO_2 lattice, we show some computational resources that can be employed in order to compute the new electronic structures, $Ti_{1-x}A_xO_2$, resulting from these doping processes.

T60.00036: Observation of a Dirac state in a half-Heusler material YPtBi

Christopher Sims, Md Mofazzel Hosen, Gyanendra Dhakal, Klauss Dimitri, Hongchul Choi, Firoza Kabir, Orest pavlosiuk, Piotr Wisniewski, Tomasz Durakiewicz, Jian-Xin Zhu, Dariusz Kaczorowski, Madhab Neupane

The prediction of non-trivial topological electronic states hosted by half-Heusler compounds makes them prime candidates for discovering new physics and devices as they harbor a variety of electronic ground states including superconductivity, magnetism, and heavy fermion behavior. Here we report a systematic study of normal state electronic properties of the superconducting half-Heusler compound YPtBi using angle-resolved photoemission spectroscopy (ARPES). Our data reveal the presence of a Dirac state at the Γ point of the Brillouin zone at 500 meV below the chemical potential. We observe the presence of multiple Fermi surface pockets including two concentric hexagonal and six half oval-shaped pockets at the Γ and K points of the Brillouin zone, respectively. Furthermore, our measurements show Rashba-split bands and multiple surface states crossing the chemical potential which are supported by the first-principles calculations. Our findings of a Dirac state in YPtBi play a significant role in establishing half-Heusler compounds as a new potential platform for novel topological phases and explore their connection with superconductivity.

T60.00037: Enhanced rectification performance of MIM tunnel diode applying an oxide semiconductor electrode

Donggun Lee, Jun-Woo Park, Youn Sang Kim

MIM DIODE using F-N tunneling-based conduction mechanism is the most promising diode device as ultra-high frequency rectifier because the electron tunneling process takes only femtoseconds. However, in spite of the ultra-fast operation of the MIM, it is difficult to increase the On / Off ratio which is the most important property of diode. Here we propose a solution to apply an oxide semiconductor film as an electrode in MIM structure in order to increase a rectification ratio of electrical currents. An IGZO thin-film, which is a well-known-type semiconductor, was formed on a HfO_2 insulator with a thickness under 20 nm. Depending on the depleted surface charge state at the IGZO / HfO_2 interface under negative voltages, the current is rectified, therefore, the rectification ratio is highly enhanced to 10^5 at 3 V. Furthermore, the conduction of electron maintains the F-N tunneling, which means our device can be operated at high frequency. We believe that the F-N tunneling-based MIS DIODE for ultra-high frequency diodes will be used in future electronic devices and wireless power transfers.

T60.00038: Thermal scanning probe lithography of topological regions in disordered Sb_2Te_3 thin films

Shihua Zhao, Inna Korzhovska, Edoardo Albisetti, Elisa Riedo, Lia Krusin-Elbaum

We demonstrate the use of thermal scanning probe lithography (t-SPL) for writing on the disordered thin (30-40nm) films of Sb_2Te_3 to define nanoscale regions of low disorder with topological signatures, such as weak antilocalization (WAL) quantum interference correction to classical Drude conductivity. We will discuss the results of non-local transport measurements and chiral effects associated with the edges.

T60.00039: Quantum electronic transport in $(Bi_{1-x}Sb_x)_2Se_3$ topological insulator nanoribbon contacted with superconducting electrodes

Heungsoon Im, Nam-Hee Kim, Hong-Seok Kim, Yasen Hou, Rui Xiao, Dong Yu, Yong-Joo Doh

The formation of spin-textured metallic edge states in topological insulators (TIs) enables highly coherent charge and spin transport. Combinations of TIs with conventional superconductors can also provide useful platforms for creating and manipulating emergent particles such as Majorana fermions, which are essential for

topological quantum computers. Here, we report electronic transport properties of $(Bi_{1-x}Sb_x)_2Se_3$ TI nanoribbon at low temperatures. With the magnetic field applied parallel to the nanoribbon axis, Aharonov-Bohm conductance oscillations were observed. In the superconducting state below the superconducting transition temperature of Al electrodes, the conductance enhancement due to Andreev reflection was observed.

T60.00040: Spin-polarized surface state transport in a topological Kondo insulator SmB_6 nanowire

Yong Zhou, Lingjian Kong, Zhimin Liao, Dapeng Yu

SmB_6, as a topological Kondo insulator, has spin-momentum-locked surface states and fully insulating bulk, which presents promising spintronic applications. Here, we report on the magnetotransport properties of individual SmB_6 nanowires. With decreasing temperature below 10 K, the surface states dominate the transport behavior as reflected by the resistance saturation. At 1.5 K, a transition from negative to positive magnetoresistance occurs with gradually increasing the bias current. The nonlocal measurements indicate that the surface state transport is spin polarized, and the spin diffusion length is as long as 0.5 μm. Bias current-modulated two-channel transport is employed to explain the observed sign reversal of the magnetoresistance.

T60.00041: SEMICONDUCTORS

T60.00042: Electronic transport in semiconductor-metal hybrid nanostructure studied by cryogenic scanning tunneling spectroscopy and ultrafast absorption measurements

Tuhin Basu, Jure Demsar, Elke Scheer

Semiconductor-noble metal core-shell hybrid nanostructures (HNs) are promising and versatile systems due to quantum confinement-induced multiple functionalities. In future nanoplasmonic devices, the interaction between the strong intrinsic optical nonlinearities of excitonic nanostructures and the ability of metallic nanostructures to locally concentrate electromagnetic fields are the most important open subjects. Moreover, the band-structure and photo-physical properties of these HNs can be engineered by changing the overall orientation of the core-shell structure. In this work, an attempt has been made to investigate the band-structure modification with the formation geometry of HNs by low temperature (4K) scanning tunneling spectroscopy at the single nanoparticle level. The band-gap and the spectral feature above the band-gap due to electronic transport exhibit a specific trend with the change in the semiconductor core size and noble-metal shell thickness. We have investigated exciton-plasmon interaction mediated charge transfer process through these modified band-structures using ultra-fast absorption spectroscopy. The charge transfer is found to occur on a picosecond time-scale and is sensitive to the change of the core-shell geometry.

T60.00043: Sub-10 nm Channel Length Field-Effect Transistors

Dongxue Chen, Kai Xu, Qian Liu, Jun He, Kaihui Liu, Dapeng Yu

Two-dimensional materials (2DMs) are competitive candidates in replacing or supplementing conventional semiconductors owing to their atomically uniform thickness. However, current conventional micro/nanofabrication technologies realize hardly ultrashort channel and integration, especially for sub-10 nm. Meanwhile, experimental device performance associated with the scaling of dimension needs to be investigated, due to the short channel effects. Here, we show a novel and universal technological method to fabricate sub-10 nm gaps with sharp edges and steep sidewalls. The realization of sub-10 nm gaps derives from a corrosion crack along the cleavage plane of Bi_2O_3. By this method, ultrathin body field-effect transistors (FETs), consisting of 8.2 nm channel length, 6 nm high-k dielectric, and 0.7 nm monolayer MoS_2, exhibit no obvious short channel effects.

T60.00044: *Transport Data Analysis in Strontium Vanadate*

Michael Milovich-Goff, Matthew Brahlek, Turan Birol, Roman Engel-Herbert

Understanding how electricity moves through material impacts technology from power transmission to the advanced functionality of a nanometer scale transistor. A full understanding of the fundamental process is only understood in subclass of materials where the electron motion is effectively non-correlated—ie the state of a single does not depend on the neighboring electrons. Here I present a study aimed to understand the electronic properties of a material that is not so simple. The material in question for this study is strontium vanadate (), a transparent conductor grown via hybrid molecular beam epitaxy (hMBE). Transport measurements for have been shown to differ from what is expected from density functional theory (DFT) calculations, which is the only means by which these materials can be studied from a theoretical standpoint. We use Ong's method to try and connect the calculated DFT values and the transport measurement data for [1]. We utilize Ong's method by the looking at the geometry of a fermi surface (FS) to determine its correlation effects. We did find that the Ong method fails in the high temperature regime due to strong electron correlations.

T60.00045: Charged Electrospray Beam Optics in the Focusing Column

Elham Vakil Asadollahei, Manuel Gamero-Castaño

Electrospray ionization process introduces a source of uniform submicron-sized nanodroplets for energetic bombardment of material. In addition to narrow size distribution, other fundamental characteristics such as low charge to mass ratio and high conductivity makes the beam of ES nanodroplets a suitable source for nano-scale microfabrication techniques such as sputtering and etching. ES beam focusing is required to achieve high energy density needed for such applications. We studied the optics of charged ES beam in electrostatic field of an experimental apparatus. A numerical simulation of projectile trajectory in the axisymmetric electrostatic field determines the Gaussian image of the source. In addition to tracing algorithms, numerical models of potential error sources, geometric and chromatic aberrations, are used to inspect the bombarded area on silicon targets for a range of accelerating voltages. The deviated size and shape of the sputtered area from Gaussian image is used to track the imperfections in the experimental setup and the inherent properties of the beam. In our presentation we discuss how each of these aberration components affects the resolution, and can be corrected or minimized using additional elements such as multipole lenses.

T60.00046: Crystal Formation and Electric Transportation of (Co,Al) Co-doped ZnO with Various Defect Concentrations

HSIEN-CHI Lin, Irina Edelman, Hsiung Chou

Electric transportation of Al- and Co-doped ZnO, $Co_{0.05}Al_{0.02}Zn_{0.93}O$ (CAZO) film as a function of the hydrogen content H_2% in the sputtered gas during growth process is studied. As H_2% is increased, the concentration of defect for hydrogen to take out part of oxygen content in the sputtering process is also increased. Therefore, the optical transmittance decreases with increasing H_2%. Using TEM investigation, we discovered that the films are in nano-rod, columnar, and polycrystalline formats for H_2%=0, 1% and 50% respectively, indicating that the generated defects lower the crystal ordering due to possible huge defect strain. XRD measurements show perfect ZnO structure for the H_2%=0 sample, while manifesting mixing phase with additional CoO nano-crystals for H_2%=50%. The resistance of H_2%=0 sample is infinite. The H_2%=1% sample exhibits the lowest resistance and the other H_2% > 1% samples show higher resistances. All resistance to temperature curves can be fitted by VRH model, indicating that defect concentration is the key factor to introduce defect states for hopping conduction. However, when the defect concentration is high, excess scattering increases the resistance.

T60.00047: Enhancement of the electrical characteristics of thin-film transistors with multi-stack zinc tin oxide channel layers produced with 2 different solution concentrations

Sunil Uprety, Shiqiang Wang, David Hanggi, Kosala Yapabandara, Vahid Mirkhani, Min Khanal, Benjamin Schoenek, Sarit Dhar, Michael Hamilton, Willis Hames, Mobassar Sk, Minseo Park

(Author Not Attending)

T60.00048: Abstract Withdrawn

Pure SnSe, 5% In doped SnSe and 5% Sb doped SnSe single crystals were grown by direct vapour transport (DVT) technique. The energy dispersive analysis of X-ray (EDAX) showed that all the samples are near stoichiometric but slightly Sn deficient. The X-ray diffraction (XRD) study of all the three as-grown single crystal samples showed that they possess orthorhombic structure and the lattice parameters are in good agreement with the reported parameters. The thermoelectric power S and d.c. electrical conductivity s variation with temperature from ambient to 573K substantiated the semiconducting nature of the all the three samples. The sign of S was positive for all three samples for all the temperature range stating the sample to be p-type semiconducting. The power factor S^2s variation with temperature showed pure SnSe having highest value compared to doped samples. Thus doping by indium (In) and antimony (Sb) does not improve the thermoelectric efficiency of the SnSe.

T60.00049: CVD Growth of Large area single-crystal and bilayer MoS_2 on Molten Glass

Zhenfeng Zhang, Yanqing Wu

The rich and diverse physics with novel optical and electrical transport properties of transition metal dichalcogenides (TMDCs) offers unprecedented opportunities for electronics and optoelectronics applications. However, large area CVD growth of multi-layer TMDC film with high mobility is still a challenge. Here, we present an approach for growing monolayer and bilayer MoS_2 with clear crystalline structures using a modified atmospheric pressure chemical vapor deposition (APCVD) method. Moreover, molten glass is utilized as a growth substrate for isotropic and smooth growth, which can significantly suppress nucleation density and promote larger domain growth. We can successfully obtain MoS_2 monolayer and bilayer with average single domain size up to 500 and 50 μm in ten minutes, respectively. This low-cost growth of high-quality large grain size of 2D TMDCs provides a pathway for high-performance 2D electronic devices.

T60.00050: Nanoscale Mapping of Thermal Gradients in MoS_2 from Plasmon Energy Shifts

Matthew Mecklenburg, Lang Shen, Steve Cronin

Using a new nanoscale thermometry technique, we observe in plane temperature gradients across suspended, few layer thick, MoS_2 sheets. The temperature gradients are measured via *in situ* experiments in a transmission electron microscope. A map of temperatures is built up by acquiring an electron energy loss spectrum at an array of points across the MoS_2. Each spectrum is then used to precisely measure the energy of the MoS_2 bulk plasmon, whose energy is sensitive to changes in temperature due to electron density changes via thermal expansion. By Joule heating two heaters on either side of the suspended sheet we are able to induce temperature gradients in either direction. By calibrating each of the heaters output power we can then infer the suspended MoS_2's thermal conductivity.

T60.00051: Exploring the Effects of Order vs. Disorder using Three Cations: the example of Al-Mg-Si-N

Mikael Rasander, James Quirk, Michelle Moram

Wurtzite structured AlN is used in ultraviolet light emitting devices and high electron mobility transistors, as well as in high temperature ceramic applications. If we replace pairs of Al atoms in AlN with Mg and Si, while fulfilling local charge neutrality around each N atom, $MgSiN_2$ will be formed. This so-called II-IV nitride forms in an orthorhombic wurtzite-derived crystal structure and it has been shown that $MgSiN_2$ has a large in-direct band gap that is similar in size to the band gap in AlN.

It is, however, possible to imagine that, rather than forming an ordered compound, Mg and Si atoms randomly occupies the cationic sublattice of the wurtzite crystal structure. Such a structure has a higher free energy while also significantly reduces the size of the band gap compared to ordered $MgSiN_2$. In this study, we have investigated the questions related to the structure of alloyed Al-Mg-Si-N systems from both experiment and first principles density functional calculations, where the composition has been varied from pure AlN to pure $MgSiN_2$. Especially, we have investigated how order and disorder in these types of systems impact the electronic properties.

T60.00052: Strain-controlled insulator-metal transition in $YTiO_3$/$SrTiO_3$ superlattices: effect of interfacial reconstruction

Xue-Jing Zhang, Bang-Gui Liu

The structural, magnetic, and electronic properties of short-period STO/YTO superlattices consisting of Mott insulator $YTiO_3$ (YTO) and band insulator $SrTiO_3$ (STO) are investigated by the density-functional-theory plus U method. It is found that an insulator-metal transition occurs when a compressive strain is applied, and no transition happens for tensile strain. Structural analyses reveal that the electronic transition accompanies a structural phase transition restoring inversion symmetry, and the strain compresses the interfacial oxygen octahedra of Ti and thus makes the *d* energy level of the interfacial Ti atoms move upward so as to induce electron transfer to the STO layer. This mechanism is supported by the fact that a similar insulator-metal transition also occurs when the on-site U is reduced. These findings can improve our understanding of structural and electronic properties of such oxide superlattices and heterostructures.

T60.00053: Electronic Structure of Thermoelectric Material ZnSb from First-Principles

Guang-Lin Zhao, Diola Bagayoko

ZnSb has been studied intensively in recent years and has shown promising features for thermoelectric applications. The figure of merit has been reported to be above one. Even though many researchers have investigated ZnSb, there are still features and behaviors of this thermoelectric material that are not well-understood. In this work, we utilized a first-principle full potential and an all electron method to calculate the electronic structure of ZnSb, which has an orthorhombic P/bca structure with Zn and Sb both in 8(c) positions. We used a density functional theory potential and the linear combination of atomic orbitals (LCAO) formalism. The calculated indirect band gap of ZnSb is about 0.56 eV; it is located at non high symmetry points and agrees with the experimental finding of 0.53 eV. The smallest direct gap, at the X point, is 0.89 eV. The calculated electron and hole effective masses in ZnSb are also consistent with the reported data from experimental works. This work was funded in part by DOE (Award # DE-NA0003679), NSF (Award # HRD 1736136) and ARO (Award # W911NF-15-1-0483).

T60.00054: Chiral magnetic effect in the absence of Weyl node

Ming-Che Chang, Min-Fong Yang

The nodal points in a Weyl semimetal are generally considered as the causes of the chiral anomaly and the chiral magnetic effect (CME). Employing a linear-response analysis of a two-band lattice model, we show that the Weyl nodes and thus the chirality are not required for the CME, while they remain crucial for the chiral anomaly. Similar to the anomalous Hall effect, the CME results directly from the Berry curvature of energy bands, even when there is no monopole source from the Weyl nodes. Therefore, the phenomenon of the CME could be observed in a wider class of materials.

T60.00055: Magneto-electronic properties of buckled monolayer GaAs nanoribbons

Hsien-Ching Chung

Magneto-electronic properties of buckled monolayer GaAs nanoribbons are studied by the developed generalized tight-binding model, where the edge orientation, buckled structure, multi-orbital chemical bondings, spin-orbit coupling, and magnetic field are considered simultaneously. Three groups of quasi Landau levels (QLLs) near the Fermi level are induced by the magnetic quantization, whose initial energies, degeneracy, energy spacings, and magnetic-field-dependence are investigated. The state probabilities of QLLs exhibit specific oscillation patterns, whose localization centers, node regularities, and energy-dependent variations of the major/minor orbitals are analyzed. The given density of states directly reflects the main characteristics of the QLL energy spectra in the structure, height, number, and frequency of the QLL peaks. The external-field-controlled gap modulations are explored in detail. These predicted magneto-electronic properties could be verified by scanning tunneling spectroscopy measurements and are helpful in designing electronic devices made of low-dimensional materials.

T60.00056: Dynamics and localization of dressed Schrodinger and Relativistic Dirac electron states in graphene

Godfrey Gumbs, Andrii Iurov, Danhong Huang, Liubov Zhemchuzhna

We have investigated the dynamics of single particle in a space-localized but periodically varying time-dependent potential $V(x,t)=\pm V_0 a \delta(x)\cos(\omega t)$ with frequency ω.
This potential may be applied to either Schr\"odinger or relativistic Dirac particles. Both numerical and semi-analytic solutions have been obtained for specific initial conditions for the probability
distribution of the particle originally around a localization center. For negative potential, we solve a bound-state problem, whereas for positive potential, the particle is scattered from a time-dependent potential barrier. From a physical point of view, this problem is relevant to space-localized electron-dressed states for a Dirac particle interacting with linearly-polarized light.

T60.00057: Ab-initio calculations of electronic, transport and bulk properties of pyrite FeS_2

Dipendra Banjara, Yuriy Malozovsky, Lashounda Franklin, Diola Bagayoko

We present results from *ab-initio*, self-consistent density functional theory (DFT) calculations of electronic, transport, and bulk properties of cubic iron pyrite (FeS_2). Our non-relativistic computations employed the Ceperley and Alder LDA potential and the linear combination of atomic orbitals (LCAO) formalism. We attained the ground state by minimizing the occupied energies with respect to the size of the basis set and the number of iterations (for a given basis set). Our calculated, indirect band gap of 0.96 eV, using a room temperature experimental lattice constant, is in excellent agreement with most accepted experimental one of 0.95 eV. Our calculated bulk modulus of 147 GPa is also in agreement with experiment. The calculated partial densities of states reproduced the experimentally observed splitting of the Fe d bands.

T60.00058: Magnetic interactions among defects on the boron-doped Si(111)-$\sqrt{3} \times \sqrt{3}$ surface

Chang-Youn Moon, Daejin Eom, Ja-Yong Koo

We study the possible magnetism on the Si(111)-$\sqrt{3} \times \sqrt{3}$ surface, which is stabilized for the highly boron-doped samples, using first-principles calculations based on the density-functional theory. When the silicon adatom on top of the boron atom is removed to form a defect structure, three silicon dangling bonds are exposed with half-filled doubly degenerate energy levels in the bandgap, stabilizing the local magnetic moment of 2 μ_B. When there are many such defect structures adjacent each other, they are found to align antiferromagnetically as expected for the exchange interaction among the half-filled orbitals. In the meanwhile, we demonstrate that the ferromagnetism can be stabilized by adjusting the number of electrons, suggesting the possibility towards spintronic applications of this unique silicon surface structure.

T60.00059: Photovoltaic Properties of Aluminum Phosphide Nanoarticles

Iris Varela, Ajit Hira, Jose Pacheco, Tommy Cathey, Ruben Rivera, Alexandra Valdez

We continue our interest in the clusters of semiconductor materials in this investigation of the physical and chemical properties of Al_mP_n cluster ($1 \le m \le 10$, $1 \le n \le 10$). Aluminum phosphide material, usually alloyed with other binary materials, has applications in devices such as light-emitting diodes, besides its use as a pesticide. The goal of this research is to reveal the trends seen in the properties of these clusters that may have implications for technological applications. We used the hybrid ab-initio methods of quantum chemistry, particularly the DFT-B3LYP model, and the Many Body Perturbation Theory (MBPT)/MP2 model, to derive the optimal geometries for the clusters of interest. We compare the calculated binding energies, bond-lengths, ionization potentials, electron affinities and HOMO-LUMO gaps for the various clusters. The optimized geometries that we obtained are various combinations of triangles, squares, rectangles, pentagons and hexagons. For the very small clusters, C_{2v} and D_{2v} symmetries dominate. The values of HUMO-LUMO gap decrease as the cluster size increases. We also investigate the effects of crystal symmetries corresponding to the bulk structures.

T60.00060: Study of silicon based 2D materials Si_2Te_3

Jiyang Chen, Keyue Wu, Xiao Shen, Jingbiao Cui

As an emerging silicon-based two-dimensional (2D) semiconductor, silicon telluride (Si_2Te_3) with unique properties and potential applications in electronics and photonics has recently attracted much attention. We will present our recent studies on this 2D material through both experimental and theoretical investigations. The Si_2Te_3 layered nanostructures was deposited by a Chemical Vapor Deposition process with Si and Te as source materials. Morphology, structure, and optical and electrical properties of the nanostructures were investigated by electron microscopy, x-ray spectroscopy, temperature dependent photoluminescence, and electrical transport measurements. Band gap emission of Si_2Te_3 was observed only at low temperatures while strong defect emission bands were present at room temperature. Electrical measurements of the nanowires showed memristive switching at room temperature, which may have potential applications in memory devices. The mechanism of the memristive switching behavior was further investigated by theoretical calculations.

T60.00061: Direct-Indirect Bandgap Transition in Monolayer MoS_2 under Hydrostatic Pressure

Lei Fu, Yi Wan, Ning Tang, Yi-min Ding, Jing Gao, Jiachen Yu, Hongming Guan, Kun Zhang, Weiying Wang, Caifeng Zhang, Jun-jie Shi, Xiang Wu, Su-Fei Shi, Weikun Ge, Lun Dai, Bo Shen

Monolayer MoS_2 is a promising material for optoelectronics applications thanks to its wide direct bandgap, strong spin-orbit coupling, large Coulomb interaction, and unique valley pseudospin degree of freedom, etc. It has a great potential for applications in spintronics, valleytronics and optoelectronics. The band structure of monolayer MoS_2 is well-known to have a direct gap at K (K') point while the second lowest conduction band minimum is located at L point which may interact with the valence band maximum at K point to make an indirect optical bandgap transition. Here we experimentally demonstrate the direct-to-indirect bandgap transition by measuring the hydrostatic pressure dependent photoluminescence spectra at room temperature for monolayer MoS_2. With increasing pressure, the direct transition shifts at a rate of 49.4 meV/GPa while the indirect transition shifts at a rate of -15.3 meV/GPa. We experimentally extract the critical transition point at the pressure of 1.9 GPa, in agreement with first-principles calculations. Combining our experimental observation with first-principles calculations, we prove that this transition is caused by the K-Λ crossover in the conduction band.

T60.00062: Characterization of Novel Optical Limiters

Donald Sakowicz, Tristan Naranjo, Joshua Reding, Kimberly de La Harpe

We report on the nonlinear response of III-V semiconductors and platinum-based dyes. The strong two-photon absorption of these materials results in a nonlinear response to increasing light intensity, resulting in self-focusing as well as increased absorption. We investigated p-type GaSb and GaAs in the SWIR and platinum-containing dyes at 532 nm using 10 ns pulses. We report the nonlinear index of refraction and the two-photon absorption coefficients of these materials using the z-scan technique. This study will help inform the ongoing assessment of these materials as passive optical limiters and the development of new materials.

T60.00063: Impact of Scratch Speed on Interface Adhesion of Thin Films
Vijaya Rana, Jay Mody, Brian Hara, Jeffrey Riendeau

As we extend towards lower technology nodes (<14nm), low-k dielectric materials (k<2.7) are widely used to reduce the RC parasitic signal losses. One way to obtain this lower-k value is by the introduction of porosity to the material structure. However, these porous materials have reduced mechanical integrity and adhesion strength thus exhibits significant processing challenges. To measure the mechanical integrity of low-k thin films, we routinely utilize nanoindentation to determine mechanical properties such as hardness and modulus. To measure adhesion failure, a Four Point Bend Test (FPBT) is utilized to determine the strain energy release rate. However, the FPBT is time-consuming and can introduce variability in results from sample preparation. Hence, we propose the Nanoscratch (NST) that exhibits tremendous potential for reducing the time needed to measure the thin film adhesion properties. We have observed that the NST does not require extensive sample preparation and thus eliminates the variability factor arising from sample preparation. In this study, we employ a ramped load NST using a conical probe equipped with a standard transducer. The effect of scratch speed on the Critical Nanoscratch Load is studied to understand the adhesion failure of the low-k thin films.

T60.00064: Bloch-Grüneisen nonlinearity of electron transport in GaAs/AlGaAs heterostructures
Anthony Hatke, Oleg Raichev, Michael Zudov

We report on nonlinear transport measurements in a two-dimensional electron gas hosted in GaAs/AlGaAs heterostructures. Upon application of direct current, the low-temperature differential resistivity acquires a positive correction, which exhibits a pronounced maximum followed by a plateau. With increasing temperature, the nonlinearity diminishes and disappears. These observations can be understood in terms of a crossover from the Bloch-Grüneisen regime to the quasielastic scattering regime as the electrons are heated by direct current. Calculations considering the interaction of electrons with acoustic phonons provide a reasonable description of our experimental findings.

T60.00065: Optical and Electrical Properties of Formamidinium Lead Bromide Perovskite LEDs
Roy Sfadia

The need for more energy-saving optoelectronics is ever-present. Perovskite light-emitting diodes (PeLEDs) are promising candidates in this regard. They are efficient, easily tunable, and have high color purity. Even more important, they do not require the energy-costly fabrication conditions and processes that traditional semiconductors do. PeLEDs' simple solution-based processing, even at ambient temperatures and pressures, is found to produce highly crystalline structure. However, perovskite devices suffer from short lifetimes. This work studies the optical and electronic properties associated with the degradation of formamidinium lead bromide PeLEDs. Specifically, we aim to optimize device architecture and efficiency, while also measuring the degradation of such optimizations. We use photothermal deflection spectroscopy (PDS) to longitudinally investigate trap states in the material as a function of device architecture. Fourier-Transform Infrared Spectroscopy also provides insight to the degradation of our devices.

T60.00066: Defect Characterization of Organic Photovoltaics
Fernando Ayala, Tyler Jones, Yannai Kashtan, Katheryn Kornegay, Sabrina Li, David Tanenbaum, Janice Hudgings

Polymer based organic photovoltaic devices (OPVs) have attracted a great deal of interest because of their mechanical flexibility, tunable material properties, and potentially low cost, with demonstrated efficiencies of up to 10.6% [1]. However, non-uniformities and defects can decrease the operating efficiency, and exposure to oxygen and moisture under working conditions can progressively degrade the cells over time. In this work, we demonstrate the use of highly spatially resolved thermoreflectance imaging to examine electrical shunts and other defects in P3HT-based devices. Examining the thermal signature of a defect in response to sweeping the cell bias conditions, together with more conventional means of characterization including IV curves and electroluminescence imaging, provides a powerful tool for characterizing the types and physical origin of defects present in the cells.

[1] Gang Li, Rui Zhu, and Yang Yang, "Polymer Solar Cells," Nature Photonics, vol. 6, March 2012, pp.153-161.

T60.00067: Charge Carrier Transport in Organic Field-Effect Transistors
Ricardo Espinoza, Ana Sofia de Olazarra, Laura Parker, Kara Martin, Kenneth Carter, Janice Hudgings

Organic optoelectronic devices such as organic field-effect transistors (OFETs) show great promise as competitive alternatives to silicon-based electronics due to demonstrated advantages from a cost and manufacturing standpoint, as well as enabling a new generation of technologies such as flexible integrated optoelectronic devices. However, charge-carrier transport in organic materials is not well-understood, preventing realization of the full potential of organic devices. The objective of this work is to use OFETs with a poly(3-hexylthiophene) (P3HT) active semiconducting layer as a model system for investigating charge-carrier transport in this material. Current-voltage curve measurements of our initial devices show an average charge-carrier mobility of 3.18 x 10^{-5} $cm^2/(V*s)$, which is about 10x smaller than lowest literature values ranging from 10^{-4} to 10^{-1} $cm^2/(V*s)$. In addition, we have developed a technique called Modulated-Amplitude Reflectance Spectroscopy (MARS) imaging, which can be used to create a spatially resolved map of charge-carrier distribution in the organic, semi-conducting layer of OFETs [1].

[1] A. R. Davis, L. N. Pye, N. Katz, J. A. Hudgings, and K. R. Carter, Adv. Mater. **26**, 4539 (2014).

T60.00068: Imperceptible and Ultra-flexible P-type Transistors and Macroelectronics Based on Carbon Nanotubes
Xuan Cao, Qingzhou Liu, Chongwu Zhou

Flexible thin-film transistors based on semiconducting single-wall carbon nanotubes are promising for flexible digital circuits, artificial skins, radio frequency devices, active-matrix-based displays, and sensors due to the outstanding electrical properties and intrinsic mechanical strength of carbon nanotubes. Nevertheless, previous research effort only led to nanotube thin-film transistors with smallest bending radius down to 1 mm. In this paper, we have realized the full potential of carbon nanotubes by making ultra-flexible and imperceptible p-type transistors and circuits with bending radius down to 40 μm. In addition, the resulted transistors show mobility up to 12.04 $cm^2V^{-1}{}_S{}^{-1}$, high on-off ratio (~10^6), ultra-light weight (< 3 g/m^2), and good mechanical robustness (accommodating severe crumpling and 67% compressive strain). Furthermore, the nanotube circuits can operate properly with 33% compressive strain. Based on the aforementioned features, our ultra-flexible p-type nanotube transistors and circuits have great potential to work as indispensable components for ultraflexible complementary electronics.

T60.00069: Low dimensional semiconductor for electronic and optoelectronic device applications
Hyosun Lee, Hyun Tae Choi, Do Kyung Hwang

Low dimensional semiconducting materials such as colloidal quantum dots (QDs) and two-dimensional van der Waals (2D vdWs) atomic crystals are an emerging class of new materials that can provide important resources for future electronics and materials sciences due to their unique physical properties.
In the first part, we report on a new approach to fabricate PbS QD sensitized IGZO hybrid phototransistors for cost-effective NIR detection. The PbS QD can be functionalized directly onto the surface of the IGZO TFT to create a new bi-functional optoelectronic device: a gate-tunable, highly sensitive, and easily integrated NIR-sensing three-terminal phototransistor. In the second part, we report on a high performance MoS_2 and BP nanosheet based nonvolatile memory transistors with polymer ferroelectric top gate insulator. The MoS_2 ferroelectric field-effect transistor (FeFET) shows a highest linear electron mobility value of 175 cm^2/Vs with a high on/off current ratio more than 10^7, and memory window more than 15 V. Our BP ferroelectric FETs (FeFETs) also exhibit a clear memory window of 15 V and a highest linear mobility value of 1159 $cm^2V^{-1}s^{-1}$ with a 10^3 on/off current ratio at room temperature in ambient air.

T60.00070: Van der Waals Heterostructures Based on Two-dimensional Materials
Shengman Li, Yanqing Wu

Two-dimensional (2D) layered materials offer a platform to build well-designed heterostructures due to their weak van der Waals interactions between each individual layer and dangling-bond-free surface. It is therefore possible to assemble high quality and multifunctional heterostructures using different 2D materials. Herein, a high performance gate tunable P-I-N heterojunction has been demonstrated using BP/WSe_2 /MoS_2 system, where the PN junction is unintentionally formed by p-type BP and n-type MoS_2, and WSe_2 thin film acts as photo carrier generation layer and carrier transportation layer. With well-designed bandgap alignment, such van der Waals heterostructure shows versatile applications integrated in one single device, including high performance optoelectronic photodetector and logic inverter. When under illumination, excellent photoresponse has been demonstrated, covering 10^3 large photocurrent-to-dark current ratio and 10^9 Jones of specific detectivity at zero bias. As a vertical complementary inverter, this device exhibits decent voltage transfer from logic 1 to logic 0. This work indicates the great potential in future functional optoelectronic applications as well as integrated logic circuits.

T60.00071: Nonvolatile Memory Based on Black Phosphorous
Xiong Xiong

Over the past few years, few-layer black phosphorus (BP) has attracted tremendous research efforts due to their extraordinary properties. The superior ambipolar properties, higher mobility than TMDCs, and comparable drain current modulation up to ~10^5 with TMDCs promises black phosphorus to be a good candidate for future flexible and transparent memory devices. In this work, we demonstrated floating memory devices based on BP FETs with patterned local bottom gate geometry and another BP nanosheet as charge trapping layer on a silicon substrate. As expected, the devices shown a significant hysteresis and a substantial memory window thanks to the superior trap capacity of the BP bottom gate stack. Meanwhile, a robust program/erase ratio of over ~10^3 and a stable endurance of more than 1000 s have been achieved. Moreover, a memory circuit of a resistive-load inverter was demonstrated. Therefore, nonvolatile memory based on black phosphorous film opens one possible way to fabricate high-performance nonvolatile memories and inverter logic circuits.

T60.00072: Nonvolatile Memory Based on Few-layer Black Phosphorous
Xiong Xiong, Yanqing Wu

Over the past few years, few-layer black phosphorus (BP) has attracted tremendous research efforts due to their extraordinary electronic and optical properties. In this work, we demonstrated floating-gate memory devices based on BP transistors with pre-patterned local-gate structures and another BP film as charge trapping layer on a silicon substrate. As expected, the devices exhibited a significant current hysteresis and a substantial memory window thanks to the superior trapping

capacity of the BP floating gate. Meanwhile, a robust program/erase ratio of over ~10^3 and a stable endurance of more than 1000 s have been achieved. Moreover, a memory circuit of a resistive-load inverter was demonstrated. Therefore, nonvolatile memory based on black phosphorous film opens a new possibility to fabricate high-performance nonvolatile memories and inverter logic circuits.

T60.00073: Quantum electronic transport in InAs semiconductor nanowire

Rak-Hee Kim, Nam-Hee Kim, Hong-Seok Kim, Jindong Song, Yong-Joo Doh

InAs nanowire provides a useful platform for developing high-mobility quantum electronic devices. In particular, the InAs nanowires, grown by high vacuum molecular beam epitaxy, exhibit conductance quantization behavior at low temperature, which is a signature of quasi one-dimensional (1D) electronic transport. When the magnetic field is applied, the spin degeneracy in the 1D subbands can be lifted due to the Zeeman effect. The strong spin-orbit interaction in InAs also can induce spin splitting of conduction subbands. Those electronic properties are essential to build 1D topological superconducting system in the nanowire. Here we report quantum electronic transport properties of InAs nanowire with varying gate voltage, temperature and magnetic field.

T60.00074: SUPERCONDUCTIVITY

T60.00075: The Study of Quantum Critical Point In $BaFe_{2-x-y}Ni_xCr_yAs_2$ Based Superconductors

Xiaoyan Ma, Dongliang Gong, Shiliang Li

Previous studies have shown that iron based superconductors may have antiferromagnetic and nematic quantum critical points, but it can not be observed directly due to the presence of superconductivity. Our previous works have shown that superconductivity in the $BaFe_{2-x}Ni_xAs_2$ system can be suppressed by dopping a small amount of chromium. At the same time, the antiferromagnetic order changes from incommensure to commensure, from short-range to long-range. Therefore, the antiferromagnetic and the nematic quantum critical points may be studied by completely suppressing superconductivity. In this poster, I will show our recent results of the antiferromagnetic and nematic phases on the chromium dopped $BaFe_{2-x}Ni_xAs_2$ by the electron resistance measurement.

T60.00076: Anisotropy of the Seebeck and Nernst coefficients in $BaFe_2As_2$ and $CaFe_2As_2$

Marcin Matusiak, Michal Babij, Thomas Wolf

In-plane anisotropic longitudinal and transverse thermoelectric phenomena in the parent compounds of iron-based superconductors are studied. Namely, the Seebeck (S) and Nernst (ν) coefficients were measured in detwinned $BaFe_2As_2$ and $CaFe_2As_2$ single crystals in the temperature range 10 – 300 K. The thermoelectric response shows sizeable anisotropy in the spin density wave (SDW) state for both compounds, while dissimilarities in the vicinity of the SDW transition can be attributed to different order of the phase transition in $BaFe_2As_2$ and $CaFe_2As_2$. Temperature dependences of S and ν can be manifestations of an influence of highly mobile, perhaps Dirac, electrons in the two-band model. The Dirac band seems to be rather isotropic, whereas most of the anisotropy in transport phenomena could be attributed to “regular” hole-like charge carriers. We also observe that the off-diagonal element of the Peltier tensor α_{xy} differs between *a* and *b* orthorhombic axis, which indicates that the widely used Mott formula is not applicable to the SDW state of iron-based superconductors.

T60.00077: Anisotropic Superconducting Properties and Pressure Effects in 1144-Structure-Type Pnictides

Kalyan Sasmal, Christian Wolowiec, Zackary Rehfuss, Yuankan Fang, Naveen Pouse, Alexander Breindel, Trevor Keiber, Sheng Ran, M Brian Maple

New Fe-based CaK-1144 superconductors (Fe-SC's) with T_c ~ 35 K were recently discovered. We grew phase-pure 1144 superconducting single crystals out of a quaternary molten solution of FeAs, self-flux. The crystal structure is determined by x-ray diffraction. The effects of pressure on T_c and the collapsed tetragonal phase transition are studied. In the superconducting state, temparature dependent magnetization and resistivity were measured under magnetic fields at different angles with respect to the basal plane. Lower critical field (H_{c1}), superfluid density (ρ_s), critical current densities, and the London penetration depth are extracted from magnetization data. Upper critical field (H_{c2}) and Irreversible field (H_{irr}) are determined by resistive transitions along *c* and *ab* directions. Various pairing gap functions were fit to the normalized $\rho_s(T)$ and specific heat data, and are compared with the nodeless two gap $s^{\pm}$ wave pairing symmetry reported by μSR and ARPES measurements. Normal-state magnetic susceptibility with characteristic *T*-dependence are used to discuss the possibility of antiferromagnetic spin fluctuations as the pairing mechanism in 1144 Fe-SC's will be presented.

T60.00078: Fourfold ab-plane torque symmetry in the superconducting state of BaFe1.82Ni0.18As2

Wei Liu, Mahmoud Abdel-Hafiez, Gang Mu, Huiqian Luo, Peigang Li, Tao Hu, Hong Xiao, Xiao-Jia Chen

We performed in-plane angular dependent torque measurements on an overdoped iron-based superconductor Ba2Fe2-xNixAs2 with x=0.18 both in the normal state and mixed state. The torque signal were measured in both clockwise and counter-clockwise rotating directions. The reversible torque is the average of the torque data measured in two rotating directions which allows the determination of thermodynamic properties. A fourfold symmetry is observed in the reversible part of the superconducting torque, which disappears when superconductivity vanishes. So we concluded that in the overdoped part of the phase diagram, torque measurements reveal signatures of a fourfold symmetry of the superconducting gap structure. In addition, the specific heat results support the existence of nodes in the gap structure. Hence, our results point to a possible d wave pairing symmetry.

T60.00079: Ultrafast Dynamics Evidence of High Temperature Superconductivity in Single Unit Cell FeSe on $SrTiO_3$

Jimin Zhao

We report the time-resolved excited state ultrafast dynamics of single unit cell (1 UC) thick FeSe films on $SrTiO_3$ (STO), with FeTe capping layers. By measuring the photoexcited quasiparticles' density and lifetime,we unambiguously identify a superconducting (SC) phase transition, with a transition temperature Tc of 68(-5/+2) K and a SC gap of Δ(0) = 20.2±1.5 meV. The obtained electron-phonon coupling strength λ is as large as 0.48,demonstrating the likely crucial role of electron-phonon coupling in the high temperature superconductivity of the 1 UC FeSe on STO systems.We further find a 0.05 THz coherent acoustic phonon branch in the capping layer, which provides an additional decay channel to the gluing bosons.If time permits, I will also address our recent progress in other superconductors.

T60.00080: Asymmetric Josephson Effect in WTe2 Weyl Semimetal

Yongbin Choi, Chui-Zhen Chen, Kumari Gaurav Rana, Mazhar Ali, Kam Tuen Law, Kin Chung Fong, Gil-Ho Lee

WTe_2 is predicted to be Type-II Weyl semimetal, hosting Weyl nodes at the contact of electron and hole pockets in a momentum space. We studied electronic transport properties of the Josephson effects mediated by WTe2 Weyl semimetal. Proximity Josephson junctions were fabricated by depositing a pair of superconducting electrodes on exfoliated WTe2 layers. Perpendicular magnetic field dependence of Josephson critical current, $I_c(B)$, (so-called Fraunhofer pattern) exhibited anomalous behaviors: 1) Slow decay of I_c lobes as B increases indicates that the transport is dominated by edge channels of WTe_2 layer. 2) Asymmetric Fraunhofer pattern, i.e. $I_c(B) \neq I_c(-B)$, suggests asymmetric Fermi velocity of each edge channel due to the inversion symmetry breaking of WTe_2.

T60.00081: Hysteresis in the I-V characteristics of overdamped topological Josephson junctions

Zhao Huang, Jia-Jin Feng, Qi-Feng Liang, Zhi Wang

We consider two one-dimensional topological superconductors with four Majorana modes gamma_{1,2,3,4}, where gamma_2 and gamma_3 are coupled by an overdamped Josephson junction and thus form a two-level system with their energy difference dependent on the Josephson phase shift phi. We find a hysteresis in the I-V characteristics which is the consequence of the Landau-Zener effect at finite V where phi oscillates, while this hysteresis disappears in the topological trivial regime due to absence of the two energy levels. This hysteresis is not blurred in presence of other channels for tunneling of Cooper-pairs in the Josephson junction, thus serving as a useful signature for the experimental search of Majorana modes.

T60.00082: Entanglement dynamics of Majorana fermions in one dimension

Takumi Ohta

We study the ground-state phase diagram and dynamics of one-dimensional Kitaev model of spinless *p*-wave superconductor with several competing interactions. We first map out the ground-state phase diagram of the model and characterize the phases by the edge modes, the correlation functions, and the entanglement spectrum. We then investigate the dynamical properties during interaction sweeps across the critical point using the time-dependent Bogoliubov theory. When the sweep speed is slow compared to the typical time scale at the critical point, both correlation function and entanglement entropy exhibit spatially periodic structures after the system passes the critical interaction strength. On top of this, we find that the degeneracy structure of the entanglement spectrum changes in time during the sweep. [1] By explicitly calculating the above quantities for excited states, we attribute these behaviors to the Bogoliubov quasiparticles excited near the critical points. We also show that the entanglement spectrum reflects the pattern of the Majorana correlation for the excited states.
[1] T. Ohta, S. Tanaka, I. Danshita, and K. Totsuka, Phys. Rev. B **93**, 165423 (2016).

T60.00083: Symmetry classes and Topological properties of 1D Superconductors

Sayonee Ray, Subroto Mukerjee

We study the topological phases and the emergence of Majorana bound states (MBS) at the edge of 1D spinless p-wave superconductor (SC). We classify these systems according to the tenfold scheme on the basis of their topology, resulting from the presence or absence of discrete symmetries. The simplest system we study belongs to the BDI symmetry class, with *Z* topological invariant and integer number of edge modes. This is reflected by the presence of MBS doublets at the edges. In our analysis, we have considered two types of spinless p-wave pairing with the same and opposite signs of p-wave order parameter for the two spins. We study the type of edge states for these two cases for different values of the chemical potential (measured with respect to the SC gap). For μ>1/2, these MBS have an oscillating part along with a decay part. For 0<μ<1/2, they are purely decaying. Adding perturbations like s-wave pairing and Zeeman fields induces transitions from one topological class to another. We show that there are 3 symmetry classes for the first type of pairing and 6 for the second, with these perturbations. We also analyse the possible perturbations and their combinations, which can place the system in the above number of classes, for each of the two cases.

T60.00084: Pairing states of spin-3/2 fermions: Symmetry-enforced topological gap functions

J.W.F. Venderbos, Lucile Savary, Jonathan Ruhman, Patrick Lee, Liang Fu

This talk reports on a study of the topological properties of superconductors with paired j = 3/2 quasiparticles. We obtain a comprehensive symmetry-based classification of topological pairing states in systems with higher angular momentum Cooper pairing. Our study consists of two main parts. First, we develop the

phenomenological theory of multicomponent (i.e., higher angular momentum) pairing by classifying the stationary points of the free energy within a Ginzburg-Landau framework. Based on the symmetry classification of stationary pairing states, we then derive the symmetry-imposed constraints on their gap structures. We find that, depending on the symmetry quantum numbers of the Cooper pairs, different types of topological pairing states can occur: fully gapped topological superconductors in class DIII, Dirac superconductors and superconductors hosting Majorana fermions. Notably, we find a series of nematic fully gapped topological superconductors, as well as double- and triple-Dirac superconductors, with quadratic and cubic dispersion, respectively. Our approach, applied here to the case of j = 3/2 Cooper pairing, is rooted in the symmetry properties of pairing states, and can therefore also be applied to other systems with higher angular momentum and high-spin pairing.

T60.00085: Unidirectional Majorana Edge Mode in 2D Chiral Superconductor with Apllied Supercurrent

Xuzhe Ying

2D chiral superconductor is known to support chiral Majorana modes. Those modes are localized at the boundary and are gapless while the bulk remains fully gapped. In this report, I will show that by applying a supercurrent, a transition from gapped to gapless bulk states is possible. At the same time, the edge modes could survive the gap closing process and have the same chirality for opposite edges. Those modes are known as unidirectional Majorana modes. It could argue that those states are stable according to the theory of classification of Fermi surfaces.

T60.00086: Bursting at the Seams: Rippled Monolayer Bismuth on NbSe2

Carolina Adamo, alan fang, S. Jia, Robert Cava, Aharon Kapitulnik

One of the heaviest semimetals in nature, bismuth ignited the interest of the materials-physics community for its potential impact on topological quantummaterial systems that utilize its strong spin-orbit coupling (SOC) and unique orbital hybridization. In particular, recent theoretical predictions of unique topological and superconducting properties of thin bismuth films and interfaces prompted intense research on the growth of sub- to a few monolayers of bismuth on different substrates. Similar to bulk rhombohedral bismuth, the initial growth of bismuth films on most substrates results in buckled hexagonal bilayers that either grow in the (111) or (110) directions, with a lattice constant close to that of the bulk. By contrast, in this paper we show a new unpredicted growth paradigm for bismuth monolayers. Using a freshly cleaved NbSe2 as a substrate, we show that the initial growth of Bi can strongly bond, 1 while conforming to the lattice constant of the top Se-layer of NbSe2, resulting in a compressed two-dimensional triangular lattice. The enormous strain is relieved during growth by developing a unique pattern of ripples and local strain, which also introduces strong marks on the electronic properties at the surface.

T60.00087: Effect of Li_2O on the microstructure, magnetic and transport properties of Tl-2223 superconductor

Fnu Shipra, Athena Sefat

The presentation will provide an account of the effect of Li_2O on the ease of phase formation and superconducting properties of $Tl_2Ba_2Ca_2Cu_2O_{10+5}$ (Tl-2223) material. Li substitution only slightly decreases the superconducting transition temperature, while the optimal concentration of 20% doping improves the critical current density (J_c) by ~ two fold. We found substantial effects on the synthesis temperature, microstructure and normal state transport properties of Tl-2223 with Li_2O addition. Short-time thermal annealing under flowing Ar+4%H_2 (1 hr.) further improves the superconducting volume fractions, as well as J_c.

T60.00088: The Effect of Disorder on the Superconducting Gap in 2d Systems

Gautam Rai, Malte Roesner, Stephan Haas

The effect of disorder on superconductivity has been a tempting avenue of study for scientists for many years. However, direct numerical computation of characteristic quantities such as the superconducting gap is traditionally limited by the large dimensions that are required for the system to have true disorder. We apply the recently developed Kernel Polynomial method as an approximate diagonalization technique to 2 dimensional superconducting Hamiltonians which improves the size of systems that can be studied from D = 10^5 to D=10^9. We present a scheme to extract the superconducting gap from the approximate density of states and benchmark our method with well understood simple systems. Lastly, we apply this method to disordered systems with the disorder coming from impurity-based perturbations added to homogeneous materialistic Hamiltonians.

T60.00089: Thermally Jammed States in Superionic Conductors

Dillon Sanders, Jacob Eapen

Superionic solids exhibit a significant increase in ionic conductivity within a certain temperature range. Studies of superionic conductors have shown the presence of dynamical heterogeneity (DH) among the mobile ions in these systems, in which groups of ions exhibit different dynamical behavior than those in nearby regions, a feature also observed in supercooled liquids. Using atomistic simulations in conjunction with the two-phase thermodynamic (2PT) method that models a system as a superposition of hard spheres (gas) and a harmonic oscillators (solid), we quantify the thermal packing fraction φ of the oxygen ions of UO_2, which exhibits superionic properties at temperatures above 2000 K. Our analysis shows that at temperatures near 2000 K, the O ions are in a jammed state with φ close to that of a random close-packed configuration (~0.64). Interestingly, at the λ-transition temperature of ~2600 K, φ for O ions attains a value corresponding to a cubic lattice (~0.52), which is consistent with the sub-lattice structure of the oxygen ions. Our work provides an alternate direction for investigating the disordering process in superionic conductors and solid materials that have significant thermal disorder.

T60.00090: Chiral p+ip triplet states existing in the graphene sandwiched by even-parity superconductor and ferromagnet

Shih-Jye Sun, Hsiung Chou

We proposed a sandwiched structure odd-parity superconductor/graphene/ferromagnet and theoretically investigated the triplet superconductivity in the hole-doped graphene. In our theory the superconducting and Kondo interactions are arose from spin fluctuations and ferromagent, respectively, and both interactions fall in a competition. Our calculations have confirmed that the triplet superconductivity is p+ip chiral state as shown in fig. 1. Our theory predicts that the critical supercurrent of the sandwiched sample varying with the magnetic field would increase to saturation in the beginning then gradually decrease to the end. The sandwiched structure is composed a buffer layer of graphene which provide an accommodation for triplet superconducting pairs to maintain. We believed that the sandwiched sample is better than the heterostructure, i.e., even-parity superconductor/ferromagnet, which could increase the possibility for detecting the triplet superconductivity.

T60.00091: Effect of Rattling Phonon on Superconductivity of KOs_2O_6

Samin Tajik, Bozidar Mitrovic

We model the electron coupling to anharmonic (rattling) mode in β-pyrochlore superconductor KOs_2O_6 by a sharply peaked electron-phonon coupling function centered at the mode energy. The strong-coupling Eliashberg equations are solved for the transition temperature and the gap function for a series of temperatures below T_c. From these solutions we obtain the temperature dependence of the gap edge, the nuclear magnetic resonance (NMR) relaxation rate and the microwave conductivity for several values of the electron-phonon coupling
parameter. The result are compared with the available experimental results.

T60.00092: Magnetic and Crystalline Electric Field Effect in $Lu_{1-x}Dy_xNi_2B_2C$ System

Wonchoon Lee

To investigate the interplay between magnetism and superconductivity, we have analyzed the magnetic isotherms curves of dilute magnetic systen such as $Lu_{1-x}Dy_xNi_2B_2C$ (x = 0 ~ 1.0) single crystals at high applied magnetic fields parallel and perpendicular to the crystallography c-axis and various low temperature. All above isostructural compounds show some magnetic transitions in magnetization isotherms at certain applied magnetic fields and temperatures above and below Neel and superconducting temperatures (T_N, T_C) where T_N/T_C varies systemetically. Comparing our results by using theoretical group analysis to the energy scheme of crystalline electric field of magnetization anisotropy at various temperatures, we have obtained some temperary low energy levels such as singlet Γ_4 and some excited Γ_5 and Γ_1. Our energy scheme analysis shows qualitative agreement between theoretical caculation and experiments only at high magnetic fields, but disagreement for x > 0.7 regime.

T60.00093: Superfluid and critical current densities of underdoped YBa$_2$Cu$_3$O$_{6+x}$ cuprates

Patricia Salas Casales, Miguel Solis

T60.00094: Abstract Withdrawn

Surface potassium dosing has recently been proven to be an effective method in tuning the electron doping and enhancing the superconducting transition temperatures in both iron chalcogenides and electron doped iron pnictides. However, it remains unknown how surface potassium dosing can affect the hole doping and superconductivity in hole doped Fe-based superconductors. Here we performed K-dosing on $Ba_{0.5}K_{0.5}Fe_2As_2$, a prototypical hole-doped iron pnictide compound, and explored the electronic structure by *in situ* ARPES measurements. Starting from the slightly over-doped $Ba_{0.5}K_{0.5}Fe_2As_2$ surface, K-dosing gradually drives the material towards optimal doping and enhances the superconductivity. Intriguingly, the increasing of superconducting gap size does not slow down at the optimal doping, and the gap further increases with K dosing even when the doping effect is saturated. Meanwhile, the scattering rate of the inner hole pockets at the zone center is reduced by higher K concentration. Our results indicate that the enhanced superconductivity by K-dosing is a collaborative effect of electron doping and reduced scattering.

T60.00095: Muon-Probing sites and states in MgO and GdBCO

Carolus Boekema, M Dam, I Lin, S Welch, A Mahajan

A computational model is used to locate the muon sites in MgO. The positive muon localizes in a vacant oxygen tetrahedron. This work supports μSR MgO [1] & MnO studies. For MnO, one μ^+ signal is observed. [2] In MgO, an extra sharp signal has been seen, suggesting extended O[-1] states. [1] Shekhter *et al* [3] found, the μ^+ reduces strongly cuprate loop currents. [4] Site-search calculations for $RBa_2Cu_3O_{7-5}$ (RBCO) [5] generated candidate Balmer (Bi) and Lin (Li) muon sites. These sites are ~1 Å away from O^{2-} ions in *insulating* regions. The B_i sites are near the BaO layer and are observed; [5] B2 is the favorite site. The L_i sites are near the CuO-chain layer and rarely cited. [4] Our ME-TF-μSR [6] GdBCO study confirms, muons probe away from the superconducting CuO_2 planes.
1] C Boekema *et al,* APS March meeting (2016). [2] YJ Uemura *et al*, Hpf Int 17-19 (1984) 339. [3] A Shekhter *et al*, Phys Rev Lett 101 (2008) 227004. [4] C Boekema *et al,* Physica C49 (2013) 136; T Songatikamas *et al*, J Supercond & Novel Magn 23 (2010) 793. [5] WK Dawson *et al*, J Appl Phys 64 (1988) 5809; Hpf Int 63 (1990) 219. [6] C Boekema & MC Browne, MaxEnt 2008, AIP Conf Proc #1073 p260.

T60.00096: Complementary response of static spin-stripe order and superconductivity to non-magnetic impurities and pressure in cuprates

Zurab Guguchia, Bertrand Roessli, Rustem Khasanov, Alex Amato, Ekaterina Pomjakushina, Kazimierz Conder, Yasutomo Uemura, John Tranquada, Hugo Keller, Alexander Shengelaya

Cuprate high-temperature superconductors (HTSs) have complex phase diagrams with multiple competing ordered phases. Understanding to which degree charge, spin, and superconducting orders compete or coexist is paramount for elucidating the microscopic pairing mechanism in the cuprate HTSs. In this talk, i will report some novel results of muon-spin rotation (μSR), neutron Scattering and magnetization experiments on non-magnetic Zn impurity and hydrostatic pressure effects on the static spin-stripe order and superconductivity in the La214 cuprates [1]. Remarkably, it was found that in these systems the spin-stripe ordering temperature T_{so} decreases linearly with Zn doping y and disappears at y ≈ 4%, demonstrating the high sensitivity of static spin-stripe order to impurities within a CuO_2 plane. Moreover, T_{so} is suppressed in the same manner as the superconducting transition temperature T_c by Zn impurities. We also observed the same pressure evolution of both T_c and T_{so} in $La_{2-x}Ba_xCuO_4$, while there is an antagonistic pressure evolution of magnetic fraction and superfluid density. These results indicate that static spin-stripe order and SC pairing correlations develop in a cooperative fashion in La214 cuprates.

[1] Z. Guguchia et. al., PRB **94**, 214511 (2016). PRL **119**, 087002 (2017).

T60.00097: NMR studies of CDW and superconducting gap structure in layered 2H-NbSe2

Douglas Wilson, Garima Saraswat, Parasharam Shirage, Rukshana Pervin, Philip Kuhns, Michael Hoch, Arneil Reyes

Single crystals of layered transition metal dichalcogenide 2H-$NbSe_2$ were probed to investigate the charge density wave CDW (T_{CDW} = 33.5 K) and superconducting states (T_c = 7.2 K) using ^{93}Nb and ^{77}Se nuclear magnetic resonance (NMR). The low temperature quadrupolar ^{93}Nb above H_{c2} shows two broadened Gaussians of unequal amplitude per transition, which is believed to be evidence of a discommensurate CDW phase. In orientations parallel and perpendicular to the applied field H_0, the spin-lattice relaxation (T_1) data of both nuclei reveal Korringa behavior above T_c, an absence of coherence peak, and a linear crossover for $T < T_c$. In both orientations, $1/T_1$ is accurately fit by a two-gap function for relaxation. A field-independent suppression in $1/T_1$ was also observed in both orientations, with deviations from Korringa behavior occurring above T_c and far above H_{c2}, implying the presence of a pseudogap. The field-dependence of T_1 in the SC state shows $1/T_1 \propto H_0$. This behavior most likely originates from the Volovik effect, which suggests 2H-$NbSe_2$ is a two-gap *s*-wave superconductor.

T60.00098: Ultra low-loss sputtered NbN films for microwave applications

Faustin Carter, Trupti Khaire, Tom Cecil, Gensheng Wang, Valentyn Novosad, Volodymyr Yefremenko, Steve Padin, Junjia Ding, Chrystian Posada, Amy Bender, Clarence Chang

We present both fabrication method and measurement details regarding low-loss NbN films fabricated at Argonne National Laboratory. We sputter Nb in the presence of N2 gas, with an RF substrate bias, directly onto high-resistivity Si wafers, and by varying N2 flow rates we control the superconducting critical temperature (Tc) to be between 8-16 K. Coplanar waveguide resonators fabricated by etching these films give quality factors greater than 1E6 at 5 GHz when driven at high power, and quality factors of order 1E4 when loaded with single-photon power levels for all values of Tc. Furthermore, in our highest Tc samples, this excellent quality factor persists at temperatures up to ~2 K. We also report on an anomalous temperature-dependent loss mechanism that affects a portion of our samples and consistently turns on at temperatures above 1 K.

(Author Not Attending)

T60.00099: Loss minimization in superconducting radio frequency cavities by artificial vortex pinning

Ivan Sadovskyy, Andreas Glatz, Alexander Romanenko

AC magnetic fields in a superconducting radio frequency (SRF) cavity may lead to parasitic penetration of magnetic flux into the cavity material. This effect depends on the frequency of the AC filed, the quality of the cavity surface, and the distribution and size of (nanometer-sized) impurities near the surface. We present a numerical study of the energy dissipation near the surface of the superconductor in the external AC field concentrating on the spatial distribution of non-superconducting defects. We employ 3D large-scale time-dependent Ginzburg-Landau approach to simulate the vortex dynamics and consequent energy dissipation. We discuss in details the influence of two generally opposite effects: (i) pinning of frozen and induced vortices by defects in the vicinity of the surface and (ii) reduction of the surface pinning potential by means of the same defects. Our findings reveal the details of flux penetration in the presence of the external AC field and provide a novel recipe for the design of next-generation SRF cavities with high quality factor.

T60.00100: Interplay between topological surface states and superconductivity in SmB6/NbN tunneling junction

Lin Zhu, Zhimin Liao, Dapeng Yu

Superconductivity and topological surface states are both exotic macro-quantum states in condense matter system. We could acquire a lot of new interesting quantum excitations if we let above two quantum states interplay in some appreciate way, such as topological superconductivity and Majorana fermion excitations. In this paper, we mainly study the interplay between Cooper pairs in superconductor NbN and topological surface states in SmB6 through magneto-transport and tunneling spectroscopy. Non-monotonic linear magnetoresistance(MR) was observed at low temperature. MR of NbN/SmB6 junction is positive as B<2T, however, MR turns to negative B>2 T. We predicated exotic interplay between Cooper pairs and topological surface states probably result in above special MR behaviors.

T60.00101: Zero Energy States at a Normal--Cuprate-Superconductor Interface Probed by Shot Noise

Michael Reznikov, Ori Negri, Moran Zaberchik, Gil Drachuck, Amit Keren

We report measurements of the current noise generated in the optimally doped, x=0.15, Au-$La_{2-x}S_xCuO_4$ junctions. For high transmission junctions on (110) surface, we observed a split zero-bias conductance peak (ZBCP), accompanied by enhanced shot noise. The ZBCP disappears and the noise decreases to the noise expected for the charge *e* with heating at temperatures well below T_c, and at voltages much smaller than the bulk superconducting gap, setting a new energy scale of 0.5 mV. We attribute this scale to a subdominant order parameter at the sample surface, which fascilitates Cooper pair transport through a disordered normal metal-superconductor interface.

Another option could be a spontanious breaking of the translational symmetry on (110) surface, and associated with it vortex formation. Motion of the vortices can lead to an excess noise.

T60.00102: Development of a Nanocluster-Graphene Proximity Device

Patrick Edwards, Vitaly Kresin

The study of metal clusters has revealed quantum nanoscale effects unique to the fully size-resolved regime. A highly notable example is electronic shell structure, akin to that in atoms and nuclei, which arises when confined conduction electrons organize into discrete energy levels. One consequence is the possibility of dramatic enhancement in electron Cooper pairing. Recent research from our group has provided evidence of this enhancement in certain free Al clusters, with the electronic transition taking place at a temperature two orders of magnitude above that of bulk aluminum. We now aim to take advantage of this phenomenon by exploring the pairing transition in size-selected nanoclusters soft-landed on an appropriate substrate. For example, a network of such superconducting nanoislands will induce superconductivity in graphene even at low coverages. Theory predicts that an array of clusters will not only support, but even enhance the Josephson current by 2-3 orders of magnitude. We will report on our progress toward the fabrication and characterization of a graphene-nanocluster device for displaying enhanced superconducting transport.

T60.00103: possible negative hubbard U in potassium doped p-terphenyl

Yuhao Gu, Jiangping Hu, Hong Jiang

Recently, a possible organic superconductor, potassium doped p-terphenyl, which was recently reported to exhibit transition temperatures in the order of 120~K, draws people's interests. By optimizing the crystal structure of $KC_{18}H_{14}$, we noticed that half of the p-terphenyl molecules are nearly coplanar while another half of p-terphenyl molecules are still tilted, while our calculation about molecular $K_xC_{18}H_{14}$ shows that benzene rings are almost coplanar in $K_2C_{18}H_{14}$ but tilted obviously in $C_{18}H_{14}$. This intriguing phenomenon indicates that there might be a negative hubbard U in potassium doped p-terphenyl. Through mean field theory, we shows that superconductivity occurs in this possible neagtive-U system at low temperatures.

T60.00104: Element substitution effects on superconductivity and charge density wave of Laves compound ZrV_2

Hirotaka Ishii, Motoki Ogawa, Tadataka Watanabe

Laves-phase compounds ZrV_2 and HfV_2 have C15-type cubic crystal structure, which contains V sublattice of corner-sharing tetrahedra (pyrochlore lattice). These compounds exhibit superconducting and charge-density-wave (CDW) transitions at T_c ~ 9 K and T_{CDW} ~ 120 K, respectively. Concerning the superconductivity of ZrV_2 and HfV_2, the NMR study suggested the presence of point nodes in the superconducting gap. To study element substitution effects on the superconductivity and CDW of ZrV_2 and HfV_2, we investigate structural, electric, and magnetic properties of polycrystalline $(Zr_{1-x}Hf_x)V_2$ and $Zr(V_{1-x}Cr_x)_2$ (x = 0 ~ 1). The experiments reveal that $(Zr_{1-x}Hf_x)V_2$ exhibits superconductivity and CDW order regardless of the Hf concentration x. For $Zr(V_{1-x}Cr_x)_2$, on the other hand, superconductivity and CDW order are found to be suppress with increasing Cr concentration x. These results suggest that, for ZrV_2 and HfV_2, V 3*d* electrons play dominant roles for the occurrence of superconductivity and CDW order. Furthermore, the experiments in $Zr(V_{1-x}Cr_x)_2$ reveal that the Cr doping suppresses the CDW order more sensitively than the superconductivity, which implies that, for ZrV_2 and HfV_2, the superconducting and CDW gaps respectively open on different portions of the Fermi surface.

T60.00105: Unconventional superconductivity in single crystals of the noncentrosymmetric superconductor La_7Ir_3

Daniel Mayoh, Toshiro Takabatake, Don Paul, Geetha Balakrishnan, Martin Lees

In superconductors, the inversion symmetry of the crystal structure plays a central role in the formation of the Cooper pairs. Systems lacking a center of inversion exhibit a nonuniform lattice potential, giving rise to a Rashba-type antisymmetric spin-orbit coupling. This can lead to exotic physics, such as time-reversal symmetry (TRS) breaking, below the superconducting transition temperature, T_c. Until recently, only two NCS compounds, Re_6Zr and $LaNiC_2$, have been shown to break TRS below T_c [1,2]. The nature of the pairing states in these superconductors continues to be a puzzling and challenging question. Now we have discovered a third NCS material, polycrystalline La_7Ir_3, that shows broken TRS below T_c [3]. Here, we report the first growth of single crystals of La_7Ir_3. We present experimental data on these single crystals that shed light on to the unconventional superconducting state of La_7Ir_3. We compare our results with other members of the La_7T_3 (T =

transition metal) family of superconductors and discuss the unconventional superconductivity in this exciting new family of materials.

[1] A. D. Hillier *et al*., Phys. Rev. Lett. **102**, 117007 (2009).
[2] R. P. Singh *et al*., Phys. Rev. Lett. **112**, 107002 (2014).
[3] J. A. T. Barker *et al*., Phys. Rev. Lett. **115**, 267001 (2015).

T60.00106: Multiple Energy Gaps via Soft Point Contact Spectroscopy of Doped $Ba_{(1-x)}K_xFe_2As_2$

Caitlyn McConnell, Oberon Wackwitz, Brett Conti, Luke Conover, Guotai Tan, Yu Song, Chenglin Zhang, Rui Zhang, Ding Hu, Pengcheng Dai, Roberto Ramos

We report progress in our measurements of multiple energy gaps in $Ba_{(1-x)}K_xFe_2As_2$ with different K, Co and P dopings. These iron-based superconductors provide a new platform where multi-band superconductivity can be studied. The observed multiple energy gaps depending on the crystal growth conditions and on which tunneling directions are made accessible during the sample preparation process. We discuss how we have made electrical contact to crystal samples obtained by applying a small amount of silver paint using a sharp-tipped wire and measuring the resulting conductance. We have been moderately successful using this technique and have observed observe peaks and broad shoulders in the conductance - which can correspond to multiple energy gaps; some peaks correlate well with data from oher groups, while other new peaks are unexplained. Finally, we report progress on exploring a micropipette-based delivery of silver paint for more controlled method of contacting crystals. All measurements in this work were performed by undergraduates.

T60.00107: MATTER AT EXTREME CONDITIONS

T60.00108: Breakdown of intermediate range order in AsSe chalcogenide glass

Azkar Saeed Ahmad

As-cast amorphous AsSe (a-AsSe) has been characterized by *in-situ* high pressure XRD and Raman spectroscopy up to the pressure of ~30 GPa using diamond anvil cell together with *ab-initio* molecular dynamics simulations. A gradual densification has been observed under compression along with the breakdown of intermediate range ordering at ~16 GPa. The whole transformation process can be divided into three relatively distinct pressure regimes from 1bar to 7 GPa, from 7 to 16 GPa and beyond 16 GPa. Our XRD results together with Raman spectroscopic studies confirm that in a-AsSe pressure tuning results in network transformations only, without sudden jump in the density. The results obtained by high pressure *ab-initio* molecular dynamics simulations demonstrate the variations in the local structures associated with the experimentally observed transformations. The amorphous-to-amorphous network transformation is found to be reversible upon decompression.

T60.00109: Work in Progress on LLNL's EOS for Metals including Beryllium

Carrie Prisbrey, Christine Wu

We are currently working on updating a number of Equation of State (EOS) tables that have been developed at Lawrence Livermore National Laboratory (LLNL) over 2 decades ago. Some of these EOS tables are still routinely used in hydro-code calculations such as Be EOS for simulating Be capsules in NIF experiments. Over the past decade, much progress has been made toward a better understanding of EOS properties. Experimentally, both static and dynamic high-pressure physics experiments have been carried out to obtain measurements at higher pressure regions. Theoretically, many first principles density functional theory (DFT) and molecular dynamics simulations have been applied to our materials of interest. We aimed to develop multiphase EOSs that would incorporate current experimental data and use the most up-to-date theory where data is not available.

T60.00110: Alkali metal incommensurate phases under pressure: phase trasisitions, stability and electronic structure

Graeme Ackland, Miriam Marques, Hongxiang Zong, Andreas Hermann, Victor Naden Robinson

The free-electron model fails when "free-electron" metals are compressed, leading to the appearance of open and complex structures under pressure. A remarkable and intriguing example are the incommensurate host-guest phases in sodium, potassium, and rubidium under pressure. The "guest" substructure forms chains of atoms interpenetrating the host so that the axial ratio (c_h/c_g) is irrational. For computational studies, commensurate unit cells are used as approximants with c_h/c_g ratios close to those seen in nature. Using commensurate structures with different c_h/c_g ratios, we assess the ability of density functional theory to describe the phase sequence in each alkali metals, and study the pressure evolution of the guest content. Topological analysis of the electron density and the electron localization function (ELF) provides insight into why nature chooses these strange phases: in addition to the guest atoms, tubes of electrons are also found in channels through the guest structure. Which channels contain electrons and which contain guest atoms depends on the material. Finally, we use molecular dynamics to simulate the phase transformation into the host-guest structure, despite its complexity, it is remarkably easy to nucleate and grow.

T60.00111: Study of structural properties of Fe and FeS at conditions of Earth's inner core

Aldemar De Moya Camacho, Carlos Pinilla, Karen Valencia

The observation of seismic waves, composition of meteorites, experimental and computational results of materials at extreme conditions indicate that the Earth's core (320-350GPa and 5000-6500K) is composed mostly of Fe with a less presence of light elements such as Si, C and S of high solubility at these conditions. The inclusion of these elements may explain the difference in density that exists between seismic data and relevant laboratory results. We have performed computational calculations based on functional density theory (DFT) to study structural, magnetic and thermodynamic properties of Fe pure phases at Earth's inner core conditions and so obtain information on thermodynamic stability. We found the hcp phase to be the most stable at inner core conditions as has been reported by many previous works (Alfe et al., 2015, Denoeud et al., 2016). Since S is one of the candidates to be incorporated into the core, this study analysis several solid phases of FeS as well as several liquid and solid solutions of FeS alloys ranging from a S concentration (3.7wt%-16wt%) In the case of solid FeS we found troilite (NiAs) to be the most stable phase at ambient conditions whereas at core conditions a CsCl becomes stable.

T60.00112: Thermoelastic properties of the "new aluminous" (NAL) phase

Michel Marcondes, Chao Yao, Zhongqing Wu, Renata Wentzcovitch

Mid-Ocean Ridge Basalt (MORB) is formed via seafloor spreading at mid-ocean-ridges. It is one of the most important rocks in the Earth's crust. Upon subduction and exposure to high pressures and temperatures (PT), the high Al_2O_3 content in MORB gives rise to a "new aluminous phase" (NAL) responsible for up to 25 w% of its composition. This phase has hexagonal structure, 21 atoms/cell, and is a complex solid solution with chemical formula $XY_2Z_6O_{12}$, where X is a large monovalent or divalent cation, e.g., Na+ or Ca2+, Y is a mid-sized cation, e.g., Mg2+, and Z is Al3+ and/or Si4+. Chemical constraints on its composition may reduce the number of end-member compounds to less than twenty. Using *ab initio* calculations, we model the iron-free NAL phase by considering seven end-members. We perform Quasiharmonic (QHA) calculations to address composition dependent thermodynamic and thermoelastic properties of this phase. These results are essential to investigate the seismic signature of subducted MORB crust into the deep mantle.

T60.00113: AN ATOMISTIC STUDY OF THE INCORPORATION AND DIFFUSION OF NOBLE GASES IN SILICATE MINERALS

Carlos Pinilla, Karen Valencia, Carolina Martinez, Aldemar De Moya, Neil Allan

Trace elements are widely used to unravel magmatic processes and constrain the chemical differentiation of the Earth. Central to this enterprise is understanding the controls on trace element fractionation between solid and liquid phases and thus the energetics of incorporating trace elements into crystals. In this contribution we focus on the incorporation of noble gases into crystals, with implications for the degassing processes in the Earth and the atmosphere. We use ab-initio and force-field methods to study the uptake of noble gases He, Ne and Ar in solid silicates. We calculate atomic defect energies of incorporation both at vacancies and at interstitial positions in the solid. We use these energies to estimate the total uptake of noble gases into the crystal as a function of temperature. Such concentrations are found to be very low (10^{-3} and 10^{-10} ppm) for He up to Ar respectively with the noble gases incorporated predicted to be more favorable at intrinsic vacancies of Si or Mg sites. We also look at the diffusion of these minerals within the lattice and estimate activation energies for such processes. Our results support the hypothesis that noble gases have very low solubilities in bulk solid minerals.

T60.00114: Ab initio calculation of electron - ion temperature relaxation in dense plasmas

Jacopo Simoni, Jerome Daligault

The last ten years have seen tremendous progress in our ability to
form and probe well-controlled warm dense matter conditions in the
laboratory thanks to better drivers and diagnostics.
By their nature, warm dense matter experiments produce transient,
non-equilibrium conditions, and measurements of equilibrium properties
may be misleading if recorded while the plasma species are still out of equilibrium.
Here we consider the electron-ion temperature relaxation rate in dense plasmas
Previous evaluations based on theoretical models have shown strong disagreement between each other.
In this work, we compute the temperature relaxation rates using
ab-initio quantum molecular dynamics across a wide range of condiitons
for dense Aluminum and Hydrogen plasmas.

(Author Not Attending)

T60.00115: Detecting the Topological Superconductivity: Pseudo Kondo Resonance in the Induced p + ip Supreconducting Surface State of Topological Insulator

Rui Wang, Wei Su, Baigeng Wang, Jian-Xin Zhu, Chin-Sen Ting, Hai Li

Topological superconductors, which can be classified due to the symmetries they respect, have drawn enormous attention recently. However, unambiguous scheme to probe or distinguish different types of topological superconductors are still in need. We propose that a quantum magnetic impurity can uncover the nature of the hosting topological superconductors. We study the Kondo effect in the surface state of a topological insulator (TI) in proximity to a s-wave superconductor, which is known to be topological similar to the intrinsic p+ip superconductor as it effectively enjoys the p + ip pairing symmetry due to the spin-momentum locking. It is found that the induced p + ip superconductor in TI surface state is more similar to the conventional s-wave superconductor rather than the intrinsic p + ip superconductor in terms of the impurity-induced states. Two distinctive features are also identified. One is the pseudogapped hybridization function and the shrinking of the Kondo region, the other is the emergence of an unusual pseudo Kondo singlet state (PKS), where the

local impurity is screened by a pseudo spin composed of true spin and orbital angular momentum index.

T60.00116: Evolutionary Optimization of PAW Data-sets for Ultra-high Pressure Simulations

Kanchan Sarkar, Peter Blaha, Renata Wentzcovitch

Employing our in-house code “Evolutionary Generator of Projector Augmented Wave data-sets” (EGPAW-1.0), we optimize PAW basis functions for some abundant planetary elements up to 100 Mbar. EGPAW-1.0 is an automated hybrid recipe that integrates evolutionary computing with density functional theory calculations. The self-learning evolutionary algorithms in EGPAW-1.0 adaptively tune some of the PAW parameters (such as different radii, and reference energies) to reproduce as close as possible all-electron equations of state (EOS) obtained with WIEN2k in desirable pressure ranges. The program imposes various constraints on logarithmic derivatives and basis sets features to avoid numerical instability, ghost states, and maximize transferability. PAW datasets obtained with this evolutionary procedure aim to maximize the accuracy of *ab initio* calculations of condensed states at extreme pressures within the favorable PAW computational framework

T60.00117: Beyond Bean’s critical state model: On the origin of paramagnetic Meissner effect

Sangjun Oh

Solving phenomenological macroscopic equations instead of microscopic Ginzburg-Landau equations for superconductors is much easier and can be advantageous in a variety of applications. However, till now, only Bean’s critical state model is available for the description of irreversible properties. Here we propose an overall macroscopic model for both reversible and irreversible properties, combining London theory and Bean’s model based on superposition principle. First, a simple case where there is no pinning is discussed, from which a microscopic basis for Bean’s model is explored. It is shown that a new concept of ‘flux share’ is needed when the field is increased above the lower critical field. A portion of magnetic flux is completely shielded, named as ‘Meissner share’ and the rest penetrates through vortices, as ‘vortices share’. We argue that the flux shares are irreversible if there is pinning. It is shown that the irreversible flux shares can be the reason for observed peculiar reversible magnetization behavior near zero field. The overall macroscopic model seems to be valuable for the analysis of fundamental physical properties as well. As an example, it is shown the origin of paramagnetic Meissner effect can be explained by the phenomenological macroscopic model.

T60.00118: Breakdown of Minimal Mean Free Path Theory in MgSiO3 Perovskite

Renata Wentzcovitch, Philip Allen, Tao Sun, Dong-Bo Zhang

Understanding the lattice thermal conductivity at high temperatures is important for many applications. We characterize phonon quasiparticles numerically through a hybrid approach that combines *ab initio* molecular dynamics and lattice dynamics. We find no lower-bound limits on phonon mean free paths in MgSiO3-perovskite. This contradicts the widely used minimal mean free path idea. The clear identification of phonon quasiparticles validates the use of the phonon gas model when phonon mean free paths are shorter than lattice constants of solids. Using the phonon quasiparticle properties, we have calculated the lattice thermal conductivity of MgSiO3 perovskite, a controversial topic of fundamental importance in geophysics.

T60.00119: Multi-scale microdiffraction and characterization of heterogeneous high-pressure syntehsis products

Barbara Lavina

The laser-heated DAC is a powerful technique to synthesize high-pressures materials. High P-T synthesis products are often too challenging to be characterized with powder diffraction techniques because high-pressure structures can be fairly complex and patterns are typically mixed phase. Microdiffraction mapping[1] allows obtaining a whole sample characterization, including grain size and phase heterogeneities, chemical and strain heterogeneities and, at the same time, robust structure factors allowing solution and refinement of relatively complex materials. By spatially resolving the sample chamber in 2D and the diffraction effects in the 3D reciprocal space we were able to solve and refine crystal structures of new polymorphs[2] and compounds [3-4] and achieve comprehensive samples characterization.

[1] Lavina et al., JoVE, 2013, e50613.
[2] Lavina et al., arXiv, 2017,1709.06667v1.
[3] Lavina et al. PNAS, 2011, 108 (42) 17281-17285.
[4] Lavina and Meng, Science Advances, 2015, e1400260.

T60.00120: Gamma-Ray Irradiation Effect on Sol-Gel Derived Zinc Tin Oxide Thin Film Transistors

Shiqiang Wang, Sunil Uprety, Vahid Mirkhani, David Hanggi, Kosala Yapabandara, Min Khanal, Ayayi Ahyi, Michael Hamilton, Mobbassar Sk, Minseo Park

Radiation-hard electronics have broad celestial applications. Zinc tin oxide (ZTO) has a wide band gap of 3.35 eV and is a promising candidate for radiation-hard electronics. The thin film transistors (TFTs) with sol-gel derived ZTO channel layers were fabricated. The effects of gamma-ray irradiation on the ZTO TFTs were investigated using dosages 10 MRad and 50 MRad. The transistor output and transfer characteristics indicated no statistically significant changes before and after irradiation. 10 MRad gamma-irradiation showed a small negative shift while 50 MRad gamma-irradiation showed a small positive shift in the threshold voltage. The maximum drain current (I_D) extracted from the transfer characteristics of the linear region showed negligible change after irradiation at any of the two dosages. A slight reduction in the field effect mobility was observed after 50 MRad irradiation. The overall result suggests radiation-hard and stable nature of the sol-gel derived ZTO TFTs under gamma-ray irradiation. Further analysis is in progress.

T60.00121: STRONGLY CORRELATED SYSTEMS, INCLUDING QUANTUM FLUIDS AND SOLIDS

T60.00122: A Generalization of Non-Abelian Anyons in Three Dimensions

Sagar Vijay, Liang Fu

We introduce both an exactly solvable model and a coupled-layer construction for an exotic, three-dimensional phase of matter with immobile topological excitations that carry a protected internal degeneracy. Unitary transformations on this degenerate Hilbert space may be implemented by braiding certain point-like excitations. This provides a new way of extending non-Abelian statistics to three-dimensions.

T60.00123: ABSTRACT WITHDRAWN

T60.00124: The impact of native defects and hydrogen on the electronic and optical properties of $BiFeO_3$

Marciano Carneiro, Iflah Laraib, Anderson Janotti

There is great interest in materials that exhibit simultaneous ferroeletric and magnetic properties, so called multiferroics, for applications in spintronics and memory devices that can be addressed both magnetically and electrically. $BiFeO_3$ (BFO) is an important example of this class of materials, despite displaying an antiferromagnetic ground state. Recent experiments indicate that BFO is also a promising material for solar cells that explores a ferroelectric photovoltaic (FPV) effect, as an alternative to conventional photovoltaic devices. A large photocurrent effect and above bandgap voltage has been observed in BFO under illumination. For these applications, the behavior of point defects and excess charge can play a major role in the materials performance. Understanding the behavior of excess electrons and holes introduced by native defects or impurities in BFO is therefore of fundamental importance to the development of these new devices. We use density functional calculations with a hybrid functional to study the impact of electrons in the conduction band or holes in the valence band on the magnetization and ferroelectric ordering, paying special attention to carrier localization. We also study the behavior of hydrogen impurities and their interaction with native defects.

T60.00125: Room temperature multiferroic SmFeO3 thin films

Yuan-Chih Wu, Yi-De Liou, Chang-Yang Kuo, Zhiwei Hu, Chun-Fu Chang, Tay-Rong Chang, Heng-Jui Liu, Yi-Chun Chen, Liu Tjeng, Jan-Chi Yang

Multiferroic materials have caught significant attention in the last decade because of its interesting properties and intriguing coupling between different order parameters. $SmFeO_3$ was predicted as a new type of room-temperature multiferroic system ever since 2012. It exhibits antiferromagnetism and significant magnetization below $T_N \sim 670$ K. However, the existence of ferroelectricity of $SmFeO_3$ single crystal is still under debate. In this work, we process the growth of $SmFeO_3$ thin films on various single crystalline substrates, which has rarely been done hitherto. An elegant combination of multiple characterizations has been conducted to identify the ferroic natures of $SmFeO_3$ thin films. Atomic force microscopy is used to check the thin film surface, certifying the layer-by-layer growth nature. The interfacial strains are calculated by using high resolution XRD. X-ray absorption spectroscopy is used to determine the electronic structures. Piezoresponse force microscopy has clearly identified the ferroelectricity of $SmFeO_3$ grown on $NdGaO_3$ substrate. Furthermore, we processed first principle calculation to determine the origin of the ferroelectricity observed in the thin films. The information pileup reveals a new room temperature single-phase multiferroic system.

T60.00126: Two relaxation rates in the Hubbard-Falicov-Kimball Model

Himadri Barman, Mukul Laad, Syed Hassan

A single transport relaxation rate governs the decay of both, longitudinal and Hall currents in Landau Fermi Liquid (FL). Breakdown of this fundamental feature, first observed in cuprates and subsequently in other correlated systems close to (partial or complete) Mott metal-insulator transitions, played a pivotal role in emergence of a non-FL (NFL) paradigm in higher dimensions d > 1. Motivated hereby, we explore the emergence of this ``two relaxation rates'' scenario in the Hubbard-Falicov-Kimball model (HFKM) using the dynamical mean-field theory (DMFT). Specializing to d=3, we find, beyond a critical FK interaction, that two distinct relaxation rates governing distinct temperature dependence of the longitudinal and Hall currents naturally emerges in the NFL metal. Our results show good accord with the experiment in vandium sesquioxide near the metal-to-insulator transition (MIT). We rationalize this surprising finding by an analytical analysis of the structure of charge and spin Hamiltonians in the underlying impurity problem, specifically through a bosonization method applied to the Wolff model and connecting it to the x-ray edge problem.

Reference : https:// arxiv.org/abs/1611.07594 .

T60.00127: Disordered Quantum Spin Chains with Long-Range Antiferromagnetic Interactions

Nicolas Moure Gomez, Hyunyong Lee, Stephan Haas, Ravindra Bhatt, Stefan Kettemann

We investigate the magnetic susceptibility $\chi(T)$ of quantum spin chains of N = 1280 spins with power-law long-range antiferromagnetic couplings as a function of their spatial decay exponent α and cutoff length ξ. The calculations are based on the Strong Disorder Renormalization Group (SDRG) method which is used to obtain the temperature dependence of $\chi(T)$ and distribution functions of couplings at each renormalization step. For the case with only algebraic decay ($\xi = \infty$) we find a crossover at $\alpha^* = 1.066$ between a phase with a divergent low-temperature susceptibility $\chi(T \to 0)$ for $\alpha > \alpha^*$ to a phase with a vanishing $\chi(T \to 0)$ for $\alpha < \alpha^*$. For finite cutoff lengths ξ, this crossover occurs at a smaller $\alpha^*(\xi)$. Additionally, we study the localization of spin excitations for $\xi = \infty$ by evaluating the distribution function of excitation energies and we find a delocalization transition that coincides with the pseudo-gap opening at $\alpha_c = \alpha^*$.

Currently we are working on the corrections necessary to obtain an α and ξ dependence on the concurrence between two spin, which is inexistent in the standard SDRG framework.

T60.00128: Quantum Monte Carlo solution of the dynamical mean field equations in real time

Igor Krivenko, Qiaoyuan Dong, Joseph Kleinhenz, Andrey Antipov, Guy Cohen, Emanuel Gull

We present real-time inchworm quantum Monte Carlo results for single-site dynamical mean field theory on an infinite coordination number Bethe lattice. Our numerically exact results are obtained on the L-shaped Keldysh contour and, being evaluated in real-time, avoid the analytic continuation issues typically encountered in Monte Carlo calculations. Our results show that inchworm Monte Carlo methods have now reached a state where they can be used as dynamical mean field impurity solvers and the dynamical sign problem can be overcome. We envisage the main use of these methods as dynamical mean field solvers for time-dependent problems far from equilibrium.

T60.00129: Measuring Distance in Quantum Many-body Wave Functions

Tianci Zhou, Xiao Chen, Cenke Xu

We study quantum chaos by investigating the growing distance of two slightly different initial states under unitary evolution. The distance $d(t)$ is defined to be that of the reduced density matrices, which undergoes a rapid growth from small initial value to the value of independent random states. A clear exponential growing regime is observed in the Floquet spin model when we turn on the non-local power law decay interactions. The operator spreading picture shows that $d(t)$ captures the same physics as the out-of-time-ordered correlator.

T60.00130: Heisenberg evolution of matrix product operators by time-dependent variational principle

Xiangyu Cao, Ehud Altman

We apply the time-dependent variational principle to study Heisenberg evolution of matrix product operators (MPO). Compared to the analogous Shroedinger evolution approach based on matrix product states recently developed by Leviatan et.al., the MPO approach presents the following advantages: it avoids the ensemble averaging; starting from a local observable, the "entanglement" of the Heisenberg-picture operator grows less rapidly. As applications, we study the chaotic wave front and the hydrodynamic diffusion of local conserved quantities.

T60.00131: Symmetry and filling enforced topological insulators in two and three dimensions

Yuan-Ming Lu, Fuyan Lu

Due to the difficulty of either analytical or numerical calculations, in more than one spatial dimensions, it proves hard to reliably predict topological states in strongly correlated systems. Here we prove a set of theorems of the Lieb-Schultz-Matthis type, which dictates the nature of a non-fractionalized insulating ground state in certain systems. More concretely, with certain crystalline symmetries, at a certain filling fraction, a non-fractionalized insulating ground state must be a topological insulator. These results shed new light on how to guide the search for topological states in strongly correlated systems.

T60.00132: Bulk-Edge Correspondence in Fractional Quantum Hall States

Bin Yan, Rudro Biswas, Chris Greene

We substantiate a complete picture of the ``bulk-edge correspondence" conjecture for topological phases. By studying the eigenstates in the entanglement spectrum for both the ideal and realistic Coulomb ground state of the fractional quantum Hall system, it is verified that the eigenstates in the universal part of the entanglement spectrum purely lie in the Hilbert space of the edge excitations projected onto the physical Hilbert space of the subsystem itself. Hence, not only the eigenlevels in the entanglement spectrum are in one-to-one correspondence with the eigenenergies of an effective dynamical edge Hamiltonian, but all the eigenstates are confirmed to be the actual (projected) edge excitations of the subsystem. This result also reveals the possibility of extracting the full information of the edge excitations from the state of the subsystem reduced from a geometric cut of the pure ground state of the total system in topological phases.

T60.00133: Efficient Estimation of Classical Spin Hamiltonian based on Bayesian Inference by using Markov Chain Monte Carlo Method

Hikaru Takenaka, Kenji Nagata, Takashi Mizokawa, Masato Okada

We propose a method for efficiently estimating a classical spin Hamiltonian based on Bayesian inference using the Markov chain Monte Carlo method. We used sampling data from the exchange Monte Carlo method for the electronic structure calculation in a triangular lattice system. We also used the multidimensional multiple-histogram method which enables the reconstruction of the density of states. Consequently, the results of model selection using all spin configurations could be efficiently reconstructed from sampling data. This suggests that our method can be generically applied to larger systems such as a large-scale numerical simulation system. This method is an extension of our previous methods [1,2].
[1] H. Takenaka, K. Nagata, T. Mizokawa, and M. Okada, J. Phys. Soc. Jpn. 83, 124706, (2014).
[2] H. Takenaka, K. Nagata, T. Mizokawa, and M. Okada, J. Phys. Soc. Jpn. 85, 124003, (2016).

T60.00134: Towards a Quantum Diode: Transport and Countertransport in an Anderson-localized System

Richard Zhu, Nicole Yunger Halpern, Gil Refael

Many-body localized systems are known to exhibit interesting transport and rectification effects. Inspired by Feynman's classic example of the Brownian ratchet and pawl system, transport effects within localized systems are studied. In particular, this work specializes to a simple model of localized single-particle hopping in a 1D disordered tight-binding model, and demonstrates regimes of transport of particle density under periodic driving dynamics. An interesting effect, termed "countertransport", is found to occur under certain parameters, where density is transported against the direction of drive. In addition, this work seeks to use generative unsupervised machine learning models to characterize the types of disorder landscapes that are conducive to transport and countertransport. A better understanding of transport dynamics in such localized systems may prove useful in experimental realizations of quantum electronics.

T60.00135: Towards Real-Time Dynamics of Typical and Untypical States in Non-Integrable Systems

Jonas Richter, Fengping Jin, Hans De Raedt, Kristel Michielsen, Jochen Gemmer, Robin Steinigeweg

Due to controlled experiments with cold atomic gases and the development of sophisticated numerical methods, the study of non-equilibrium dynamics in many-body quantum systems has experienced an upsurge of interest. Particularly for closed systems, there has been immense theoretical effort to answer fundamental questions about equilibration and thermalization. Since such systems are isolated from their environment, out-of-equilibrium conditions can only be induced by the preparation of suitable initial states. In this context, we investigate the real-time dynamics for a class of non-equilibrium pure states in the spin-1/2 XXZ chain. Such states have been recently studied for integrable models [1,2], and relying on the concept of typicality, allow a comparison with results from linear response theory. By introducing an additional next-to-nearest neighbor interaction, we discuss the effect of integrability vs. non-integrability on the dynamics. Furthermore, the role of the specific initial state realization is analyzed in terms of internal randomness, entanglement entropy, and local density of states.

[1] R. Steinigeweg *et al.*, Phys. Rev. B **95**, 035155 (2017).

[2] R. Steinigeweg *et al.*, Phys. Rev. E **96**, 020105(R) (2017).

[3] J. Richter *et al.*, in preparation.

T60.00136: Dynamics of Typical Pure States in Integrable Quantum Many-Body Systems

Robin Steinigeweg, Fengping Jin, Daniel Schmidtke, Hans De Raedt, Kristel Michielsen, Jochen Gemmer

The real-time broadening of density profiles starting from non-equilibrium states is at the center of transport in condensed-matter systems and dynamics in ultracold atomic gases. Initial profiles close to equilibrium are expected to evolve according to linear response, e.g., as given by the current correlator evaluated exactly at equilibrium. Significantly off equilibrium, linear response is expected to break down and even a description in terms of canonical ensembles is questionable. We unveil that single pure states with density profiles of maximum local amplitude yield a broadening in perfect agreement with linear response, if the structure of these states involves randomness in terms of decoherent off-diagonal density-matrix elements. While these states allow for spin diffusion in the XXZ spin-1/2 chain at large exchange anisotropies, coherences yield entirely different behavior [1]. In contrast, charge diffusion in the strongly interacting Hubbard chain turns out to be stable against varying such details of the initial conditions [2].

[1] R. Steinigeweg, F. Jin, D. Schmidtke, H. De Raedt, K. Michielsen, J. Gemmer, Phys. Rev. B **95**, 035155 (2017).

[2] R. Steinigeweg, F. Jin, H. De Raedt, K. Michielsen, J. Gemmer, Phys. Rev. E **96**, 020105(R) (2017).

T60.00137: Current-controlled-negative-differential-resistivity, insulator to mixed metal-insulator state switching and power dissipation in self-heated VO_2 single crystals.

Bertina Fisher, Larisa Patlagan

The outstanding features of the insulator-metal-transition (IMT) in VO_2 at T_{IMT}=340 K include a large negative thermal emissivity in the infrared over the transition. Under an applied current, the resistance drops due to Joule heating, the voltage reaches a maximum and a current controlled negative differential resistivity (CC-NDR) regime sets on. The mixed insulator-metal phase appears within the NDR regime. The stability of I(V) of a sample in this regime is governed by the load resistance (R_L) in series with the sample. For small enough R_L the sample switches from the last steady state with maximal Joule heating power (P_{max}) to a state with minimal Joule heating power (P_{min}). Instead of hot filaments that are formed upon switching in thin films, the mixed state of single crystals consists of dynamic or static metal-insulator domains with boundaries that cross the width of the crystal at favorable inclinations. The results derived from I-V characteristics of several VO_2 single crystals show that: 1. P_{max} / P_{min} may exceed by far the ratio between the emissivity in the infrared of the insulator to that of the metal and 2. Beyond the minimum, P increases with increasing current due to sliding domains but this increase as well as sliding are suppressed by damage.
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T60.00138: Effects of Surface Plasmonic Electric Field Enhancements on Thin Film Vanadium Dioxide's Insulator to Metal Transition.

Scott Madaras, Jason Creeden, Salinporn Kittiwatanakul, Jiwei Lu, Irina Novikova, Rosa Lukaszew

We investigate the effect that the surface plasmonic electric field enhancement will have on insulator to metal transition (IMT) in vanadium dioxide (VO_2) films. We have observed using this method that we can photo-induced the IMT with laser powers of 5mW. The possibility of surface plasmons inducing an IMT in a VO_2 film could be the basis of a new type of efficient photo switch or sensor. Our theoretical model predicts that in a glass/Au/VO_2 thin film structure, a strong electric field enhancement of 89 times the field at the glass-Au interface will occur in VO_2 at 1064nm laser wavelength. A model of the SP electric field enhancement effect in VO_2 coupled with the differences in fractional amounts of VO_2 converted between metal and insulator is being used to guide the design of experimental samples and from experimental results fits to within 50%. The study involves two different samples with structures consisting of a 31nm Au film and 10nm VO_2 film and a 31nm Au film and 5nm VO_2, both deposited on a glass substrate.

T60.00139: Unusual Charge Density Wave coupled to a metal-to-metal transition in $Ce_3Co_4Sn_{13}$

Amol Singh, Hsiao-Yu Huang, Y. Chin, Y. Liao, TingChun Huang, Jun Okamoto, Wen-Bin Wu, H. Lin, Ku-Ding Tsuei, R Wang, Frank de Groot, C N Kuo, H Liu, ChinShan Lue, C. Chen, Di-Jing Huang, Ashish Chainani

We study the electronic structure of the skutterudite $Ce_3Co_4Sn_{13}$, which exhibits a charge density wave transition (CDW ; T_{CDW}~160 K) coupled to a metal-to-metal transition. We use temperature dependent HAXPES and XAS to investigate the occupied and unoccupied electronic states of $Ce_3Co_4Sn_{13}$. The Co 2p and Sn 3p core level spectra show small but finite shifts in energy positions across T_{CDW} but Ce 3d core level spectra do not show any change across the transition. The Ce M-edge XAS spectrum compared with calculations indicate a typical trivalent ionic Ce^{3+} spectral shape, ruling out Kondo screening in $Ce_3Co_4Sn_{13}$. In contrast, the Co 2p L-edge XAS spectrum compared with calculations shows evidence for hybridization with neighbouring Sn atoms in a trigonal prismatic co-ordination. Temperature dependent XAS across the Co 2p L-edge shows a small shift across T_{CDW}, consistent with HAXPES results. The Co 3d states are observed at a binding energy of ~2 eV while the Ce 4f states occurs within 0.5 eV of the Fermi level as a weak feature. The results indicate an unusual CDW coupled to a metal-to-metal transition in $Ce_3Co_4Sn_{13}$.

T60.00140: Electron dressed states in black phosphorus and dice lattices

Liubov Zhemchuzhna, Andrii Iurov, Godfrey Gumbs, Danhong Huang

Electron dressed (or Floquet) states, which are due to the interaction between electrons with off-resonant electromagnetic radiation have been investigated for recently fabricated anisotropic black phosphorus as well as 2D pseudospin-1 dice lattices. Our analytic calculations were performed for the low-energy electronic states. Optical dressed states for both linear and circular polarizations of the incoming radiation have been investigated for both of these lattices. We also discuss electron tunneling and the Klein paradox for the obtained states.

T60.00141: Electric-Field-Induced Insulator to Metal Transition in α-MoO_3

Yuechen Zhuang

Layered α-MoO_3 is well known for its intriguing optical and electrical properties based on two dimensional (2D) character. Here we show the reversible metallization and pronounced structural changes of MoO_3 thin film by electrolyte gating. The resistivity of the gated thin film is tuned by five orders of magnitude at room temperature and a clear insulator-to-metal phase transition is observed accompanied by the change in out-of-plane lattice constant.

T60.00142: Spin-Level Hybridization between Ising and XY Models: A Monte Carlo Study

Manal Al-Ali, Fawaz Hrahsheh

We develop a classical spin model by hybridizing the well studied Ising and XY models at the spin level. We investigate the phase transition and the critical phenomena of a clean two-dimensional system of this XY-Ising hybrid spin model by means of large-scale Monte Carlo simulations. Preliminary results suggest that the order phase is purely Ising-like and a ferromagnetic phase transition occurs at a critical temperature ($T_c\simeq 1.7$) smaller than that of the clean two-dimensional Ising model ($T_{c}^{Ising}\simeq 2.269$). This phase transition is accompanied by the formation of Ising ferromagnetic domains confined by energetically cheap XY walls (Ising-XY ferromagnetic domains). This picture of domains persists for significantly high temperatures producing a novel paramagnetic phase. By increasing the temperature in this paramagnetic phase, the Ising-XY ferromagnetic domains do not completely transform into Ising-like paramagnetic domains or a globally mixed paramagnetic bulk phase but rather they undergo a continuous splitting into smaller ones. We also investigate the critical properties of our system in detail and compare them to those of the clean parent models and their universality classes.

T60.00143: Emergent Bloch Excitations in Mott Matter

Nicola Lanata, Tsung-Han Lee, Yong-Xin Yao, Vladimir Dobrosavljevic

We develop a unified theoretical picture for excitations in Mott systems, portraying both the heavy quasiparticle excitations and the Hubbard bands as features of an emergent Fermi liquid state formed in an extended Hilbert space, which is non-perturbatively connected to the physical system. This observation sheds light on the fact that even the incoherent excitations in strongly correlated matter often display a well defined Bloch character, with pronounced momentum dispersion. Furthermore, it indicates that the Mott point can be viewed as a topological transition, where the number of distinct dispersing bands displays a sudden change at the critical point. Our results, obtained from an appropriate variational principle, display also remarkable quantitative accuracy. This opens an exciting avenue for fast realistic modeling of strongly correlated materials.

T60.00144: Anomalous Dimensions for Gauge Fields in the Strange Metal of the Cuprates

Philip Phillips, Kridsanaphong Limtragool

One of the cornerstones of theoretical physics is that conserved currents cannot have anomalous dimensions. However, a recent proposal[1] for the ubiquitous strange metal phase in the cuprates argues just the opposite. Namely, all of the properties of such `strange metals' can be understood if the current has an anomalous dimension. My talk will focus on trying to understand this claim. To demystify this claim, I will first show[2] that even in the standard formulation of gauge theories, there is a loop-hole in Noether's theorems which has remained `almost' (Noether was aware of it) un-noticed until now, that can allow, in principle, for the current to have any allowable dimension. However, I will show that the only quantum theories to date which exhibit such odd behaviour are holographic models that are derived from a gravity theory that lives in higher dimensions. The corresponding boundary theory is inherently non-local as dictated by the exception to Noether's theorems. The existence of currents having anomalous dimensions, a direct probe of the existence of extra `hidden' dimensions, can be tested with the Aharonov-Bohm effect. I will describe this effect and its potential impact for unlocking the secret of the strange metal in the cuprates.

T60.00145: Peierls instability in linear carbon chains calculated by quantum Monte Carlo

Matteo Barborini, Ludger Wirtz

Linear carbon chains are known to occur in two different structures: the semi-metallic cumulene (characterized by identical double bonds between the carbon atoms) and the semiconducting dimerized polyyne (characterized by the alternation of triple and single bonds). The Peierls instability that triggers the transition from cumulene to polyyne[1,2] is reflected in the instability of the Longitudinal Optical (LO) mode at Γ[3] and is influenced by the long-range correlation between electrons, such as the highest optical phonon mode at the high-symmetry point K in graphene.[4]
Since Density Function Theory (DFT) is known to under- or over-estimate the instability according to the different exchange-correlation functionals, to better assess their behavior, we present here unbiased Variational Monte Carlo (VMC) calculations studying the relative stability of the infinite carbon-atom chain in the two conformations (cumulene and polyyne) as a function of the stretching and we study the variation of the LO frequency at Γ.

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T60.00146: Impact of the charge-density-wave state in the electrodynamic response of $ZrTe_{3-x}Se_x$: optical evidence for a pseudogap phase

Leonardo Degiorgi, M. Chinotti, C. Petrovic

The emergence of superconductivity upon progressively suppressing the long-range, charge-density-wave (CDW) order characterises the phase diagram of several materials of interest in the on-going solid-state physics research. Se-doped $ZrTe_{3-x}Se_x$ compounds provide the most recent, suitable arena in order to investigate the interplay of otherwise competing orders in layered-like two-dimensional systems. We present an optical study of the CDW state in $ZrTe_{3-x}Se_x$ at selected Se-doping, based on the measurement of the reflectivity from the far-infrared up to the ultraviolet, as a function of temperature. We particularly focus our attention to the redistribution of the spectral weight, which images the impact of the CDW state within the optical conductivity across the phase diagram of the title compounds. The electrodynamic response is consistent with a scenario based on a long-range CDW condensate at low Se-doping. Upon increasing the Se content, this then gives way to precursor effects as consequence of local, short range order CDW segments. Our spectral weight analysis reveals the presence of a pseudogap phase, as fingerprint of the CDW precursor effects and thus shaping the charge dynamics of the title compounds in their normal state, preceding the onset of superconductivity.

T60.00147: Quantum Singwi-Tosi-Land-Sjoelander (STLS) approach for interacting inhomogeneous systems under electromagnetic fields

Taichi Kosugi, Yu-ichiro Matsushita

As a natural extension of the original semi-classical STLS approach for an electron gas[1],
we derive the linear equation for response functions in a quantum mechanical manner[2] for inhomogeneous interacting electronic systems under a time-dependent electromagnetic perturbation.
In this study, we choose an analytically solvable interacting two-electron system as the target for which we examine the validity of the approximation.
We compare the STLS response function and the exact one.
The interaction energy calculated from the STLS response function is also discussed.

[1] K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjoelander, Phys. Rev. **176**, 589 (1968)
[2] T. Hasegawa, and M. Shimizu, J. Phys. Soc. Jpn. **35**, 18 (1973); T. Hasegawa and M. Shimizu, J. Phys. Soc. Jpn. **38**, 965 (1975)

T60.00148: Suppression of weak ferromagnetism in ultra-thin iridates by interfacial engineering of octahedral rotations

Wei Guo, Dianxiang Ji, Zhengbin Gu, jian zhou, Yuefeng Nie, Xiaoqing Pan

The *5d* transition metal oxide Sr_2IrO_4 has been predicted to be a new type of high-*Tc* superconductor upon electron doping, and exhibits many behaviors similar to cuprates. However, no direct evidences (zero resistance and Meissner effects) of superconductivity have been observed up to date. A major difference between irdates and cuprates is the sizable IrO_6 octahedral rotations and weak ferromagnetic ordering (considerable net magnetic moments) in the IrO_2 plane, which may hinder the formation of cooper pairing. To suppress the IrO_6 octahedral rotations, we grew epitaxial $SrIrO_3$ films on cubic $SrTiO_3$ substrate by reactive molecular-beam epitaxy. Via the interfacial clamping effect imposed by substrates, low-energy electron diffraction (LEED) measurements exhibit no octahedral rotations in 2 and 1 unit-cell $SrIrO_3$ films. *In-situ* angle-resolved photoemission spectroscopy (ARPES) and first principle calculations suggest an intriguing antiferromagnetic ground state with no canted magnetic moments in these ultra-thin $SrIrO_3$ films. Our work provides a new path to explore superconductivity in iridates.

T60.00149: Quantitative Evaluation of "Diracness" from the Quantum Oscillations in PbTe

Kazuto Akiba, Atsushi Miyake, Hideaki Sakai, Keisuke Katayama, Takuya Sakamoto, Noriaki Hanasaki, Sadao Takaoka, Yoshiki Nakanishi, Masahito Yoshizawa, Yoshiya Uwatoko, Masashi Tokunaga

The Dirac electron systems, which are characterized by their highly mobile carriers governed by the relativistic Dirac equation, have been one of the biggest topics in condensed matter physics. Still, it has not been clear how to identify them experimentally. Recent theoretical study proposed a quantitative prescription to experimentally evaluate "Diracness" of materials, which focuses on the ratio of Zeeman energy to cyclotron energy (ZC ratio). In this context, we focus on lead telluride (PbTe) to investigate physical properties tuning Diracness by external parameters. We investigated quantum oscillations in various physical quantities (resistivity, magnetization, sound velocity, and ultrasonic attenuation) in high magnetic fields, and determined ZC ratio of PbTe as 0.52. Further, we investigated the pressure dependence of the quantum oscillations, and obtained an indication that PbTe approaches the Dirac system by applying pressure.

T60.00150: Magnetostriction Measurements to Clarify High-Temperature Phase Boundary in $CeOs_4Sb_{12}$

Pei-Chun Ho, Marcelo Jaime, John Singleton, M Brian Maple, Tatsuya Yanagisawa

The filled skutterudite compound $CeOs_4Sb_{12}$ displays Kondo insulating behavior with accompanied by a ~1 K antiferromagnetic (AFM)/ Spin-Density-Wave (SDW) order state. In penetration depth and magnetic susceptibility measurements, we found a Fermi-surface reconstruction in $CeOs_4Sb_{12}$ and an unusual phase boundary in the temperature T vs magnetic field H diagram associated with the valence transition from the Ce^{4+} to Ce^{3+} state. However, the phase boundary between 5 and 15 K, currently described by the susceptibility data, is hard to define. Since a valence transition can strongly influence the electron-phonon coupling, we performed additional magnetostriction measurements to clarify this intriguing phase boundary.

T60.00151: Shubnikov de Haas oscillations and magnetic properties of p type polycrystalline $ZrTe_5$

Mandeep Hooda, C. S. Yadav

We report the magnetoresistance and magnetic properties of the polycrystalline p-type $ZrTe_5$. We observed Shubnikov de Haas (SdH) oscillations in the compound with the small cyclotron effective mass of ~ $0.05m_e$ and high mobility of ~ 2.2×10^4 cm^{-2}/V-s. Magnetoresistance data shows three dimensional Weyl semimetal like behavior. Kohler's rule is obeyed at low temperatures ≤ 10K. The fast Fourier transform analysis of SdH oscillations show a single predominant oscillation frequency. The paramagnetic peak in M/H versus H data extends in broad field range up to 4 Tesla at 1.8 K, field range and size of peak decreases with increasing temperature. We have compared our results on p-type polycrystal with bipolar single crystal $ZrTe_5$ reported in the literature.

References:
1. G. N. Kamm et al., Phys. Rev. B **31**, 7617 (1985).
2. A. Pariari, and P. Mandal, Scientific Reports **7**, 40327 (2017).
3. G. Zheng et al., Phys. Rev. B **93**, 115414 (2016).

T60.00152: Characterization and transport measurements of bulk and surface conduction of La and Eu doped SmB_6 using multi-terminal Corbino devices

Juniar Lucien, Yun Suk Eo, Alexa Rakoski, Dmitri Mihaliov, Cagliyan Kurdak, Priscila Rosa, Boyoun Kang, Beongki Cho

Transport properties of topological Kondo insulator SmB_6 can be altered by either introducing vacancies or substitutional atoms such as La or Eu in the Sm site. In the case of samples with vacancies, we found the activated behavior at low temperatures to be independent of vacancy concentrations whereas we have observed differences in the high-temperature Hall coefficients. In this study, we have extended our transport experiments to samples with magnetic and non-magnetic doping. In the heavily doped samples such as $Sm_{0.6}La_{0.4}B_6$, both the bulk and surface transport measurements were polluted by the presence of cracks. We, therefore, focused on the dilute doping limit and found introduction as little as 3% of La can alter the magnitude of the Hall resistance at all temperatures including the sign at low temperatures. In addition to Hall measurements, we will present transport results from multi-terminal Corbino devices including inverted resistance measurements.

T60.00153: Interplay between topology and disorder in a two-dimensional semi-Dirac material

Pallasena Viswanathan Sriluckshmy, Kush Saha, Roderich Moessner

We investigate the role of disorder in a two-dimensional semi-Dirac material characterized by a linear dispersion in one, and a parabolic dispersion in the orthogonal, direction. Using the self-consistent Born approximation, we show that disorder can drive a topological Lifshitz transition from an insulator to a semi-metal, as it generates a momentum independent off-diagonal contribution to the self-energy. Breaking time-reversal symmetry enriches the topological phase diagram with three distinct regimes-- single-node trivial, two-node trivial and two-node Chern. We find that disorder can drive topological transitions from both the single- and two-node trivial to the two-node Chern regime. We further analyze these transitions in an appropriate tight-binding Hamiltonian of an anisotropic hexagonal lattice, by calculating the real-space Chern number. Additionally we compute the disorder-averaged entanglement entropy which signals both the topological Lifshitz and Chern transition as a function of the anisotropy of the hexagonal lattice. Finally, we discuss experimental aspects of our results.

T60.00154: Experimental investigation of Co_2MnGa: candidate for the first intrinsic, three-dimensional topological magnet.

Ilya Belopolski, Daniel Sanchez, Guoqing Chang, Kaustuv Manna, Benedikt Ernst, Suyang Xu, Songtian Sonia Zhang, Hao Zheng, Jiaxin Yin, Bahadur Singh, Guang Bian, Daniel Multer, Xiaoting Zhou, Shin-Ming Huang, Baokai Wang, Arun Bansil, Hsin Lin, Claudia Felser, Zahid Hasan

To date, the field of topological phases of matter has focused on band inversions driven by spin-orbit coupling (SOC). An open frontier is the search for topological invariants driven instead by magnetism. Since magnetic exchange splitting can be much larger than SOC, band inversions in magnetic systems may allow robust topological transport at room temperature. Magnetism also allows new topological phenomena. For instance, the configuration of topological objects may change with the direction of sample magnetization. Recently, we used density functional theory (DFT) to predict that the ferromagnet Co_2MnGa hosts a magnetic topological phase with a network of topological line nodes. Here we present a preliminary experimental investigation of Co_2MnGa using transport and angle-resolved photoemission spectroscopy (ARPES). We observe a robust ferromagnetic order with a high Curie temperature of ~ 700 K. Our ARPES measurements are consistent with DFT in the magnetic phase, confirming that we access the magnetic band structure in ARPES. Our findings pave the way for the discovery of the first intrinsic, three-dimensional topological magnet in Co_2MnGa.

T60.00155: Sequential Topological Phase Transitions of J_1-J_2 Integer Spin Chain

Shota Fubasami, Yasuhiro Hatsugai

Phase diagrams of the integer spin Heisenberg chains with nearest neighbor (J_1) and next nearest neighbor (J_2) interaction are considered numerically for S = 1, 2, 3 and 4. The Berry phase associated with twisting several local bonds is quantized to 0 or π (Z_2) due to the time reversal symmetry, which is a topological order parameter assuming the gap is finite. Since it is an adiabatic invariant even for a finite system, the phase boundaries are well defined for the finite system. This Z_2 Berry phase is a topological order parameter for the short range Symmetry Protected Topological (SPT) phases. Several Z_2 Berry phases are evaluated by choosing a combination of local bonds. Sequential quantum phase transitions by changing J_2/J_1 are observed which implies reconstruction of local singlets.

T60.00156: Single crystal growth and study of the magnetic properties of the mixed system $Ba_{(3-x)}Sr_xCr_2O_8$

Alsu Gazizulina, Diana L. Quintero Castro, Andreas Schilling

We describe the growth of $Ba_{(3-x)}Sr_xCr_2O_8$ single crystals with x=2.9 and x=2.8 in a four-mirror type optical floating-zone furnace and the influence of chemical disorder on their magnetic and structural properties studied by magnetization and heat-capacity measurements. Inelastic neutron scattering measurements on single crystalline $Ba_{(3-x)}Sr_xCr_2O_8$ with x=2.9 show three excitation modes, corresponding to the three twinned domains that confirm a monoclinic distortion. The interaction constants were determined from a random phase approximation (RPA) model, and the results are compared to the pure $Sr_3Cr_2O_8$ and $Ba_3Cr_2O_8$ systems. The intradimer interaction constant for $Ba_{0.1}Sr_{2.9}Cr_2O_8$ is found to be J_0 = 5.332(2) meV, about 4% smaller than that of the pure $Sr_3Cr_2O_8$ compound, while the interdimer exchange interaction Je is smaller by 6.9%. These results show a noticeable change in the magnetic properties by a random substitution effect.

T60.00157: Majorana zero modes and long range edge correlation in interacting Kitaev chains: analytic solutions and density-matrix-renormalization-group study

Jian-Jian Miao, Hui-Ke Jin, Fu-Chun Zhang, Yi Zhou

We study the interacting Kitaev chain model with open boundary condition by using exact analytic methods as well as using density-matrix-renormalization-group (DMRG) method. At the symmetry point △=t and zero chemical potential, the interacting model is mapped onto a noninteracting fermion model by applying two Jordan-Wigner transformations and a spin rotation and is diagonalized exactly. For generic parameters, we resort to DMRG to study the model. We suggest and examine an edge correlation function of Majorana fermions to characterize the long range order in the topological superconducting states and study the phase diagram of the interating Kitaev chain.

T60.00158: COMPLEX STRUCTURED MATERIALS, INCLUDING GRAPHENE

T60.00159: Length Distribution of DNA-Wrapped Boron Nitride Nanotubes
Johnathan Weicherding, Geyou Ao

Boron nitride nanotubes (BNNTs) are an emerging nanomaterial with promising properties for applications in elevated temperature and hazardous environments. BNNTs are mechanically robust and have extraordinary thermal and chemical stability. However, the structure polydispersity of BNNTs presents special challenges for its processing and applications. In this work, the length distribution of various aqueous dispersions of BNNT wrapped by DNA (DNA-BNNTs) is evaluated as a start of its liquid phase processing. Additionally, we performed the length separation of BNNTs using a polymer precipitation method previously developed for carbon nanotubes [1]. The attempt at length separation was done using polyethylene glycol (PEG) as a crowding agent. The PEG concentrations ranged from (1.4 -5.2) % by mass. We used scanning electron microscopy, as well as UV-vis optical spectroscopy to characterize the length distribution of various samples. An average length of 276 nm was found for the initial tip sonicated aqueous dispersion of DNA-BNNTs.

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T60.00160: Probing the temperature dependent transport in colloidal MoS_2 nanocrystals
Souvik Biswas, Subhrajit Mukherjee, Samit Ray

The quantum confinement effect leads to interesting phenomenon in colloidal MoS_2 nanocrystals (NCs), specifically, size-tuneable optical and electronic properties. In addition the ability to be solution processed makes the NCs ideal for commercial flexible and tuneable LEDs, photodetectors, solar cells and transparent electronic devices. In this work, we made temperature dependent (10K-350K) two probe I-V measurements on MoS_2 NC assemblies (without gate bias) to estimate parameters (from non-linear fitting) such as mobility, conductivity, activation energy, etc. and study their temperature and size dependence, which showed a transition from Nearest Neighbour Hopping (NNH) at higher temperatures (where Arrhenius like behaviour was seen) to Variable Range Hopping (VRH) at lower temperatures. Spontaneous phase transition of MoS_2 from trigonal prismatic to octahedral (which was monitored by X-ray photoelectron spectroscopy, Raman and UV-Vis spectroscopy), and restoration of 2H-phase by ex-situ thermal annealing was also studied. Our results indicate that for microelectronics, 1-T might be more suitable due to its higher mobility over 2-H, which remains the better choice for optoelectronics.

T60.00161: Lateral WSe_2/$MoSe_2$ Heterostructures Grown by a Two-step CVD Method
Yuhang Cai, Kai Xu, Wenjuan Zhu

Recently, atomically thin transition metal dichalcogenides (TMDs), as well as their heterostructures, have attracted great attention due to their unique properties. In this work, we systematically investigate the impact of the growth conditions on the morphology of the MoS_2 and WSe_2 grown by chemical vapor deposition (CVD) using solid precursors. Large domain sizes (100 μm) of WSe_2 are synthesized. We further demonstrate WSe_2/$MoSe_2$ heterostructure growth by using a two-step CVD method, where MoS_2 was synthesized first followed by an epitaxial growth of WSe_2 on the edge. During the WSe_2 growth, a Se–S ion exchange occurs in the MoS_2 region, converting the MoS_2 into $MoSe_2$. The Raman and photoluminescence spectra, and atomic force microscope (AFM) images, of the synthesized structure indicate that the film is a monolayer lateral heterostructure. These heterostructures will have broad application in nanoscale electronic and photonic devices, including tunneling field effect transistors, photodetectors, and solar cells.

T60.00162: Unveiling the electronic dispersions in layered MoS_2 by electron energy loss spectroscopy
Chien-Ting Wu, Chuan-Yu Wei, Chin- Wei Tsao, Cheng-Yen Wen, Cheng-Hsuan Chen, Ming-Wen Chu

Electronic dispersions of free-standing MoS_2 layers have been investigated by momentum-resolved electron energy-loss spectroscopy with an improved q resolution. With the fine q resolution and extensive q range, we were able to explore the plasmon dispersion characteristic of 2D collective excitations along the two principal in-plane directions, ΓM and ΓK. Here, we report the q-dependent EELS analysis on the free-standing layered MoS_2 thin films from long-wavelength to large-momentum transfer. Also, the E-q map experiments of MoS_2 are exhibited. It was found to display the square root of the q dispersion characteristic of the collective excitation of the 2D electron systems, and further unveil an in-plane electronic anisotropy. Furthermore, the STEM-EELS studies show that the predominant excitations at ~8.5, ~23 and ~12 eV arise from the respective resonances of bulk and surface plasmons in aloof mode. Calculations elucidating the q-resolved EELS analysis are also discussed.

T60.00163: A Multi- and few-layer graphene growth on Si(100) by pulsed laser deposition
Saidjafarzoda Ilhom, Trason Carter, Khomidkhodzha Kholikov, Zachary Thomas, Ali Er

A multi- and few-layer graphene were successfully prepared by pulsed laser exfoliation of highly ordered pyrolytic graphite (HOPG) using nanosecond Q-switched Nd:YAG laser. The effect of laser energy density, substrate temperatures, wavelength, and background pressures were investigated. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) were used to analyze the topography and thickness of the films. AFM and SEM measurements showed that amorphous carbon, few-layer graphene and thin graphite films were formed as the laser power increased. Laser wavelength of 532 nm produced better quality films compared to 1064 nm pulses. Raman spectroscopy results confirmed the graphene film formation as well as the quality. Ongoing reflection high energy electron diffraction (RHEED) will also be presented. This study presents new insights to better understand the growth mechanism of graphene via laser exfoliation; an alternative, controllable, and efficient synthesis route.

T60.00164: Supercell DFT calculations of charged defects in monolayer h-BN
Pradip Niraula, Angelo Bongiorno

We use density functional theory (DFT) calculations to study the structure, energy stability, and electronic properties of point charge defects in monolayer hexagonal boron nitride (h-BN). We introduce and use a novel scheme based on atomistic models and polarizable force fields to correct the formation energy of charged defects resulting from our supercell DFT calculations. The parameters of the polarizable force field are selected to reproduce the in- and out-of-plane static dielectric constants of monolayer h-BN, equal to 6.0 and 1.9, respectively. Using this scheme, we find that the correction energies range between 11 up to 50% of the uncorrected energies of vacancy and substitutional charged defects in h-BN. These corrections have a significant impact on the energy vs. Fermi level stability diagrams of the point defects considered in this study. We conclude this paper with an outlook on future research on point defects in multilayer hybrid materials obtained by combining graphene and h-BN.

T60.00165: Tunable band gap coupling in 2D heterostructures based on ternary alloys of transition metal dichalcogenides
Florence Nugera, Prasana Sahoo, Yan Xin, Humberto Gutierrez

Transition metal dichalcogenides (TMDs) ternary alloys have composition dependent electronic properties. For instance, their bandgap as well as their electrical response (n-type or p-type conductivity) can be continuously tune with the chemical composition. However, these advantages of individual ternary alloys can be greatly expanded if we combine them into a heterostructure, and the number of possible materials combinations is larger than for binary TMDs heterojunctions. In this work we performed a systematic study to explore the production of ternary alloy heterostructures of the type $MoS_{2(1-x)}Se_{2x}$-$WS_{2(1-x)}Se_{2x}$ (where x is the composition of the chalcogen atom). We demonstrate the successful and continuous tuning of the band gap for both materials forming the heterostructure. We identified conditions in which in-plane or vertically stacked 2D heterostructures can be *in situ* fabricated. The alloy-based heterostructures were extensively studied by Raman, PL and Transmission Electron Microscopy.

T60.00166: The normal-auxeticity mechanical phase transition in graphene
Qing Peng, Binghui Deng, Jie Hou, Hanxing Zhu, Sheng Liu, Emily Liu, yunfeng Shi

When a solid object is stretched, in general, it shrinks transversely. However, the abnormal ones are auxetic, which exhibit lateral expansion, or negative Poisson ratio. While graphene is a paradigm 2D material, surprisingly, graphene converts from normal to auxetic at certain strains. Here, we show via molecular dynamics simulations that the normal-auxeticity mechanical phase transition only occurs in uniaxial tension along the armchair direction or the nearest neighbor direction. Such a characteristic persists at temperatures up to 2400 K. Besides monolayer, bilayer and multi-layer graphene also possess such a normal-auxeticity transition. This unique property could extend the applications of graphene to new horizons.

T60.00167: Structural Phase Transformation in Strained Monolayer $MoWSe_2$ Alloy
Pankaj Rajak, Aravind Krishnamoorthy, Rajiv Kalia, Aiichiro Nakano, Priya Vashishta

Molecular dynamics (MD) simulations are performed to examine atomistic mechanisms of defect formation and crack propagation in a strained monolayer $MoWSe_2$ alloy. The system consists of a 1.0 m x 1.0 m $MoSe_2$ monolayer with a pre-crack and random patches of WSe_2. Under strain, the crack meanders as it propagates through the system and branches into two daughter cracks when it crosses the $MoSe_2$/WSe_2 interface and enters the WSe_2 patches. The most dramatic change occurs in the process zone around the crack tip, where large stress concentration and the resulting biaxial tensile strain trigger an irreversible local structural phase transformation from the ground state 2H crystal structure to the 1T crystal structure. This is consistent with experimental observations in an $MoWSe_2$ alloy.

T60.00168: One-pot growth of 2D lateral superlattices via vapor phase modulation
Prasana Sahoo, Shahriar Memaran, Yan Xin, Luis Balicas, Humberto Gutierrez

Here, we developed a one-pot synthesis strategy for the continuous fabrication of TMDs lateral superlattices ($MoSe_2$-WSe_2 and MoS_2-WS_2). These superlattices are sequentially created by only changing the composition of the reactive gas environment in the presence of water vapor. Water vapor allows selective oxidation

and volatilization of Mo compound whereas reducing gas (H_2) facilities the vaporization of W compounds. The switching cycle between the water vapor and H_2 allows us to control the Mo and W domains, respectively, and hence the superlattice structure. The exact role of water vapor in the selective oxidation and reduction of solid precursor will be discussed. We found that this carrier gas switching cycle is very crucial for obtaining atomically sharp interfaces. Raman and Photoluminescence spatial mapping confirm the chemical and optical homogeneity of the distinct TMD domains in the heterostructures. Photoluminescence line scans revealed the effective modulation of the electronic transitions across the heterostructures. Transmission electron microscopy confirm high quality seamless lateral connectivity within a single-crystal heterostructure.

T60.00169: Study of Contact Properties for Semiconducting TMDCs Using Via Contacts Embedded in h-BN

Min Sup Choi, Younghun Jung, Daniel Rhodes, Bumho Kim, James Teherani, James Hone, Won Jong Yoo

The semiconducting transition metal dichalcogenides (TMDCs) are considered as a promising candidate for Si-based electronics. However, it is notorious particularly for a contact of semiconducting TMDCs especially when their thickness scales down to extreme thinness such as mono- to tri-layers. There have been some reports on contact issue and its remedy but most of them are discussed on multi-layered structures. According to our study, even though it showed a linear behavior at room temperature, a non-linear behavior could be observed at low temperature. Thus, it is very valuable to study contact properties to achieve ohmic contact even at low temperature. In this study, we evaluated the electrical properties of semiconducting TMDCs from mono- to tri-layers with different metals embedded in hexagonal boron nitride (h-BN) so as to uncover its contact properties. The fabricated devices show the higher performances in terms of current value and stability due to the lower contact resistance and ultraflat surface of h-BN so as to allow us to trace the intrinsic carrier transport and unique properties of the TMDCs.

T60.00170: Synthesis, Characterization, and Device Application of Antimony-Substituted Violet Phosphorus

Franziska Baumer, Yuqiang Ma, Chenfei Shen, Anyi Zhang, Liang Chen, Yihang Liu, Daniela Pfister, Tom Nilges, Chongwu Zhou

Two-dimensional (2D) nanoflakes have emerged as a class of materials that may impact electronic technologies in the near future. A challenging but rewarding work is to experimentally identify new 2D materials and explore the properties of them. Here, we report the synthesis of a new layered material $P_{20.56}Sb_{0.44}$, with systematic study on characterizations and device applications. This material demonstrates a direct bandgap around 1.67 eV. Using laser-cutting method, the thin flakes of this material can be separated into multiple segments. We have also fabricated field effect transistors based on few-layer $P_{20.56}Sb_{0.44}$ flakes with thickness down to a few nanometers. Interestingly, these field effect transistors show strong photoresponse within wavelength range of visible light. Under room temperature, we have achieved good mobility values (up to 43.08 $cm^2/V\bullet s$), reasonably high on/off current ratio (~10^5), and intrinsic responsivity up to 10 μA/W. Our results demonstrate the potential of $P_{20.56}Sb_{0.44}$ thin flakes as a new two-dimensional material for applications in visible light detectors.

T60.00171: High Responsivity Graphene/MoS_2 Flexible Photodetectors

Domenico De Fazio, Ilya Goykhman, Duhee Yoon, Matteo Bruna, Anna Eiden, Silvia Milana, Ugo Sassi, Matteo Barbone, Dumitru Dumcenco, Kolyo Marinov, Andras Kis, Andrea Ferrari

We present a flexible photodetector for visible wavelengths fabricated by stacking chemical vapor deposited (CVD) graphene and CVD MoS_2 onto a flexible polyethylene terephthalate (PET) substrate, where MoS_2 acts as an absorber and graphene is used as a conductive channel. When electron-hole pairs are generated in MoS_2 upon illumination of the stack, MoS_2 donates electrons to the p-doped graphene channel [1], resulting in a decrease of the total source-drain current. In this configuration, the device responsivity can be enhanced either by promoting the injection process from MoS_2 to graphene through side-gating using a polymer electrolyte [2, 3], or by applying larger source-drain voltage. The device shows responsivity as high as ~570A/W at 642nm. The reported responsivity is at least two orders of magnitude higher than the values obtained in the bulk-semiconductor flexible membranes [4] and other flexible photodetectors based on graphene and layered materials [5]. The photocurrent is stable for radii of curvature down to ~1.4cm.

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[3]S. Das et al., Nat. Nano. **3**, 210 (2008)
[4]W. Yang et al., Appl. Phys. Lett. **96**, 121107 (2010)
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T60.00172: Extrinsic Light Emission of 2D Semiconductor for Multi-Index Optical Sensing

Shun Feng, Chunxiao Cong, Ting Yu

Two-dimensional transition metal dichalcogenides (2D TMDs) possess a tunable excitonic emission that varies with extrinsic electrostatic or chemical doping, which is beneficial to 2D material based optical sensing applications. Here we revealed the interaction between DNA nucleobases and monolayer WS_2 by investigating the change of the photoluminescence (PL) emission of WS_2 with the coatings of nucleobases solutions. The p-type doping of WS_2 by introducing adenine is clearly evidenced by both evolutions of the PL spectra and the electrical transport behaviors. Besides the tunability of PL spectra shapes, we also demonstrated the tailoring of valley degree of freedom by electrostatic and optical doping. We performed the circular polarized PL measurement on monolayer WS_2 with various carrier densities at 80 k. The doping induced 5-fold increase of polarization degree of charged exciton emission is achieved even under off-resonance laser excitation, without the requirement of cryogenic temperature or magnetic field. Our findings fill the gaps in previously reported optical biosensing methods and indicate rich possibilities for developing optical sensing platform with both excitonic and valleytronic indices.

T60.00173: Building a Better Graphene Loudspeaker

Donez Horton-Bailey, Stephen Gilbert, Hu Long, Zhen Guo, Stanley Liu, Alex Zettl

Electromechanical resonator devices made from suspended graphene sheets have many applications such as gas sensing and information processing. Previous work in our group has demonstrated that graphene possesses several useful properties for audio devices such as microphones and loudspeakers. It has been demonstrated that the low mass of graphene ensures good high-frequency response, while its high strength allows for free-standing diaphragms large enough for effective low-frequency response. Multilayer graphene (tens of layers) being less brittle than single-layer graphene is ideal for the scaling of these devices. In this work, various methods are used to manipulate the physical properties of graphene, and we consider the effects of these methods on overall device performance.

T60.00174: Characterization of MoS_2/Si and WS_2/Si Heterojunction Photodetectors Fabricated by High-Working Pressure Plasma-Enhanced CVD

Soyeong Kwon, Jungeun Song, Dongrye Choi, Eunah Kim, Yonghun Kim, Byungjin Cho, Dong-Wook Kim

Trilayers of MoS_2 and WS_2 were grown on p-type Si wafers using high-working pressure plasma-enhanced chemical vapor deposition technique. Dark current-voltage measurements of the MoS_2/Si and WS_2/Si heterojunctions showed rectifying behaviors, indicating formation of diodes. While illuminating the samples with a green laser (wavelength: 532 nm), both of the heterojunctions exhibited large (negligibly small) photocurrent under reverse (forward) bias conditions. The measured photocurrent was linearly proportional to the laser power at 80 K as well as at room temperature. This suggested that trapping and detrapping of the photo-generated carriers at interface defects and surface adsorbates could not significantly suppress the collection of photo-carriers. We also studied dynamics of photocurrent behaviors using a chopper. Both of the heterojunctions showed fast photoresponse: the rising and decaying time constants were ~ 1 ms. All these results showed that our plasma-enhanced growth technique could be very useful to produce high quality MoS_2/Si and WS_2/Si heterojunctions for optoelectronic applications.

T60.00175: Temperature Dependent Infra-red Detection in Graphene – Tellurium Nanowire Binary Hybrid with Ultra-high Sensitivity

Avradip Pradhan, Ahin Roy, Shalini Tripathi, Anirban Som, Depanjan Sarkar, Jayanta Kumar Mishra, Kallol Roy, Thalappil Pradeep, Narayanan Ravishankar, Arindam Ghosh

Single layer graphene serves as a good candidate for ultra-sensititve photodetection by virtue of its high carrier mobility and lifetime. Also because of spatial charge separation and large optical gain, the optoelectronic performance of graphene based hybrid devices always becomes superior than usual photodetectors. Tellurium nanowire (TeNW), having a narrow direct bandgap (~ 0.65 eV) is an excellent potential candidate for near infra-red (NIR) detection. In this work, we report a maximum photoresponsivity ~ 10^6 AW^{-1} at 175K for a graphene - TeNW binary hybrid in the NIR regime (920 nm - 1720 nm). The extracted noise equivalent power (NEP) can be as low as 2×10^{-18} $WHz^{-1/2}$ and specific detectivity value exceeds 5×10^{13} Jones. A systematic temperature dependence of the photoconductivity has also been performed and we have observed a suppression of the photoconductivity at higher temperature by virtue of the conduction through the NWs. But the optimal operating range of temperature can still be improved by controlling the inter-wire electronic coupling and the defect density inside the TeNWs.

T60.00176: Ionic selectivity and filtration from fragmented dehydration in multilayer graphene nanopores

Subin Sahu, Michael Zwolak

Selective ion transport is a hallmark of biological ion channel behavior but is a major challenge to engineer into artificial membranes. Here, we demonstrate, with all-atom molecular dynamics simulations, that bare graphene nanopores yield measurable ion selectivity that varies over one to two orders of magnitude simply by changing the pore radius and number of graphene layers. Monolayer graphene does not display dehydration-induced selectivity until the pore radius is small enough to exclude the first hydration layer from inside the pore. Bi- and tri-layer graphene, though, display such selectivity already for a pore size that barely encroaches on the first hydration layer, which is due to the more significant water loss from the second hydration layer. Measurement of selectivity and activation barriers from both first and second hydration layer barriers will help elucidate the behavior of biological ion channels. Also, for separation of ions from water, one can exchange longer, larger radius pores for shorter, smaller radius pores, giving a practical method for maintaining exclusion efficiency while enhancing other properties (e.g., water throughput).

T60.00177: Measuring the Barrier Height at Transition Metal Dichalcogenide Heterojunctions

Upendra Rijal, Arthur Bowman, Kraig Andrews, Michael Koehler, David Mandrus, Zhixian Zhou

Transition metal dichalcogenides (TMDs) have attracted much interest in recent years as channel materials for high performance Field Effect Transistors (FETs). However, a large Schottky barrier tends to form at the interface of TMD channels and most conventionally used metal contacts. Chuang et al. demonstrated low-resistance Ohmic contacts to WSe_2, MoS_2, and $MoSe_2$ channels by inserting a degenerately doped TMD at the contact areas.[1] While the low contact resistance suggests a substantially reduced barrier, a systematic study is necessary to probe the reduction of the Schottky Barrier Height (SBH) and better understand the mechanism of carrier injection at TMD heterojunctions that enables the success of the 2D-2D contact strategy. In this work, we investigate how the band alignment affects the Schottky barrier Height.

While ohmic contacts are achieved between degenerately -doped MoS_2 drain/source and WSe_2 channel, a SBH in the range of tens to hundreds of meV is observed for individual 2D/2D junctions consisting of -doped WSe_2 contact and $MoSe_2$ channel. For comparison, we also study isolated Schottky barriers at TMD/metal junctions by fabricating asymmetrically contacted WSe_2 FETs consisting of a 2D/2D ohmic contact and a TMD/metal Schottky contact.

T60.00178: Electrical detection of spin-polarized states conduction in $ZrTe_5$

Wei Wang, Wanli Peng, Liang He

(Author Not Attending)

T60.00179: Abstract Withdrawn

The manipulation of carrier density for semiconducting transition-metal dichalcogenides (TMDs) is crucial to control the electrical properties and create the electric/optoelectric devices in the two-dimensional material systems. Here, by utilizing a locally reversed ferroelectric polarization of the supporting $BiFeO_3$ (BFO) substrate within an isolated WSe_2 sheet, we obtain an additional degree of freedom to strongly modify the electron confinement and thus create a WSe_2 diode defined by a lateral *pn* homojunction. This ferroelectricity-controlled WSe_2 *pn* homojunction is demonstrated by optical and scanning probe methods in ambient environment and by scanning photoelectron micro-spectroscopy. In particular, a defect-free junction interface is a direct manifestation of this profile, which can be quantitatively understood by an ideal rectifying behavior with an estimated ideality factor near unity. Complementing previous approaches to confine carriers by carefully gate biasing on TMDs, the nonvolatile confinement of carriers and associated gate-free *pn* homojunction are a new addition to the two-dimensional electron-photon toolbox, paving the way to laterally develop 2D electronics and photonics.

T60.00180: High-Performance Sub-Micron Channel WSe_2 Field-Effect Transistors Prepared Using A Flood-Dike Printing Method

Fanqi Wu, Liang Chen, Anyi Zhang, Chongwu Zhou

Printing technology has potential to offer a cost-effective and scalable way to fabricate electronic devices based on two-dimensional transition metal dichalcogenides (TMDCs). However, limited by the registration accuracy and resolution of printing, previously reported printed TMDC field-effect transistors have relatively long channel lengths (13-200 μm), thus suffering low current-driving capabilities (≤ 0.02 μA/μm). Here, we report a "flood-dike" self-aligned printing technique which allows the formation of source/drain metal contacts on TMDC materials with sub-micron channel lengths. This technique involves three steps, including (i) printing gold ink on WSe_2 to form the first electrode, (ii) modifying the surface of the first gold electrode with self-assembled monolayer (SAM) to lower its surface tension, and (iii) printing gold ink close to the SAM-treated first electrode with a certain distance. During the third step, the gold ink would firstly spread toward the first electrode and then get stopped by the hydrophobic SAM coating, forming a sub-micron channel. With this printing technique, we have successfully downscaled the channel length to ~750 nm, and achieved enhanced on-state current densities of ~0.64 μA/μm (average) and high on/off current ratios of ~$3x10^5$ (average).

T60.00181: Temperature and Magnetic Field Dependence of the Raman Spectra of $TaSe_2$

Hamna Ali, Sugata Chowdhury, Heather Hill, Angela Hight Walker, Jeffrey Simpson

A layered, transition-metal dichalcogenide (TMD), $TaSe_2$ continues to attract interest for advanced device applications. In bulk form, metallic $TaSe_2$ exhibits transitions between commensurate and incommensurate charge-density wave (CDW) phases. In the present work, we extend our opto-thermal Raman measurements[1] on MoS_2 to include bulk $TaSe_2$ in both 1T and 2H crystallographic phases. A novel, magneto-Raman microscope system affords measurement of low-frequency (down to 10 cm^{-1}) vibrational modes as a function of both temperature (100 to 400)K and magnetic field (0 to 9)T. The dependence of the observed Raman-active phonons on temperature and magnetic field will be presented and compared with earlier results on MoS_2. Specifically, we observe the appearance of low-frequency, zone-folded modes in the CDW state, which soften with temperature similar to the higher frequency, in-plane E_{2g} mode. Additionally, we compare the measured magneto-Raman results to calculations using *ab initio*, density functional theory.

[1] R. Yan, J. R. Simpson, *et al*., ACS Nano **8**, 986 (2014).

T60.00182: Multi-Valley Superconductivity in Ion-Gated MoS_2 Layers

Domenico De Fazio, Erik Piatti, Dario Daghero, Srinivasa Tamalampudi, Duhee Yoon, Renato Gonnelli, Andrea Ferrari

Charge carrier concentrations~$10^{14}cm^{-2}$ induce a superconducting state in MoS_2 [1, 2]. Here we report low-temperature transport measurements in electrical double layer-gated MoS_2 flakes from 4 to 10 layers. We observe two kinks in the resistivity as a function of doping, which indicate the crossing of the spin-orbit split sub-bands Q_1 and Q_2 [3]. Superconductivity does not appear until both spin-orbit split sub-bands are simultaneously populated.

[1] J. T. Ye, et al., Science **338**, 1193 (2012).
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T60.00183: Water/RTIL Sorption interaction in Nanoporous Carbon Electrode Materials

Jose Espitia

A unique feature of CDC is it's fine-tuned pore size in the subnanometer range, which depends on the initial carbide (TiC) and annealing conditions. Where at low temperatures there is a formation of small pores with a narrow size distribution, while higher temperatures result in larger pore sizes. Recent reports of water's diffusional dynamics dependence on CDC pore size indicate confinement effects similar to observed in pores of 16 Angstroms.Though other studies have gleaned insights into the porous structure of CDC, there is currently no direct structural information on the sorption of water at intermediate stages between completely empty and full. Small angle X-ray scattering was used to study the degree to which pores may be filled with room temperature ionic liquids (RTILs) and with water (H2O) at different RTIL/water. We present models being developed to reproduce the SAXS data and extract information on 1) the structure of CDC, consisting of subnanometer and meso-pores, 2) the kinetics of water sorption in porous media 3) the interaction between (RTILs) and (H2O). The bahavior of water/RTIL mixtures in confinement, and their role in supercapacitors is still not fully understood.

T60.00184: Characterization of itinerant ferromagnet Fe_3GeTe_2

Paul Malinowski, Zaiyao Fei, Bevin Huang, Xiaodong Xu, Jiun-Haw Chu

I present the results of characterization of bulk single-crystals of Fe_3GeTe_2, an itinerant Ising ferromagnet with a layered, hexagonal crystal structure and bulk magnetic ordering below T_c ~ 221K. Comprehensive magnetization and electrical transport measurements reveal a large magnetic anisotropy with an out-of-plane easy axis and a pronounced anomalous hall effect (AHE). Angle resolved magneto-transport measurements and first-order reversal magnetization curve measurements identify relevant scattering mechanisms and probe the behavior of magnetic domains during saturation. The links between the large AHE response and the topological properties of the band structure and concepts of Berry curvature are discussed.

T60.00185: Orbital Selectivity and Particle-Hole Asymmetry of the Charge Density Wave Energy Gap in Transition Metal Dichalcogenides

Kapila Wijayaratne, Junjing Zhao, Jasper van Wezel, Utpal Chatterjee

Angle Resolved Photoemission Spectroscopy (ARPES) study of the incommensurate Charge Density Wave (CDW) material, *2H*-TaS_2, is presented in comparison to a similar *layered transition metal dichalcogenide* (TMD) *2H*-$NbSe_2$. Similarities were observed in the selective appearance of CDW energy gap about some specific symmetry points in the momentum space, particle-hole asymmetry of this gap and the persistence of a *pseudogap* above CDW transition temperature. As per differences, in *2H*-TaS_2, the gap was significant for all momentum locations about a symmetry point, while in the case of *2H*-$NbSe_2$ the gap opened up only in specific momentum locations. Analysis of momentum and temperature dependence of the electronic band dispersion shows many body renormalization due to a *phononic* origin. As the model of *Fermi surface nesting* was unable to explain above observations, a tight binding model with emphasis on orbital selectivity and strong electron-phonon coupling was utilized. In the light of similar behaviors exhibited by other related material, we suggest that this model can be generalized for a wide spectrum of CDW materials beyond TMDs.

T60.00186: Distinct surface and bulk charge density waves in ultrathin 1T-TaS_2

Zhipeng Ye, Rui He, Gaihua Ye, Heidi Anderson, Junichi Okamoto, Xia Dai, Xianxin Wu, Jiangping Hu, Yu Liu, Wenjian Lu, Yuping Sun, Abhay Pasupathy, Adam Tsen

We employ variable temperature low-frequency Raman spectroscopy to study the nearly commensurate (NC) to commensurate (C) charge density wave (CDW) transition in 1T -TaS2 ultrathin flakes protected from oxidation. We identify additional modes originating from C-phase CDW phonons that are distinct from those seen in bulk 1T -TaS2. We attribute these to CDW modes from the surface layers. By monitoring individual modes with temperature, we find that surfaces undergo a separate, low-hysteresis NC-C phase transition that is decoupled from the transition in the bulk layers. This indicates the activation of a secondary phase nucleation process in the limit of weak interlayer interaction, which can be understood from energy considerations.

T60.00187: Transition-Metal Effects on the Electronic Dirac Cone in Intercalated Bilayer Graphene

Chloe Chicola, Alexander Balatsky, Jason Haraldsen

In this study, we examined the affect of intercalated transition-metal atoms on the electronic properties of bilayer graphene. Through a comparison of single, double, and triple layer graphene, we set out to investigate the integrity of the Dirac cone with the substitution of Mn, Fe, Co, and Ni. Using density functional theory, we calculated and analyzed the electronic structure for each material. Contrary to expectations, the Dirac cone was not destroyed by the presence of transition-metal atoms, but experiences a shift in the chemical potential that, in turn, lowers the Dirac cone by about 1 eV. Therefore, it may be possible to produce a spintronic device that couples to d Dirac symmetries.

T60.00188: Emergent wave phenomena in coupled elastic bars: from extreme attenuation to realization of elastodynamic switches

Qianli Chen, Ahmed Elbanna

Metamaterials with acoustic and elastic band gaps are of great interest to scientists and engineers. Here, we introduce a novel mechanism for emergence of multiple band gaps with extreme attenuation by coupling continuous one-dimensional elastic structures. We show that it is possible to develop extreme attenuation at several frequencies from coupling two homogenous bars of different elastodynamic properties even though each bar individually possesses no such gaps. Moreover, if each bar is a composite on its own, multiple resonant band gaps appear in the compound system which do not exist in either bar. We verify our results by conducting numerical simulations for the elastodynamic response and show that the resonant gaps are efficient in attenuating wave propagation. Furthermore, we show that by carefully tailoring the properties of the coupled bars we may construct elastodynamic signal choppers. These results open a new gate for designing *Metamaterial* with unique wave modulation properties.

T60.00189: Cluster-Inspired Magnetic Materials Composed of Manganese

Purusottam Jena, Hong Fang

Magnetic materials have always played an important role in both scientific research and practical applications. Many of these materials involving the transition element manganese (Mn) have attracted considerable interest due to the large magnetic moment of the element. In addition, the strongly correlated *d* electrons of Mn enable various magnetic coupling and states in different crystal environments. Here, we study the magnetic properties of a series of nano-materials composed of Mn. These include zero dimensional clusters, one dimensional chains and two dimensional materials, as well as a Mn-cluster supported on 2D substrate. Our motivation is to investigate the possibility of modifying the magnetic properties of materials by using the Mn-clusters instead of the Mn atom as building blocks.

T60.00190: Polymer Mediated Nucleation of Minerals: A Molecular Dynamics Study

Shayna Hilburg, Kirill Shmilovich, Alfredo Alexander-Katz

Biomineralization creates complex structures with advantageous properties, such as the superior toughness seen in nacre. In biomineral nucleation, calcium carbonate or calcium phosphate ions are directed by organic macromolecules, often leading to the growth of thermodynamically unfavorable polymorphs and/or specifically shaped crystals that contribute to the materials' properties. To investigate how macromolecules guide crystal formation in complex biological systems, we probed the pre-nucleation nanoscale interactions in a simplified computational model that may govern overall precipitation and crystallization. We performed atomistic molecular dynamics simulations of calcium carbonate solution with charged polymers as analogs to the proteins that have been shown to influence crystallization. By analyzing resulting polymer and ion configurations in this system, we found that ion aggregate size and order are increased by the polymer's presence, and this effect is a function of ion concentration and polymer properties such as hydrophobicity, chain flexibility, and charge.

T60.00191: Atomic-Scale Structure and Optical Properties of Rare-Earth (RE =Pr, Nd, Er) Doped Sodium Ultraphosphate Glasses

Kanishka Marasinghe, Faisal Amir, Chris Benmore, Richard Brow, Stanley May

The atomic-scale structure of a series of $(Re_2O_3)_x(Na_2O)_y(P_2O_5)_{1-x-y}$ glasses (Re = Pr, Nd, Er) where $0.005 \leq x \leq 0.05$ has been characterized via high-energy X-ray diffraction (HEXRD) technique. In addition, Differential Thermal Analysis (DTA), Fourier Transform Infrared (FTIR) spectroscopy, and absorption and emission spectroscopy in visible and near IR ranges have been used to validate HEXRD results. Coordination numbers for P-O, Na-O, O-O, and P-P were found to be independent of the Re_2O_3 content. In contrast, the Re-O coordination number decreases with Re_2O_3 concentration. However, the glass transition temperature increases with increasing Re_2O_3 content. Even at these very low rare earth concentrations, depolymerization of the glasses at Q^3 tetrahedral sites was observed. Quantum efficicencies as high as 70% were observed at certain concentrations. Emission spectra of these glasses show that their florescence efficiency decreases with increasing rare-earth content suggesting that concentration quenching of lasing action may be present even at these very low rare earth concentrations.

T60.00192: Structural Role of Zirconium in Zirconium-Doped Lithium Silicate/Borate Glass-Ceramics

Kanishka Marasinghe, Changhyeon Yoo, Carlo Segre, Richard Brow

A series of Zr-doped (~3–10 mol%) lithium silicate (ZRLS) glass-ceramics and their parent glasses and a series of Zr-doped (~2–6 mol% ZrO_2) lithium borate (ZRLB) glasses were investigated using Zr K-edge EXAFS and X-ray Absorption Near Edge Structure (XANES) spectroscopy. Unusual thermo-physical properties of these materials make them good candidates for applications which demand low thermal expansion coefficients. Zirconium ions play an important role in determining those thermos-physical properties. Immediate coordination environments of all ZRLS glasses are remarkably similar for different compositions. For the nearest oxygen shell, the Zr-O coordination number ranges between 6.1 and 6.3 for nucleated and crystallized samples, respectively. Also, the Zr-O mean distance remains similar around ~2.10 Å. For these glasses, the composition dependence of structural parameters was small. Small changes in the coordination environment were observed for ZRLS glass-ceramics after thermal treatments. In contrast, Zr coordination environment in ZRLB glasses appear to depend appreciably on the Zr concentration. For the nearest oxygen shell, the Zr-O coordination number increased from ~6.1 to ~6.8 and the Zr-O distance decreased from ~2.18 to ~2.14 Å with decreasing ZrO_2 content.

T60.00193: Machine-Learning for Optical Identification of Two-Dimensional Structure

Xiaoyang Lin, Zhizhong Si, Wenzhi Fu, Jianlei Yang, Yuan Cao, Jin Zhang, Peng Liu, Xinhe Wang, Kaili Jiang, Weisheng Zhao

Two-dimensional (2D) materials and heterojunctions, with fascinating properties and abundant applications, have attracted numerous interest and triggered revolutions of corresponding device applications. However, facile methods to realize accurate and intelligent characterizations of these 2D structures are still highly desired. Here, we report the successful application of machine-learning strategy in the optical identification of 2D structures, including graphene, molybdenum disulfide and heterojunctions of these two materials. The machine-learning optical identification method (MOI method) relies on trainable and automatic identifications of the RGB information in the optical photograph of 2D structures. The MOI method enables accurate characterizations of 2D structures, including identifications of the thickness, the existence of impurities, and even the stacking order. Together with the progress in optical techniques, this intelligent identification method with significantly high accuracy and high throughput can certainly promote the fundamental research and device application of 2D structures.

T60.00194: Nanowire Optical Cavities by Fermi Liquid Pseudo-Mirror

Kiana Montazeri, Zhihuan Wang, Bahram Nabet

Surface plasmon Polaritons (SPPs) are density oscillations of electrons at the surface of a dielectric. Materials such as noble metals including Au and Ag are considered as the most promising plasmonic material candidates because of their high optical conductivity and low ohmic loss. A heterojunction is the interface that occurs between two layers or regions of dissimilar crystalline semiconductors with unequal bandgaps which provides a mature system of extremely high mobility electrons. At the interface of the core-shell nanowires, a heterostructure can be formed which results in 6 sheets of 2D and 6 pillars of 1D charge, forming the plasmonic boundary of the optical cavity. This method can produce better optical cavity quality factor, as well as enhance emission and absorption of radiation. A comparison among this plasmonic medium and noble metallic surfaces is conducted to show that 2DEG at the interface has similar effects as the well-known plasmas. Plasmonic resonant modes in sub-wavelength geometries in CSNWs can be used in THz nanowire laser applications. Additionally, control of charge density leads to design of tunable nanowire cavities.

T60.00195: Reaction Time Study of Zinc Stannate Growth on Conducting Substrates

Fouad Albadrasawi, Sarath Witanachchi, Domingo Mateo, Aayat Sabah, Pritish Mukherjee

Lead Zirconate Titanate, $Pb[Zr_x\ Ti_{1-x}]O_3$ (PZT), is a widely studied piezoelectric material with a wide array of applications ranging from medical instruments to capacitors. Adversely, this material contains lead which poses many consequential health concerns. $ZnSnO_3$, Zinc Stannate (ZTO), shows a deformed perovskite phase similar to that in Lithium Niobate, an alternative lead-free ferroelectric material with the general formula $ANbO_3$ making it a possible replacement for PZT due to its non-toxic composition. The goal of this project is to exploit the piezoelectric properties of ZTO and explore its potential for replacing PZT. To do this, a silica nanosphere monolayer, coated on top with aluminum-doped zinc oxide nanocolumns, is used as a growth template. ZTO was grown chemically from a low temperature solvo-thermal process and previous research discovered that it would grow into the desired LN-type phase of nanowires when the reaction was performed on highly conductive substrates. A reaction time study will determine the tunability of ZTO structure and nanowire aspect ratios as a function of time grown on indium tin oxide substrates. A structural study of ZTO films grown at different reaction times will be performed using XRD and SEM will be used to study the nanowire dimensions.

T60.00196: Deformation mechanisms in nanotwinned nanopillars/nanotubes in body-centered cubic tungsten

Shuozhi Xu, Saeed Chavoshi, Yanqing Su

Coherent twin boundaries (CTBs) are known to play a significant role in deformation mechanisms of metallic nanopillars/nanotubes. While numerous molecular dynamics (MD) studies have been devoted to investigating nanotwinned face-centered cubic (FCC) nanopillars, very few MD work in the literature concern the body-centered cubic (BCC) metallic nanopillars containing CTBs. On the other hand, recent studies confirmed that nanotwinned nanopillars/nanotubes in BCC systems have mechanical properties distinct from those in FCC lattices. Here, using MD simulations, we explore the uniaxial deformation mechanisms of nanopillars/nanotubes in BCC tungsten, as a function of cross-sectional area/shape and CTB spacing. Results show a strong tension-compression asymmetric deformation in nanotwinned BCC nanopillars, with the smallest CTB spacing (= 1 nm) leading to unusual mechanical responses than those with larger CTB spacing. Particularly under tensile loading, the detwinning process on {112} planes results in the formation of incoherent twin boundaries on {111} planes. This process hasn't been observed in any FCC metal, nor in BCC metals such as Fe.

T60.00197: Tunable optoelectronic properties of triply-bonded linear and graphynic carbon structures

Himanshu Chakraborty, Deepak Kumar Rai, Alok Shukla

In quest of novel materials for opto-electronic device applications, in this paper we present a computational study of electronic structure and optical properties of triply-bonded hydrocarbons with linear, and graphynic structures. Employ- ing a correlated electron methodology based upon the Pariser-Parr-Pople model Hamiltonian, and configuration interaction (CI) approach, structures containing up to 42 carbon atoms were studied. Our calculations, based upon large-scale CI expansions, reveal that the linear structures have intense optical absorption at the HOMO-LUMO gap, while the graphynic ones have those at higher energies. Thus, the opto-electronic properties depend on the topology of the graphynic structures, suggesting that they can be tuned by means of structural modifications. Our results are in very good agreement with the available experimental data.

T60.00198: Ab initio and Theoretical Study on Electron Transport through Polyene Junctions in between Angled-cut Carbon Nanotubes

Yiing-Rei Chen

We investigate the surface Green's function and layer-by-layer local density of states (LDOS) of the armchair carbon nanotube (CNT) leads from the rim into the bulk tube. We find the 3-layercycle oscillation of the cross-cut cases, and that the angled-cut cases, exhibiting a zigzag rim at the cut, possess not only the oscillation, but also evanescent edge states that decay into the bulk tube. We study the single-polyene and two-polyene molecular junctions bridging the angled-cut armchair CNT leads, with both *ab initio* and tight-binding model approaches, and look into the interference effect between effective transport channels.

T60.00199: Electronic Properties of Carbon Nanotube Bundles

Yang Li, Mikito Koshino

Abstract: We use the effective continuum model to study the electronic properties of single-walled carbon nanotube(CNT) bundles, an array of CNTs with their axises parallel to each other, including both commensurate bundles and incommensurate ones. Moiré pattern can appear on the interface between two neighboring tubes by adjusting their chirality. We find that this moiré pattern results in band distortion and in gap opening up to 20 meV. The condition when the distortion is significant is given. In addition, we investigate the interference of phases associated to the orientation of constituent CNTs and to their relative position, which provides a degree of freedom to tune the band structures. This interference in an infinite bundle can either enhance a gap by 6 times or close another gap. Besides, we show that deformation of CNTs under pressure will intensify the band distortion.

T60.00200: Probing Plasmons by EELS in Chiral Array of Graphene Nano-Ribbons

Oleksiy Roslyak, Vassilios Fessatidis, Antonios Balassis, Godfrey Gumbs

We have obtained the energy loss spectra of a graphene nano-ribbon array (GNR) in the effective media approximation. The GNR layer conductivity becomes a tensor, with a strong nonlocal component. This approach is valid in the long wavelength limit where one can neglect the polarization across the GNR. The quasi 1D longitudinal plasmons are probed using electron energy loss spectroscopy (EELS). In the perfectly aligned configuration the plasmonic propagation constant is contracted along oblique directions. This allows for plasmon probing with much lower electron energies as compared to the uniform graphene and offers drastic modification of the energy loss probability. The system is similar to a thin uni-axial crystal supporting extraordinary refracted beams with negative group velocity. We investigate the existence of plasmonic resonances by probing the system with a parallel moving electronic beam using EELS. We argue that EELS is capable of picking up two different resonances when there is a mismatch between the direction of the beam and that of the GNR. For several twisted GNR layers one may observe peculiar interference effects between the ordinary and extraordinary plasmon modes.

T60.00201: Effect of Ion Intercalation on Bulk Fullerene Structure

Oleg Sapunkov, Venkat Viswanathan

T60.00202: Abstract Withdrawn

We report low magnetoresistance (MR) measurements of conducting Poly-aniline (PANI) and multi-walled carbon nanotubes (MWCNT) composites. we have used in-situ oxidative polymerization method to synthesize hydrochloric acid doped PANI composites with MWCNT weight percentage 0%,5%,10% and 15%. The temperature dependence of resistivity is studied from room temperature to 4.2K and analysed by Mott Variable range hopping (VRH) model. The temperature dependence of resistivity shows five orders of magnitude change from $1.1\times10^{-3}\Omega$m at 300K to 65.75 Ωm at 4.2K for pure PANI, whereas for PANI composite with 15% MWCNT shows less variation from $4.6\times10^{-4}\Omega$m to $3.5\times10^{-2}\Omega$m. The huge change in resistivity is due to localization of charge carriers in presence of disorder. At 4.2K MR shows transition from positive to negative with higher MWCNT loading. Samples with 5% and 10% MWCNT shows positive MR , where as 10%and 15% MWCNT loaded samples shows negative MR. . Also at higher temperature like 10K, 20K and 30K both positive MR and negative MR is reduced to smaller value .The positive and negative MR is discussed in terms of wave function shrinkage effect and quantum interference effect on variable range hopping conduction.

T60.00203: Plasticity of Carbon Nanotubes under a Combined Axial and Torsional Stress

Masafumi Yamanashi, Masayuki Toyoda, Susumu Saito

Plasticity of carbon nanotubes (CNT) under a combined axial and torsional stress is studied. We apply a dislocation theory to CNT under a combined axial and torsional stress. It has been known that a pure axial tension can change chirality from (n,m) to (n,m-1). It is now revealed that any of six dislocation directions that change chiral indices from (n,m) to (n+1,m), (n-1,m), (n,m+1), (n,m-1), (n+1,m-1) or (n-1,m+1) can become the most energetically favorable direction depending on applied combined stress. In the hexagonal carbon network, a 5/7/7/5 dislocation dipole can be nucleated by a π/2 rotation of a single C-C bond (Stone-Wales transformation) and the motion of a 5/7 defect which is equivalent to a dislocation core allows above transformations to occur. This work is a general and important extension of previous study of CNT under tension and can explain molecular dynamics studies reported so far. From our results, one can estimate a combined stress optimized for any of six transformations to occur. The present finding therefore opens the way to manipulate the chirality of CNT and consequently their electronic transport properties.

T60.00204: Dual Interpretation of the Pseudo-Spin and Moment of Electrons in Graphene

Gerd Bergmann

The electrons in graphene can be described by a two-dimensional Dirac theory. The Dirac formalism (DF) transforms an injected spinless electron into an electron with a (pseudo) spin and magnetic moment (for finite mass m). According to Dirac's formalism the (z component of the) angular momentum is only conserved in combination with the spin. In this consistent description the pseudo spin and magnetic moment of an electron in graphene are real. On the other hand the origin of the pseudo spin and moment can be traced in graphene to distorted magnetic Landau energies. For example the n=0 Landau term has zero kinetic energy because only one of the two sub-lattices A and B is occupied. The solid state system graphene offers an insight into the microscopic working of Dirac's theory. For graphene it shows that spin and moment are an illusion.

T60.00205: Graphene Enhanced Raman Scattering effect of RhB adsorbed on graphene oxide thin films by spectral mapping deconvolution

Francisco Berrellez-Reyes, Monica Acosta-Elías, Susana Alvarez-Garcia

Graphene Enhanced Raman Scattering (GERS) of adsorbed organic molecules on graphene oxide (GO) substrates is associated to a chemical enhancing mechanism. Several works reported relative intensity variations of Raman signatures of organic molecules depending on the GO thickness or the degree of reduction. In this work, we get further insight in GERS effect through spectra deconvolution of Raman mappings of Rhodamine B (RhB) adsorbed on GO. Aqueous/ethanol solution of synthetized GO was deposited on hydrophilic Si/SiO_2 substrates by spin coating. Simultaneous noncontact AFM and Raman mapping studies were performed in areas around 20 μm^2. AFM shows uniform GO films with 5 nm thickness and 1.27 nm roughness. By means of spectra Raman deconvolution we got maps of intensity, width and central position of G and D bands of GO. RhB molecules were adsorbed by immersion in an aqueous solution. In the GO-RhB sample, AFM shows no presence of adsorbed molecules, however Raman mapping allows to discriminate areas with different amount of RhB fluorescence suppression and Raman enhancing. We identify several RhB Raman bands overlapping with the GO ones. We performed a detailed spectral deconvolution and maps of intensity, width and central position shift of different Raman bands are reported.

T60.00206: Interaction of Oxygen Adsorbates via Graphene

Jason Bub, Dmitry Solenov

Understanding the state of the surface of graphene is crucial for applications that rely on charge mobility. A graphene surface can be drastically changed by the presence of adsorbates, altering the transport and chemical properties of the surface. Our investigation focuses on one of the most prevalent adsorbates found on graphene, oxygen. Through the use of first principle density functional calculations and analytical Green's functions, we show that the interaction of the bivalent oxygen adsorbates differs significantly from monovalent adsorbates, such as fluorine.

T60.00207: Influence of electric fields on electronic specific heats of armchair and zigzag graphene ribbons

Chang Ting Liu, Kuo En Chang, Feng Lin Shyu, Yuan Cheng Huang, Chih Wei Chiu

We use the tight-binding model to study the effect of transverse electric field on the electronic specific heat for armchair and zigzag graphene ribbons. For the zero field, the electronic specific heat exhibits rich temperature dependence, mainly owing to the special band structures. The thermal property strongly depends on the geometric structures, the edge structure and the width. There is a simple relation between the ribbon width and the electronic specific heat for the metallic or semiconducting armchair ribbons. However, it is absent for the zigzag ribbons. As for the presence of the electric fields, they change the energy dispersion, the density of states, and the electronic specific heat. Comparisons with the other systems are discussed. The predicted results could be verified by the experimental measurements.

T60.00208: Tuning graphene structures and electronic properties by Ion beam irradiation

Kosuke Nakamura, Tomoaki Nishimura, Kazuyuki Takai

Irradiation of ion-beam into graphene is interesting in view of defect-introduction and chemical modification of graphene. However, it is necessary to fabricate a sacrificial layer on graphene for decelerating ions and position them at the graphene surface due to high energy ion beam penetrating the substrate through graphene. In this study, we designed appropriate sacrificial layer and evaluated the effect of irradiation of air stable Au ion on the structure of graphene. The sacrificial layer thickness giving the least damage and the largest population of Au on graphene is determined by Monte Carlo simulation (SRIM2013). Au ion irradiation of $1\times10^{15}/cm^{-2}$ were performed at 200 keV under 10^{-5} Pa by a tandem accelerator. Rutherford backscattering spectrometry revealed Au is successfully distributed near the surface of the substrate after irradiation in the case of photoresist sacrificial layer irradiated by Au ion. However, the resist layer becomes unremovable due to its change into amorphous carbon indicated by Raman spectra and XPS. The results using ZnO and NaCl as an alternative sacrificial layer will be also presented, where it has been confirmed that they could be removed by HCl and water respectively, even after Au ion irradiation.

T60.00209: Hydrogen termination of defects in graphene

Yoshinori Obata, Kazuyuki Takai

Defect introduction is one of the important strategies to tune the properties of graphene. Although, the number of defects is usually focused, and the chemical structure of defects has been not well considered in graphene. Actually, vacancies in graphene become magnetic depending on the number and position of termination hydrogen atoms. In this study, atomic vacancies are introduced into graphene as defects, and its hydrogen termination is investigated in order to clarify how chemical structure of vacancies affects graphene.
Atomic vacancies were introduced into the surface of graphite and epitaxial graphene grown on SiC as a model graphene by sputtering with Ar ion beam after pre-annealing. Adsorption of hydrogen molecules, atomic hydrogen and atmospheric exposure were performed on the sample. The Oxygen content is much smaller for the graphite surface exposed to atomic hydrogen and hydrogen molecules immediately after the defect introduction, compared with the samples exposed to air. This suggests we can control the termination atoms of defects by atmosphere after defects introduction to graphite surface.

T60.00210: Examination of the magnetic interactions between divacant Fe dimers in graphene

Ronald Putnam, Jason Haraldsen

T60.00211: Abstract Withdrawn

The role of electronic states at the graphene-SiO_2 interface is investigated using the STM/S. The local tunnel spectra show two minima, due to tip-gating, which evolve with the back gate voltage. This evolution is modeled using tip-gating and interface states. A broad energy dependent interface states' density, D_{it} (E) leads to an effect similar to a reduction in the Fermi velocity while the narrow D_{it} (E) leads to the pinning of the Fermi energy close to the Dirac point. Such inhomogeneity in D_{it} (E) amounts to an inhomogeneous screening of the gate electric field experienced by graphene. Further, the evolution of conductance maps with back-gate voltage shows a systematic reversal of contrast in some places and sharp changes in cross-correlations between topographic and conductance maps as the Fermi level approaches the Dirac point. This again is attributed to the change in charge-state of interface defects. The spatial correlations in the conductance maps, described by two different length scales and their growth during the approach to Dirac point, show a qualitative agreement with the screening theory of graphene. We also found reversible handle on doping by manipulating the charge state of interface defects.

T60.00212: Observation of one-dimensional ballistic valley transport in the curved boundary of bilayer graphene

Edrian Mania, Alisson Cadore, Kenji Watanabe, Takashi Taniguchi, Leonardo Campos

Bilayer graphene is a two-layered hexagonal crystal of carbon atoms that shows novel and interesting valley-based phenomena. The manipulation of the valley degree of freedom in graphene have been proposed by different methods such as by exploiting topological confined zero-mode states at domain walls or by creating graphene nanoribbons with zig-zag boundaries. Future dissipationless valleytronic devices require absence of short range disorder, in order to achieve a ballistic valley transport, and it is desirable that they have a channel with atomic width dimensions. In this work we show strong evidences that a ballistic valley conduction may be achieved in a one-dimensional channel formed along the curved boundary of a folded bilayer graphene. In our high quality devices of graphene encapsulated in between h-BN crystals, we measured a ballistic conductance near of $G=4e^2/h$ with zero-magnetic fields. We envision that such new ultra-thin valleytronic platform could either be exploit as a novel dissipationless electronic quantum device as well could let to the discovery of novel exciting properties of matter, such as graphene-based superconducting effects.

T60.00213: Impurity Screening by a Graphene Monolayer Under Uniaxial Strain

Paula Fekete, Dipendra Dahal, Godfrey Gumbs

We examined the static and dynamic shielding of charged impurities by monolayer graphene which is subject to uniaxial strain. The graphene layer is positioned on top of a dielectric and conducting substrate. Results will be presented for the screened impurity potential for a variety of directions in which strain can be applied and for the distance Z_0 of the impurity from the graphene sheet. For dynamic screening, we consider the role played by the underlying bulk plasmons in the conducting substrate.

T60.00214: Inter-subband Landau level couplings induced by in-plane magnetic fields in trilayer graphene

Satoru Masubuchi, Yuta Asakawa, Naoko Inoue, Kenji Watanabe, Takashi Taniguchi, Tomoki Machida

We observed broken-symmetry quantum Hall effects and level crossings between spin- and valley- resolved Landau levels (LLs) in Bernal stacked trilayer graphene. When the magnetic field was tilted with respect to sample normal from $\theta = 0^\circ$ to 66°, the LL crossings formed at the intersections of zeroth and second LLs from monolayer-graphene-like and bilayer-graphene-like subbands, respectively, exhibited a sequence of transitions. The results indicate the LLs from different subbands are coupled by in-plane magnetic fields ($B_{\parallel}$), which was explained by developing the tight-binding model Hamiltonian of trilayer graphene under $B_{\parallel}$. [Y. Asakawa *et al.*, Phys. Rev. Lett. **119**, 186802 (2017).]

T60.00215: Terahertz Driven Ultrafast Photo-carrier Dynamics in Single-Layer Graphene

Ali Mousavian, Byounghwak Lee, Andrew Stickel, Yun-Shik Lee

The unique electronic structure of Graphene gives rise to its remarkable electrical and optical properties such as high carrier mobility and strong absorption of electromagnetic waves over a broad spectral range, which suggest its promising application to ultra-highspeed photonic devices. We demonstrate extraordinary ultrafast carrier dynamics of optically excited photocarriers in single layer CVD-grown suspended graphene induced by strong THz fields. Both strong THz fields and photoexcitation enhance the THz transmission of graphene mainly due to the increase of carrier scattering rates. However, the relaxation of photocarriers show opposite effect of the THz fields and photoexcitation. Photoexcitation increases the relaxation time via the reabsorption of optical phonons by photocarriers, while strong THz fields reduce the relaxation time because the field induced redistribution of electrons opens up unoccupied states in the conduction band and consequently enhances the relaxation and the phonon emission.

T60.00216: Towards Fast Readout and Control of Single-electron Pumps Based on CVD Graphene

JINGGAO SUI, Jack Alexander-Webber, Charles Smith, Stephan Hofmann, Malcolm Connolly

The two-dimensional character of graphene makes it a promising material for realizing high-accuracy single-electron pumps for applications in quantum metrology[1]. Double quantum dots etched from exfoliated flakes, however, lack the scalability and reproducibility required for high-current generation and their ultimate accuracy remains to be seen. We present a fabrication process and low-temperature radiofrequency reflectometry setup for detecting error rates in scalable DQDs based on CVD graphene. To improve device reproducibility we use atomic layer deposition of aluminium oxide with *in situ* gaseous water pretreatments to achieve negligible gate hysteresis, low doping levels, and lower disorder compared to as-fabricated flakes[2]. Using radiofrequency reflectometry we probe single-electron tunnelling rates in DQDs with high sensitivity and at millikelvin temperatures. Using the same setup we also perform low temperature experiments and discuss the advantages of an alternative type of graphene single-electron device based on magnetically confined state in the quantum Hall regime[3].

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T60.00217: Van der Waals proximity induced structural polymorphism in atomically thin MoS_2

Tanweer Ahmed, Mit H Naik, Simran Kumari, Umesh V Waghmare, Manish Jain, Arindam Ghosh

Selective reversible structural switching of a crystal among its various polymorphs, is a fascinating problem in atomics scale crystal engineering. Atomically thin molybdenum disulphide (MoS_2), which can exist in two main coordination, namely octahedral (1T) and trigonal prismatic (1H) structures, is being endorsed as building blocks of future technologies. While both 1H and 1T polymorphs exhibit a remarkable range of physical properties, stabilizing octahedral polymorphs has been challenging. We show that thermodynamically stable octahedral phase of monolayer MoS_2 can be achieved at temperatures below ~ 500 K using van der Waal epitaxy. At room temperature, ~ 10-15% of 2 × 1 1T' octahedral phase, reversibly switchable to 1H by heating, is revealed by our temperature dependent Raman spectroscopy. Conducting-mode atomic force microscopy suggests that the octahedral phase forms a network of elongated (~ 100 nm) patches/stripes within the 1H matrix. We attribute this, with support from density functional theory calculations, to local lattice relaxation due to incommensurability-driven stress fields. Our experiment establishes the van der Waals epitaxy as new tool for crystal structure engineering in atomic membranes.

T60.00218: Lithium Intercalation in Graphene-MoS_2 Heterobilayers

Daniel Larson, Ioanna Fampiou, Gunn Kim, Efthimios Kaxiras

Using first-principles calculations, we investigate the structural and electronic properties of lithium-intercalated graphene/MoS_2 bilayers. Three distinct phases for MoS_2 have been considered, namely 2H, 1T, and 1T'. We vary the number of Li atoms between the layers, and establish a potential energy surface which predicts the stable low-energy sites for Li binding and indicates that diffusion barriers between the sites will enable forward and reverse intercalation. Increasing the number of Li atoms, up to the maximum of 1 Li per Mo atom, decreases the energy difference between the 2H and 1T' phases. Our study shows that electron carrier doping of graphene (MoS_2) up to a maximum level of $n_C = 3.6 \times 10^{14}$ cm^{-2} ($n_{MoS2} = 6.0 \times 10^{14}$ cm^{-2}) is energetically allowed. This carrier doping pushes the Fermi level into the conduction band of the semiconducting 2H phase. We also find evidence for interesting electronic interactions between graphene and metallic 1T'-MoS_2. This points the way for tailoring device heterostructures through varying intercalant concentration and layer polymorphs.

T60.00219: Ce decorated 2D materials

David Groh, Ravindra Pandey

A density functional calculations using Crystal14 were performed with cerium (Ce) and beryllium (Be) decorated 2D materials (graphene, boron-nitride, and silicene). Ce and Be are both charge +2, but Be is physically much smaller. Ce sits above one graphene ring (a little off-center) and centrally sits above boron nitride and silicene. Be does not bond to graphene or boron-nitride. It embeds itself in the center of a silicon ring. When the metal ion sits above a ring, charge transfer makes the band structure insulating. When the metal ion embeds in a ring, the system stays conducting.

T60.00220: Spin-orbit coupling effects on the electronic properties of stanene and fluorinated stanene armchair nanoribbons

Jagger Rivera-Julio, Gonzalo Usaj, Bart Partoens, Francois Peeters, Alexander Hernandez-Nieves

We have studied the electronic properties of armchair stanene and fluorinated stanene nanoribbons by using first principle calculations including the spin-orbit coupling (SOC). In the case of stanene we found that the band gaps oscillate with the width of the nanoribbon due to the quantization condition. While, for fluorinated stanene nanoribbons the band gap decreases monotonically with increasing width and tend to zero if we included the SOC. We also studied the real space charge distribution. For analyzed sizes of stanene nanoribbons we did not find a localization of the charge distribution at the edges when we include the SOC. On the contrary, there is a charge localization at the edges in fluorinated stanene nanoribbons when we include the SOC. The above results shows that fluorinated stanene shows a behavior typical of a Topological Insulator.

T60.00221: The effect of strain on graphene-on-hBN moire heterostructures

Elaheh Mostaani, Marcin Szyniszewski, Neil Drummond, Andrea Ferrari, Vladimir Falko

Double-layer devices based on graphene-on-hBN (SLG/hBN) are of great interest for electronic and optical applications. We present calculations of the binding energy (BE) curves of SLG/hBN for five different configurations using variational and diffusion quantum Monte Carlo (DMC) calculations as implemented in the CASINO code [1]. We also investigate the effects of strain with lattice mismatch. We evaluate the DMC BE as functions of local lattice mismatch and the results are used to find an approximate expression for the energy as a functional of strain in the layers [4].
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T60.00222: Diffusion quantum Monte Carlo study of excitonic complexes layered transition-metal dichalcogenides

Elaheh Mostaani, Marcin Szyniszewski, Cameron Price, Ryo Maezono, Mark Danovich, Ryan Hunt, Neil Drummond, Andrea Ferrari, Vladimir Falko

The nonhydrogenic nature of the excitonic energy spectrum is due to lateral polarization effects in layered material (LM) crystals, which modify the form of the Coulomb interaction between charge carriers. We use quantum Monte Carlo (QMC) methods implemented in CASINO code [1] to extend Mott-Wannier models to provide numerically exact binding-energy (BE) data for all nonlocal screening strengths, including an analysis of limiting behavior. We classify the types of trions and biexcitons that can be observed in different transition-metal dichalcogenides (TMDs). We also investigate donor- and acceptor-bound charge-carrier complexes in TMDs, such as quintons and donor-bound biexcitons. These have similar binding energies to the experimentally measured biexciton BE, suggesting that larger charge-carrier complexes could be responsible for the observed peak ascribed to biexcitons [2].
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T60.00223: Spin and Valley Hall Effect in Monolayer WSe_2 Transistors at Near-Room Temperature

Elyse Barré, Jean Anne Incorvia, Suk Hyun Kim, Connor McClellan, Eric Pop, Philip Wong, Tony Heinz

Monolayer transition metal dichalcogenide (TMDC) crystals have exciting potential for spintronic applications due to their distinct spin and valley properties. Due to their inversion asymmetry and the strong spin orbit coupling, they are predicted to exhibit a coupled spin and valley Hall effect (SVHE) [1,2,3]. We investigate *p*-type monolayer WSe_2 transistors. We observe distinct spin-valley polarization along the two sides of the FET channel at a temperature of 240 K which a spatial distribution that indicates long spin diffusion length. Our study complements earlier reports of the Valley Hall Effect (VHE) in gated bilayer MoS_2 at 30 K [3] by showing that the SVHE can be observed near room temperature. For use in practical electronic applications, it is necessary to control the SVHE and push it towards room temperature. Our results demonstrate the robustness of the SVHE effect and the potential for spin and valley device applications.

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T60.00224: Anomalous Behavior of Valley-Selective Optical Stark Effect Near Resonance in WS_2

Paul Cunningham, Aubrey Hanbicki, Kathleen McCreary, Berend Jonker

Broken inversion symmetry in 2D transition metal dichalcogenides produces valley-specific optical selection rules that fuel interest in future valleytronic applications. Recently, it was discovered that by breaking time-reversal symmetry with intense circularly polarized light fields the K and K' valley degeneracy can be lifted and each valley can individually tuned via a valley-selective optical Stark effect. This effect produces a blue-shift of the A-exciton resonance absorption at the K-valley while under the influence of a strong sub-resonant right-hand circularly polarized light field. Based on application of the dressed-atom picture, a red-shift is predicted for above-resonant light fields. Here, we examine the optical stark effect in monolayer WS_2 for exciation near the A-exciton resonance. We show the K-valley absorption is blue-shifted even for above resonant co-circularly polarized light fields. The blue-shift is resonantly enhanced, reaching 40 meV under moderate excitation at 610 nm. No Stark shift is observed for the opposite valley, which rules out the influence of intervalley biexcitons. We discuss our findings in terms of breakdown of the two-level dressed-atom picture.

T60.00225: Non-equilibrium steady state and current saturation of Dirac electrons in graphene

Jiajun Li, Jong E Han

We investigate the strong-field transport phenomena in graphene, particularly concentrating on the case when the system is at the charge-neutral point. The non-equilibrium momentum distribution of electrons is shown for both samples which are on/off the Dirac point. It is revealed that the system away from the Dirac point shows current saturation due to optical phonon interaction, whereas the current does not saturate in the system on the Dirac point. On the contrary, the graphene sample on the Dirac point shows a crossover from "super-linear" $I \sim V^1.5$ behavior to an approximately linear behavior as optical phonon interaction is turned on. We also unveil the different behaviors of effective temperature while current saturation occurs.

T60.00226: Photoluminescence quenching and spin-orbit coupling in graphene/WSe_2 heterostructure

Everardo Molina, Bowen Yang, David Barroso, Jeongwoo Kim, Mark Lohmann, Ludwig Bartels, Ruqian Wu, Jing Shi

Strong spin-orbit coupling (SOC) can be introduced into graphene by putting transition metal dichalcogenides (TMDs) like WSe_2 onto graphene. Due to the proximity effect, graphene can inherit the strong SOC from TMDs. We find the strength of the acquired SOC depends on the stacking order of the heterostructures when we use boron nitride (BN) as the capping layer, i.e., SiO_2/graphene/WSe_2/BN exhibits a stronger SOC in graphene than SiO_2/WSe_2/graphene/BN. We utilize photoluminescence (PL) to characterize the interaction between WSe_2 and graphene by investigating the PL quenching of monolayer chemical vapor deposition grown WSe_2 in these two stacks. We observe much stronger PL quenching in the graphene/WSe_2/BN stack than in the WSe_2/graphene/BN stack. We attribute the much reduced PL quenching in the latter stack to the increased interlayer distance between graphene and WSe_2. Consequently, we see a strong WAL effect in the former stack but a small or vanished WAL in the latter one. Our observations and hypothesis are further supported by first principles calculations, which show a clear difference in the interlayer distance between graphene and WSe_2 of these two stacks and therefore the resulting SOC strength.

T60.00227: SUPERLATTICES, NANOSTRUCTURES, AND OTHER ARTIFICIALLY STRUCTURED MATERIALS

T60.00228: Vertical Strain-Driven Antiferromagnetic to Ferromagnetic Phase Transition in Self Assembled $EuTiO_3$-Eu_2O_3 Nanocomposite Thin Film on $SrTiO_3$

Yisong Lin

A broad spectrum of functionalities in oxide thin films can be tailored by strain engineering, the strain-enabled multiferroic $EuTiO_3$ thin film is one typical example. Differ from previous reported lateral strain introduced by substrates, vertical strain imposed by novel vertically aligned nanocomposite structure (VAN) has been used to cause tetragonal distortion of $EuTiO_3$, thus tuned its magnetic phase from antiferromagnetic to ferromagnetic. Meanwhile, by a combination of other literature data, the magnetic phase diagram of $EuTiO_3$ has been proposed to illustrate the relationship between strain-enabled tetragonal distortion and different magnetic phase region.

T60.00229: Microwave Synthesis of Cu, Ni, and Cu/Ni Core/Shell Nanoparticles From Triethylene Glycol Solutions of Metal Acetates

Jerome Troy, Christian Sutton, Jie Ren, Gerald Poirier, Klaus Theopold, Karl Unruh

Elemental Cu, elemental Ni, and bimetallic Cu core/Ni shell nanoparticles have been prepared from triethylene glycol solutions of metal acetates in a microwave reactor. Unlike thermal heating, microwave heating allows more rapid heating profiles and, therefore, can more efficiently isolate intermediate reaction products. For example, very small phase pure Cu_2O nanoparticles are initially obtained at reaction temperatures from 200-225 °C which, after 5-10 minutes, rapidly decompose to larger elemental Cu nanoparticles. In comparison, elemental FCC Ni is the initial reaction product at 250 °C with a slow subsequent conversion to HCP Ni (or, perhaps, a hexagonal nickel carbide) at longer reaction times. The relatively clean separation between the temperatures at which Cu and Ni nanoparticles form makes it possible to prepare Cu core/Ni shell nanoparticles from mixed Cu and Ni acetate solutions first heated to 225 °C for a period of 5-10 minutes followed by an additional 5 minute reaction time at 250 °C.

T60.00230: Amino acids conjugated gold clusters: Interaction of Au_8 and Au_{20} clusters with Tryptophan and Alanine in the gas and aqueous phases

Marwa Abdalmoneam, Kevin Waters, Nabanita Saikia, Ravindra Pandey

T60.00231: Abstract Withdrawn

Tunable THz metamaterials have shown great potential to solve the material challenge due to the so called "THz gap". However, the tunable mechanism of current designs relies on using semiconductors insertions, which inevitably results in high ohmic loss, and thereby significantly degrades the performance of metamaterials. In this work, we demonstrate a novel tunable mechanism based on polymerric microactuators. Our metamaterials are fabricated on the surface of patterned pillar array of flexible polymers embedded with magnetic nanoparticles. The transmission spectrum of the metamaterial can be tuned as the pillars are mechanically deformed through an applied magnetic field. We observed and measured several types of deformation including bending, twisting and compressing when the applied magnetic field is polarized along different directions with respected to the axis of the magnetic particles. Compared to previous semiconductor based tunable mechanism, our structure has shown much lower loss.

T60.00232: Thermal Noise Spectrum for Near-Surface Nitrogen Vacancy Diamonds with Liquid Top Layer

Philip Chrostoski, Jaime Cardona, Deborah Santamore

Nitrogen vacancy center diamonds have become a popular topic recently with their applications in magnetic field sensors and quantum computing. Experiments have found that noise becomes a serious problem when an NV center is placed near the surface. This noise arises from fluctuations in both the electric and magnetic fields. We investigated the electric field noise caused by thermal fluctuation since it will be the main cause of noise at room temperature. Our model consisted of the NV-center with liquid on the surface. We examined three-different surface liquids; water/air, D-glycerol, and propylene carbonate to compare with recent experiments [PRL 115, 087602 (2015)]. Using the fluctuation dissipation theorem, we obtained the noise spectrum. At low frequencies, less noise is generated for glycerol and propylene carbonate than water/air. However, while water and propylene carbonate begin to follow a power law $1/\omega^{1.5}$ around 0.1 MHz reducing noise further, glycerol's power law is much weaker and soon reaches relatively constant noise. Throughout the noise spectrum, propylene carbonate has the best reduction in noise until frequencies reach 10 MHz. At this point, water drops lower than propylene carbonate as the two noise spectra begin to flatten.

T60.00233: Controlling Surface Plasmon Propagation in Space and Time

Wayne Hess, Yu Gong, alan joly, patrick El-Khoury

We discuss directional control of surface plasmon polaritons (SPPs) propagating in space and time on noble metal surfaces using femtosecond laser photoemission electron microscopy (PEEM) and its and time-resolved variant. We demonstrate laser light coupling and interferometric focusing of SPPs using nanohole arrays and show how the array geometry (diameter, pitch, and number of rows/columns) influences plasmon focus and PEEM images. We demonstrate directed SPP launching, from both simple symmetric trench and hemispherical cap nanostructures. These studies reveal competition between SSPs and localized surface plasmon (LSP) modes and infer effects of laser polarization on the SPP and LSP coupling and interplay. Our time-resolved PEEM experiments use phase-locked femtosecond pump-probe pulses to generate movies with a 210 attosecond frame rate. The recorded movies of the PSP allow us to directly measure various SPP properties, including its carrier wavelength and group velocity (0.95c) in concert with finite-difference time domain simulations. Finally we discuss plasmon propagation across a material discontinuity (trench) and show enhanced plasmon signal detection using a heterodyne-like detection scheme.

T60.00234: Thermoplasmonic Dissipation in Gold Nanoparticle-Polyvinylpyrrolidone Thin Films

Tyler Howard, Jeremy Dunklin, Gregory Forcherio, Donald Roper

Thermal dissipation of plasmon energy from gold nanoparticles (AuNPs) dispersed in transparent polymers is important to biotherapeutics, optoelectronics, and sensing. This work evaluated heat dissipated by 16 nm AuNPs with negligible Rayleigh scattering cross-sections dispersed into sub-wavelength, 70-nm polyvinylpyrrolidone (PVP) films at interparticle spacings much less than the resonant wavelength. Compared to super-wavelength films with interparticle spacing near the resonant wavelength, measured optical extinction and temperature increase on a per NP basis decreased as AuNP concentration increased; change in temperature per NP decreased 22% and optical extinction per NP decreased 35% as AuNP concentration increased from 1.01 to 5.06 x 10^{15} NP/cm^3. The trend and magnitude of measured values were consistent with those from *a priori* description of optical extinction per NP derived from Maxwell Garnett effective medium theory (EMT) and from coupled diode approximation (CDA). Comparison of EMT, CDA, and finite-element analysis measured results showed the contributions to plasmon-resonant optical extinction and heat dissipation. These results support design and adaptive control of thermal dissipation from plasmonic films.

T60.00235: Nanophotonic designs for efficient propulsion and radiative cooling of the Starshot Lightsail

Ognjen Ilic, Cora Went, Artur Davoyan, Deep Jariwala, Michelle Sherrott, William Whitney, Joeson Wong, Harry Atwater

T60.00236: Abstract Withdrawn

We study the edge dispersion relations between two lattices of gyromagnetic resonators under opposite biased magnetic field. This system by topological argument is promising to have two non-reciprocal edge modes. In long wavelength limit, these lattices can be mapped to two homogenous gyromagnetic domains and their interface similarly supports two non-reciprocal edge modes. We found that such effective medium system can reconstruct the two surface modes near the center of the surface Brillouin zone. Based on the analysis of coupled dipole theory, we reveal that the difference in the edge dispersion relation is mainly contributed by lattice effect. In addition to dispersion relation, we also study the possible field information carried by the effective medium. In one of the edge modes of the lattice case, the spatial average electric field in any time flame does vanish near the zone center. This is in agreement with the zero electric field nature of the corresponding edge mode in the effective medium case.

T60.00237: Theoretical and numerical investigation of the interaction between phase-shaped electron probes and plasmonic modes

Hugo Lourenco Martins, Giulio Guzzinati, Johan Verbeeck, Mathieu Kociak

Electron energy loss spectroscopy (EELS) in the low-loss region has attracted a large interest due to its efficiency in resolving plasmonic resonance at the nanometer scale. However, standard low-loss EELS remained intrinsically unable to detect plasmonic optical activity. Nevertheless, phase shaped electron probes constitute a perfect candidate to overcome this limitation and measure the dichroic behavior of plasmons in an electron microscope. Moreover, it has been recently demonstrated that such probes can be created in an electron microscope by tailoring the phase of the beam. In the present work, we developed a semiclassical formalism describing the interaction between an electron probe with an arbitrary phase profile and a plasmonic mode. We showed that the equation ruling this interaction takes the elegant form of a transition matrix between two electron states mediated by the eigenpotentials of the plasmon modes. In this contribution, we will present the theoretical formalism and a wide variety of numerical studies of interactions between different nano-structures (e.g. helix, rod) and phase shaped electron probes (e.g. vortex beams, HG-like beams...), with a special emphasis on the experimental feasibility of the proposed geometries.

T60.00238: Green's Function for Scalar Wave Propagation Through a Nano-Hole in a Plasmonic Semiconductor Layer

Desire Miessein, Godfrey Gumbs, Harry Lenzing

An integral equation has been established to describe scalar wave propagation through a nano-hole in a plasmonic semiconductor 2D layer in terms of a Helmholtz scalar Green's function. An exact solution of this integral equation is obtained analytically in closed form for the Green's function and its associated dispersion relation for this structure.

T60.00239: Subwavelength imaging of collective modes in silicon nanopillar honeycomb lattices

Siying Peng, Nick Schilder, Sophie Meuret, Femius Koenderink, Albert Polman, Harry Atwater

Dielectric Mie resonators enable resonant light coupling into nanoscale volumes with low loss and therefore have had significant impact as antenna motifs for dielectric metasurfaces. They hold promise for diverse applications including optical interconnects, bioimaging and metasurface. We investigate coupling between silicon Mie resonators using angle-resolved cathodoluminescence (CL) microscopy and spectroscopy. Silicon resonators arranged in monomer, dimer, hexamer and honeycomb lattice configurations with <50nm features on 10nm free standing Si_3N_4 membranes yield sharp, high quality coherent cathodoluminescence images upon electron beam excitation of optical resonances. We directly visualize redistribution of optical modes resulting from hybridization between resonances in individual Mie resonators. Using angle resolved Fourier space cathodoluminescence spectroscopy measurements, we observe photonic band structures that can be excited selectively at specific frequencies and lattice sites. Our experiments show clear evidence that collective modes can be excited in arrays of dielectric Mie resonators, and the image and spectroscopy results illustrate these features with high spatial, spectral and angular resolution.

T60.00240: Study of precursor concentration ratios on low temperature solvothermal process for growth of $ZnSnO_3$ Nanowire Arrays.

Aayat Sabah, Fouad Albadrasawi, Domingo Mateo, Sarath Witanachchi

Lead Zirconium Titanate Oxide (PZT) is a widely used piezoelectric and ferroelectric material yet its environmental hazardous potential limits future prospects. $ZnSnO_3$ (ZTO) or Zinc MetaStannate, shows a deformed perovskite phase similar to that in Lithium Niobate, an alternative lead-free ferroelectric material with the general formula $ANbO_3$ making it a possible replacement for PZT due to its non-toxic composition. The synthesis method for growth of LN-type ZTO vertically aligned nanowires uses a low temperature solvothermal process. Previous work proved that in basic conditions and on conductive substrates, a mass ratio of Zn precursor to Sn precursor of 0.9 leads to the formation of desired nanowires but growth is random across the substrate with little tunability of nanowire formation. A spatially ordered monolayer template of Aluminum doped Zinc Oxide nanocolumns on Silica Nanospheres adds another source of zinc to the reaction and will be studied to understand the effects of reaction precursors on the reaction products. The study of reaction products at different Zn and Sn precursor ratios will be measured with XRD and SEM along with EDS will be used to study the reaction products to determine which phase, either LN-type $ZnSnO_3$ or cubic perovskite $ZnSn(OH)_6$,will grow.

T60.00241: Tunable Mechanical Metamaterial with Ultra Effectiveness Based on Jamming State Honeycomb Structure

Xiangying SHEN, Lei Xu, Xinliang Xu

Mechanical metamaterials are sorts of artificial materials that can achieve unconventional properties due to the certain structures of arraying their unit cells. Many progresses are reported so far, including negative Poisson ratio, negative compressibility transitions, ultra-stiff and ultra-light materials, and also materials with tunable mechanical responds. However, almost all the researches focused on ordered crystallized structures, and the disordered systems are lack of investigations. We generated several honeycomb structures consisting of a number of nodes and bonds that connect each nodes, referring to the jamming transitions, which are very different from the formation of crystalline solids. We have noticed these engineered cellular solids with random porosities and structures are ultra sensitive to the applied loads when some certain bonds are replaced or removed. The phenomenon permits us to tune the modulus of such disordered structures in a large range just by subtracting a small fraction of the bonds. We perform the experiments and realize these honeycombs by using springs and hinges. Thus, from both simulations and experiments, we track the steps of bonds reducing, and find some regularities to help us establish a theoretical model to clarify the mechanism.

T60.00242: Toward Two-Dimensional Dirac Half-metallic MX3 for Spintronics

Qilong Sun, Nicholas Kioussis

The development of two-dimensional (2D) materials with the coexistence of intrinsic half-metallic and Dirac features will be of great realistic significance for next-generation spintronic nano-devices. Using first-principles calculations, we demonstrate that the pristine 2D MX_3 are the highly desired Dirac half metals and feasible in experiment. All MX_3 monolayers possess Dirac cone in the conducting spin channel with high Fermi velocities, while the other spin orientations have large energy gaps. The evaluated Curie temperature indicate MX_3 monolayers can maintain their ferromagnetism beyond room temperature. Remarkably, our results show that some monolayers exhibit large magnetocrystalline anisotropy (MCA). When including the spin−orbit coupling, the Dirac cones open small gaps and give rise to topologically nontrivial states with nonzero Chern number (-1), indicating MX_3 MLs are the Chern insulator and Chern half-metals. This work not only highlight the promising candidates for future spintronic applications, but also paves the way for the realization of integrating the long-craved qualities and quantum anomalous Hall effect (QAHE) in pristine 2D layers.

T60.00243: Regulation of near magnetic field distribution by using ultra-subwavelength magnetic metamaterials

Li Tongyu

We propose a method to locate the frequency where the best magnetic field uniformity is achieved of ultra-subwavelength magnetic metamaterials (MMs) with different laying patterns. Frequency bandwidth of MMs retrieved from time-domain experiments and two statistics of magnetic field distribution narrow frequency scope greatly. The result of magnetic field distribution demonstrate MM's powerful regulation of near magnetic field in wirelessly power and information transmission, including the enhancement of power transfer efficiency and variation of field distribution.

T60.00244: Atomistic simulations of tungsten nanotubes under uniform tensile loading

Travis Trusty, Shuozhi Xu, Irene Beyerlein

Nanotubes (NTs) are generally lighter than nanowires (NWs) and can possess equal or greater strength, despite this, body-centered cubic (BCC) NTs have been scarcely studied. In this work, molecular dynamics simulations are performed to investigate the tensile loading of BCC tungsten NTs and NWs. NTs (of various

thicknesses) and NWs with outer radii 5 nm, 10 nm, 15 nm, and 20 nm are uniformly stretched at 300K in the <100>, <110>, and <111> directions, respectively. Our simulations show that some NTs possess higher yield stress and yield strain than their NW counterparts. Specifically, (i) NTs with 5 nm outer radius exhibit consistently superior strength across examined thicknesses -- maximums being a 40% increase in yield stress and 5% increase in yield strain compared to the NW with the same outer radius; (ii) NTs oriented along <100> have consistently higher yield strains compared with the corresponding nanowires; (iii) when the experimental temperature is set at 800K, there is an increase in Young's modulus for all orientations and a ductile brittle-transition in the 15 nm NW case.

T60.00245: Light Scattering Nanoparticles: Plasmonic Resonances on Spheres and Regular Polyhedra Through the Theory of Characteristic Modes

Dimitrios Tzarouchis, Pasi Ylä-Oijala, Ari Sihvola

The optical properties of nanoscatterers have generated increasing research interest due to the recent advances in nanotechnology. In particular, an interesting case of resonant nanoscatterers are the plasmonic nanostructures, i.e., particles able to support localized charge oscillations, known as surface plasmons [1]. The appearance of these resonances is highly influenced by the material and morphological characteristics. In this presentation we will focus on the theoretical study between two plasmonic nanopolyhedra, the hexahedron and the octahedron [2], highlighting their connection with the resonant spectrum of a plasmonic sphere. Key feature of the analysis is the implementation of the Theory of Characteristic Modes (TCM) for the case of plasmonic scatterers [2]. The results obtained reveal the existence of bright and dark resonant plasmonic modes, triggered by their particular morphological characteristics.

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T60.00246: What is the effect of liquid coarse-graining on the Kapitza conductance at the interface between water and non-polar surfaces?

Vikram Reddy Ardham, Frédéric Leroy

Quantities like heat capacity and thermal conductivity are largely reduced when one performs coarse-graining of the molecular systems by removing certain of degrees of freedom. However, it is not clearly known what influence coarse-graining has on energy transport through the interfaces. To address this issue, we compute Kapitza conductance (or thermal boundary conductance) of water-graphite interfaces, using two model resolutions (fully atomistic and coarse-grained) of water at a wide range of wetting strengths. Rather surprisingly, we observe that, the removal of liquid degrees of freedom only has a marginal influence on the Kapitza conductance. We notice that the first adsorbed water layer plays the most crucial role in determining the interfacial conductance. Similarities in adsorbed water layer structure and vibrations explain the similarity in conductance. Through spectrally resolved heat flux, we also identified that, most of the heat transport is made possible by the coupling of low frequency vibrations. These insights are a first step in the direction of understanding the influence of coarse-graining on interfacial energy transport and could pave ways to develop multiscale models to study large scale systems with high density of interfaces.

T60.00247: *Ultrafast optical study of surface acoustic waves up to 50 GHz on patterned layered nanostructures*

Brian Daly, Michael Colletta, Wanjiru Gachuhi, Erik Szwed, George Antonelli, Weili Cui

We report ultrafast optical pump-probe measurements of surface acoustic waves (SAWs) on patterned layered nanostructures. These very high frequency SAWs ranging from 5 to 50 GHz were generated and detected on the following patterned film stack: 25 nm Al / 60-112 nm a-SiO2 / Si (100). The Al was etched to form lines of rectangular cross section with pitches ranging from 1000 nm down to 140 nm and the lines were oriented parallel to the [110] direction on the Si. The absorption of ultrafast pump pulses from a Ti:sapphire oscillator operating at 800 nm generated SAWs that were detected by time-delayed probe pulses at 800 nm or 400 nm via a reflectivity change (ΔR). We compared our results to an isotropic elastic calculation and a molecular dynamics simulation. In all cases we identified a Rayleigh-like SAW with wavelength equal to the pitch and frequency in the range of 5 GHz – 24 GHz. In some samples, we identified additional SAWs or independent modes of the Al lines with frequencies close to 50 GHz. We also describe the effects of probe beam polarization on the measurement's sensitivity to the different surface modes.

T60.00248: Thermal Properties of Alkali Halide Nanowires for Energy Storage Applications

Mack Adrian Dela Cruz, Gary Pennington

Recently arrays of NaCl nanowires have been shown to self-assemble on the surface of porous materials. In addition, salts have been found to act as an effective thermal energy storage material, finding application in the storage of heat generated from solar cells with high efficiency and long storage times. It is of interest to determine how nanoscale salt structures, such as arrays of alkali halide nanowires, might be applied in such energy storage applications. In this work we will present simulation of the heat capacity and thermal conductivity of an alkali halide nanowire. A rigid shell model is used to determine the phonon spectrum of the nanowire and thermal properties are simulated using the phonon transport Monte Carlo formulation. Scattering mechanisms included are phonon-phonon scattering and phonon boundary scattering. Results will indicate how size affects the thermal properties of alkali halide nanowires and how these materials can be leveraged as nanoscale heat storage materials.

T60.00249: Finite-Frequency Noise of a Time-Dependently Driven and Interacting Quantum Dot

Niklas Dittmann, Janine Splettstoesser

We derive the current-noise spectrum stemming from a quantum dot weakly tunnel-coupled to a nearby electronic reservoir and driven by a time-dependent gate voltage. This experimentally relevant setup is frequently applied as an on-demand emitter of single electrons into a mesoscopic conductor. The presence of Coulomb interaction poses an additional challenge for a theoretical description. In this work, we extend a real-time diagrammatic technique to obtain the symmetric finite-frequency current noise. The derived noise spectrum reveals a rich interplay between different energy scales of this system, defined by the interaction strength, the tunnel-coupling strength, the temperature and the driving frequency. We discuss how the noise frequency probes features related to these energy scales.

T60.00250: Phonon Transmission Calculation in Nano-Phononic Crystals

Ruiyuan Ma

Nano-phononic crystals and diameter-modulated nanowires have attracted significant attention due to their low thermal conductivities and their potential application as thermoelectric materials. Tuning the geometry of these nanostructures to change the scattering mechanics and thus engineering a lower thermal conductivity has been proven in recent publications. However, the modal phonon transmission coefficients across these geometrically irregular nanostructures and the effect of nanostructure geometry on thermal transport has not been fully understood. In this work, a harmonic lattice dynamics and scattering boundary method based atomistic modeling tool was created to calculate phonon spectra and modal phonon transmission coefficients in nano-phononic structures and diameter-modulated nanowires. Three key geometrical parameters including the size ratio of irregularity, the length of periodicity, and the number of irregularity have been studied in this work. The phonon transmission results in the three studies gave direction on how to achieve lower thermal conductivity in these nanostructures.

T60.00251: Control of the energy gap in a molecular junction for making a molecular rectifier

Colin Van Dyck, Mark Ratner

Molecular junctions are the constitutive components of Molecular Electronics circuits. For any potential application, the energy gap in the junction, i.e., the accumulated energy difference between the electrode Fermi level and the two frontier energy levels of the molecule, is a key property. In this presentation, we show that the gap of the molecule inserted between electrodes can differ largely from the gap of the same molecule, at the isolated level. It can be widely compressed by the alignment mechanism at each metal/molecule interface.

This behavior is important to consider for characterizing and designing molecular junctions. We show that this is particularly true for a new mechanism of rectification that we recently introduced. This latter opposes resonant to non-resonant tunneling and is based on the control of the energy gap in junction. We show that both the structure of the molecule and the anchoring group drive the value of this gap, at equilibrium and under bias. In the end, this will highlight the crucial importance, and benefit, of the contact for Molecular Electronics.

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T60.00252: Magnetic Field Enhancement of Cooper Pair Cotunneling in InSb Nanowire Josephson Quantum Dot Devices

Chunlin Yu, Mingtang Deng, Philippe Caroff, Hongqi Xu

Magnetic fields will suppress superconductivity via the spin paramagnetic effect and the orbital effect. However, the observations of magnetic-field-enhanced superconductivity in superconductor nanowires and thin films were reported by several groups. Although the origin of the field-enhanced superconductivity still remains ambiguous, it is predicted that the interaction between the Cooper pairs and the magnet impurities in the superconductors plays a crucial role. Here, we have realized superconductor-sandwiched InSb nanowire quantum dot devices, in which the dot manifests itself as a magnetic impurity when it is occupied by an odd number of quasiparticles. The spin -1/2 quantum dot interacts with the superconductor leads via the spin-exchange effect, i.e., the Kondo correlation. We have observed an magnetic field enhanced Cooper pair cotunneling in each of the Kondo valleys that are associated with proper Kondo temperatures, which cannot be explained by magnetic field induced quantum phase transition. The corresbonding dot-lead coupling, bias voltage and temperature dependence measurements are systematically performed. The Josephson quantum dot supplies us a platform for the investigation of the subtle relation between Cooper pair and magnetic impurities in superconductors.

T60.00253: Magnetoelectricity in Epitaxial Manganite/Piezo Thin Films

Yanette Navarrete, Bo Truong, Charles Zhang, Susan Trolier-McKinstry, John Wei, Guo-meng Zhao, Oscar Bernal

Multilayer thin films of $La_{0.7}Ca_{0.3}MnO_3/BaHf_{0.045}Zr_{0.045}Ti_{0.91}O_3$ were grown on [100] Nb-doped $SrTiO_3$ substrates by pulsed laser deposition using KrF excimer. Two multilayer configurations: LCMO/BHZT and LNO/LCMO/BHZT were fabricated to achieve different magneto-electric effects (where LCMO = $La_{0.7}Ca_{0.3}MnO_3$, BHZT= $BaHf_{0.045}Zr_{0.045}Ti_{0.91}O_3$, and LNO = $LaNiO_3$). The multilayers were characterized by high-resolution transmission electron-microscopy and x-ray diffraction. Electrical transport (resistivity and Hall effect) and magnetic measurements show that the LCMO layer is ferromagnetic with a reduced Curie temperature of about 230 K, which is about 40 K lower than the bulk value. Our preliminary experiments show significant magneto-electric effects in both multilayer configurations.

T60.00254: Lateral Size Confinement Effect on Charge Transport at the Interface of $LaAlO_3/SrTiO_3$

Tsung-Chi Wu, Ming-Chin Chen, MingYuan Song, Akhilesh Singh, Wei-Li Lee

As shown in some earlier works, an additional lateral charge confinement of 2-dimensional electron liquid (2DEL) at the interface of $LaAlO_3/SrTiO_3$ (LAO/STO) has revealed several intriguing phenomena, such as exotic electron pairing outside of the superconducting regime and a mysterious boost in electron mobility. In this study, we have grown ten unit cells of epitaxial LAO films on the TiO_2-terminated STO substrates by the oxide molecular beam epitaxy (MBE) technique. We also

developed a feasible fabrication procedure to define the macroscopic 2DEL at the LAO/STO interface into micro-meter sized Hall-bar patterns with different line widths. The sheet resistances were found to be inversely proportional to the line widths as expected, where the sheet carrier density could be largely tuned by applying gate voltage via a bottom gate. The influence of additional lateral size confinement on magneto-transport properties of the 2DEL will be presented and discussed.

T60.00255: Observation of Step-like Conductance Plateaus in a Molecular Film
Sreetosh Goswami, Thirumalai Venkatesan

We explore the transport properties of a film made of a Ru-complex displaying memristive response where the switching in film conductance is controlled by the ligand redox states of the film molecules, while the counter ions account for the hysteresis. As temperature is lowered, the hysteresis in *J(V)* gradually decays below 145K till ~5K where it completely quenches. In the temperature range of 135K to 110K, we observe well resolved conductance plateaus at different applied bias with sharp transition in between them. The number of plateaus *N* in the *J(V)* follows the empirical rule of *N= d[nm]/5* where *d* is the film thickness in nm. The conductance plateaus correspond to a correlation of $[J_0]^N$, with J_0 = current of the first plateau. Each of the plateaus are characterized by *in-situ* Raman spectroscopy as well as photoluminescence (PL) measurement which scale as $N \times I_0$, where I_0 is the PL/Raman intensity of the first plateau. These observations indicate a layer by layer electron doping in the film where layers of around 5 nm get doped sequentially. By reducing the van der Wall radius of the counterion this step can be reduced to a single layer ~ 1.5nm! This is an unprecedented result in an amorphous film which might have significant implication in neuromorphic computing.

T60.00256: Silicene-Inspired Study of the Electronic and Reactivity Properties Silaaromatic Molecules
Martin Mosquera, Yang Yang, George Schatz, Mark Ratner, Tobin Marks

This talk presents a comprehensive study of the electronic and reactivity properties of a series of silicon-aromatic molecules including single- and fused-ring structures, and hybrid molecules containing carbon. These structures could be used in the potential design of new molecular materials for nanoelectronics applications. Previous studies reveal that the buckling conformation of silicene and all-silicon aromatic molecules reduces their conducting properties in comparison with graphene and its nanoflakes; hence physical/chemical modification is required to correct this problem. This study shows that for the hybrid silicon-carbon molecular structures the ratio between carbon and silicon, as well as their particular locations, strongly influence the HOMO-LUMO gaps. We suggest that nitrile, fluorine, and trifluoromethyl substituents are promising to confer air-stability to silaaromatic molecules. Finally we discuss hybrid molecules with planar configurations, delocalized Si=Si pi bonds, low HOMO-LUMO gaps, and their potential applications.
Reference: J. Phys. Chem. A., 120, 9476.

T60.00257: Theoretical investigation on the formation of hexagonal, honeycomb, and kagome superlattices of binary 1D nanoparticles
Younghoon Oh, Sung-Hwan Lim, Sung-Min Choi, Bong June Sung

Superlattices that consist of binary nanoparticles have attracted attention for their potential applicability. However, the synthesis of superlattices composed of two different types of one-dimensional (1D) nanoparticles is still challenging. In this study, we investigate the formation of superlattices composed of binary component 1D nanoparticles by experiments and theory. Our experiments demonstrate that two different superlattices (AB_2 and AB_3 types) can be obtained by tuning particle diameter and mixing ratios. We develop a mean field theory to understand the thermodynamics of the superlattices self-assembly. We calculate the free volume of three different phases (AB_2, AB_3 and random phases) at given size and number ratios, and estimate free energy per site of two types of coexisting phases (AB_2 + random and AB_3 + random). The theory shows that the different types of superlattices formation (observed in experiments) can be understood in terms of the free volume entropy-driven process. Based on the calculated free energy per site, we determine the thermodynamically favorable phase at given particle diameter and mixing ratio, which is consistent with experiments.

T60.00258: Study of Self-Assembled Polymer Grafted Nanoparticles
Yiwen Qian, Marco Eres, Xingchen Ye, Paul Alivisatos, Ting Xu

Compared to using alkyl-chain-based ligands decorating the surfaces of the nanocrystals, polymeric ligands offer distinct advantages, as they allow for more precise tuning of the effective size and 'interaction softness' through changes to the polymer's molecular weight, chemical nature, architecture, persistence length and surrounding solvent. Here the formation of polystyrene grafted nanoparticles, conditions for self-assembly of single-component superlattices and their scaling behavior with GISAXS, DLS and TEM analysis are discussed. Polystyrene grafted nanoparticles with different chemical nature (gold and iron oxide), core diameter (3-25nm) and brush thickness (1-10nm) are synthesized and the procedure of self-assembly is largely improved by liquid-air interface assembly. The softness of the polymer shell thus the interparticle distance as well as the ordering of self-assembled monolayers can be easily tuned by adjusting the solvent composition. This study can help to throw light onto the rational design of functional particle brush solids with controlled nanoscale interfaces and mesostructures.

T60.00259: Self-assembly of Dispersed Gold Nanorods and Shape Complementary Mechanism
Yong Xie, Yujia Liang, Xiaochun Wu, Ziyu Chen, Ivan Smalyukh, Qian Liu

Nanoparticle self-assembly promises scalable fabrication of composite materials with unique properties, but the device-size, dynamics process and symmetry control of assembly structures remain challenges. By adjusting the interactive forces and assembly conditions, we realize centimeter-scale self-assembly monolayer of the octagonal gold nanorods. The self-assembly dynamics are investigated by successive optical imagings in the critical stage of a droplet drying containing the dispersed gold nanorods. Shape complementarity is the primary way to control the symmetry of nanoparticle assemblies. Using it, tetragonal superlattice, breaking through the only hexagonal symmetry of the superlattice is realized. Multiscale modeling reveals that the governing forces arise from hierarchical molecular and colloidal interactions. These assembly strategies might be instructive for designing assembly of various nanoparticles and realizing diverse assembly structures with pre-engineered properties.

T60.00260: Investigation of CdS/Se Surfaces: How Dipole Interaction and Impurities Influence the Growth Process
Can Ataca, Wenze Gu, Brenda Rubenstein

Nanoparticles can spontaneously assemble into larger, microscale structures due to direct specific interactions and/or indirectly through the environment. Experimentally we synthesized core/shell CdS/Se structure tetrahedral building blocks which led to bernal spine structure, hexagonal wire and fcc/bcc superlattices. In order to understand the self-assembly mechanism, we conducted several theoretical simulations. Using ab-initio first principles calculations, we predicted the surface orientations of tetrahedral building blocks by calculating surface energies, magnetic ordering and dipole moments. In order to replicate the experimental environment in our simulations, we passivated the dangling bonds of tetrahedral building blocks with different materials at various concentrations. (single-H, multiple-H, water molecules, acetic acid and phosphonic acid) For each type and concentration of passivation, we determined the binding mechanism and the effects on the dipole moment. Sequentially by training our monte carlo code (which takes into account the dipole interaction and energetics of passivation) with ab-initio calculations, we manage to predict the conditions for formation of different self-assembly geometries and verified our experimental results.

T60.00261: Optical Devices based on Plasmonic Nanoparticles
Mohammad Abdul-Moqueet, Mahmoud Mahmoud

T60.00262: Abstract Withdrawn

One-dimensional nanostructures such as nanowires have become the focus of intensive research owing to their unique diameter and orientation dependent electrical properties. Lead Zirconium Titanate (PZT) is a ferroelectric material and one of the most widely used piezoelectric materials due to its high piezoelectric constant, and operating temperature relative to other commonly used piezoelectric materials. Using a combination of Glancing angle Deposition and Pulsed Laser Deposition, we constructed nanostructures on a silicon substrate. Glancing Angle Pulsed Laser Deposition (GAPLD) is a technique where the plume of an ablated target is deposited at an oblique angle on a substrate which form randomly spaced slanted nanowires due to ballistic shadowing. XRD, EDS, and SEM will be used to characterize the nanostructure. Specifically for piezoelectronic application where manipulation of the depletion layer is desired, nanostructures are useful due to their piezoelectric surface charges being proportional to the nanocolumnar aspect ratio. Future plans are to replicate these nanostructures on silica nanospheres to see how spatial ordering affects ferroelectric properties in nanostructures.

T60.00263: Small Silver Clusters Ligated by DNA Bases: Computational Study of Electrochemical and Structural Properties
Mohammed Jabed, Svetlana Kilina

Silver clusters grown in single-stranded DNA are promising new fluorophores for applications in bio-labels and bio-imaging, due to their highly emissive properties from visible to the near-infrared range and good biocompatibility. Photophysical properties of small silver clusters are largely size, charge, and structure dependent. We have performed Density Functional Theory (DFT) calculations to study 4 to 20 atoms Ag cluster. Calculations show that the geometry of clusters and their interactions with bases depend on the oxidation state. For uniform capping, the cytosines exhibit stronger binding to the cluster than guanines. Redox potentials predict higher stability for singlet configurations of clusters with the even number of Ag atoms, while doublet configurations are more energetically favorable for clusters with the odd number of atoms. The difference in the redox potential between clusters in their singlet and doublet spin configurations decreases with increasing the cluster size. Calculated absorption spectra show that the doublet optical transitions are significantly red-shifted, compared to singlets. However, the optical intensity of the first doublet peak decreases with the cluster size increase, and become completely optically forbidden when increases up to 17-20 atoms.

T60.00264: Ferroelectrically driven nonvolatile memory by interfacing 2D semiconductors with ferroelectric thin films
Zainab Zafar, MeiYing Liu, Amina Zafar, YuMeng You

Integration of 2D semiconductors with ferroelectrics can provide a route towards control of polarization switching by piezoelectric effect which allows the realization of exciting features of next-generation optoelectronic devices. The domains are written and read on the ferroelectric film using a piezoresponse force microscopy (PFM). We propose the use of typical Raman/PL imaging to predict the effect of phase change of ferroelectric on 2D materials. This mechanical writing not only controls the local surface charge but also tunes the electric fields into the channel arising from the polarization dipole. The two different ferroelectric polarization states with the stable current retention and fatigue characteristics make the present molecular ferroelectric based FET suitable for nonvolatile memory applications. The findings reveal that it is possible to obtain working of transistor with polar surfaces and possible to integrate 2D electronics with functional oxides.

T60.00265: Ab inito study of core-level shifts in nanoclusters and their correlation with the absorption energies on the surface.
Alexey Tal, Weine Olovsson, Alvaro Posada-Borbon, Henrik Grönbeck, Igor Abrikosov

XPS techniques are widely used for nanoclusters characterization. However, the comprehensive investigation of the spectral features and their origin has not been performed. In this work, we investigate the shifts of the core-level binding energies in small gold nanoclusters by using ab initio density functional theory

calculations. The shift of the 4f states is calculated for magic number nanoclusters in a wide range of sizes and morphologies. We find a non-monotonous behaviour of the core-level shifts in nanoclusters depending on the size. We demonstrate that there are three main contributions to the Au 4f shifts, which depend sensitively on the interatomic distances, coordination and quantum confinement. They are identified and explained by the change of the on-site electrostatic potential.
In order to investigate the correlation between the shifts of the core states and catalytic activity, we have studied Pd nanocluster with icosahedral and octahedral morphology. The absorption of ethylene was modelled for different sites and it was shown that it is well correlated with the core-level shifts. Thus, we show that XPS spectra may provide means for characterization of nanoclusters catalytic properties.

T60.00266: Thermoelectric characterization of PVDF:Bi_2Se_3:Au nanocomposites

Sam Bleser, Jacob Marke, Alem Teklu, Gregory Smith

We designed, fabricated, calibrated, and automated a system to characterize thin-film thermoelectric samples at room temperature. The apparatus characterizes the Seebeck coefficient, electrical conductivity, and the power factor. We fabricated polymer nanocomposite samples with a blend of Bi_2Se_3 nanoplatelets and Au nanorods in PVDF. Pristine samples of PVDF:Bi_2Se_3 exhibited poor electrical conductivity that we attribute to discontinuities in the conduction pathways between ends of the sample. We blended small quantities of gold nanorods into the samples to facilitate better conductivity between neighboring Bi_2Te_3 domains. We used an atomic force microscope and a scanning electron microscope to image and analyze the morphology of the thin-film samples.

T60.00267: Non-linear quantum effects in a triple quantum dot shuttle: hybrid entanglement properties

K Chagollan, Ernesto Cota, Fernando Rojas

We study non-linear mechanical (Duffing quantum oscillating model) effects on the current and quantum correlations in a triple quantum dot shuttle system (TQDS), consisting of three linearly arranged quantum dots with an oscillating central dot. Quantum entanglement of the TQDS for the eigenstates is characterized by the Schmidt number (K) and is studied as a function of voltage difference across the system. A geometrical visualization representation of a three level charge subsystem (qutrit) is discussed and the cases with K larger than 2 are fully studied to provide a visual representation of the class of entangled charge-oscillation states in the model.

T60.00268: Plasmonic Excitations in Nanoscale Clusters

Zhihao Jiang, Roelof Groenewald, Malte Roesner, Stephan Haas

In this poster, we discuss the plasmonic excitations in nanoscale clusters in the presence of an applied external electromagnetic field. The nonlocal dielectric function is calculated in real space within the random phase approximation, with the electronic energy levels and wavefunctions determined from tight-binding models. The resonant frequencies of plasmons are then identified using a self-consistent field approach. Our aim is to understand the effects of quantum tunneling and Coulomb interactions on the plasmonic excitations in nanoscale clusters. By changing the separation between clusters and embedding them into tunable dielectric backgrounds, we are able to control these two effects.

T60.00269: The Collective Excitations in Quasi-N-Dimensional (N ≤ 2) Electron-Gas Systems: The Competition Between the Inelastic Electron Scattering and the Inelastic Light Scattering

Manvir Kushwaha

The most fundamental approach to an understanding of electronic, optical, and transport phenomena in condensed matter physics is generally founded on two experiments: the inelastic electron scattering and the inelastic light scattering. We embark on establishing
a systematic framework for the theory of inelastic electron scattering and of inelastic light scattering from the electronic excitations in GaAs/Ga1−xAlxAs quasi-N-dimensional (N ≤ 2) electron systems (QNDES). To this end, we start with the Kubo's correlation function
to derive the generalized dielectric function and the inverse dielectric function within the framework of random-phase approximation.
After trying and testing the general analytical results, we compute the full excitation spectrum, loss functions for the inelastic electron scattering, and Raman intensity for the inelastic light scattering. It is observed that the dominant contribution to both the loss peaks
and the Raman peaks comes from the collective (plasmon) excitations. This leads us to infer that the inelastic electron scattering can
be a potential alternative of the inelastic light scattering for investigating collective excitations in QNDES.[See, e.g., M.S. Kushwaha,
AIP Advances **2**, 032104 (2012); **3**, 042103 (2013); **4**, 127151 (2014); **6**, 035014 (2016).]

T60.00270: Optical Transitions and Excitonic Properties of $Ge_{1-x}Sn_x$ Alloy Quantum Dots

Denis Demchenko, Umit Ozgur, Indika Arachchige

Using hybrid functional calculations and experimental characterization we analyze optical properties of 2-3 nm $Ge_{1-x}Sn_x$ alloy quantum dots, synthesized by colloidal chemistry methods. Hybrid functional theory, tuned to yield experimental bulk band structure of germanium, reproduces directly measured properties of $Ge_{1-x}Sn_x$ quantum dots, such as lattice constants, energy gaps, and absorption spectra. Time-dependent hybrid functional calculations yield optical absorption in good agreement with experiments, and allow probing the nature of the dark excitons in quantum dots. Calculations suggest a spin-forbidden dark exciton ground state, which is supported by the changes in the photoluminescence lifetimes with temperature and tin concentrations. The synthesis and theoretical understanding of $Ge_{1-x}Sn_x$ alloy quantum dots will add to the overall tool box of low to non-toxic, silicon compatible Group IV semiconductors with potential application in visible to near infrared optoelectronics.

T60.00271: How an Electrically Active and Magnetically Quantized Quantum Wire Can Act As an Optical Amplifier

Manvir Kushwaha

The fundamental issues associated with the magnetoplasmon excitations are investigated in an electrically active quantum wire characterized by a confining harmonic potential and subjected to a perpendicular magnetic field in the symmetric gauge. Essentially,
we embark on the device aspects of the intersubband collective (magnetoroton) excitation which observes a negative group velocity
between the maxon and the roton. A comprehensive study of the effect of an applied magnetic field and an electric field reveals some fascinating features regarding the existence of the magnetoroton excitation, which is crucial to track the action. The computation of
the gain coefficient suggests an interesting and important application: the electronic device based on such magnetoroton modes can
act as an optical amplifier. [See, for example, similar studies but in an electrically passive quantum wire in: M.S. Kushwaha,
Phys. Rev. B 78, 153306 (2008); J. Appl. Phys. 109, 106102 (2011); Mod. Phys. Lett. B 28, 1430013 (2014).]

T60.00272: Al_2O_3-Y_2O_3 ultrathin multilayer stacks grown by atomic layer deposition as perspective for optical waveguides applications

Javier Alonso Lopez Medina, Hugo Borbón Nuñez, Eder Lizarraga Medina, Eduardo Murillo Bracamontes, Roberto Machorro, Nicola Nedev, Heriberto Márquez, Gerardo Soto, Mario Farías Sánchez, Hugo Tiznado

Nanolaminate multilayers made of Al_2O_3 and Y_2O_3 bilayer slabs were grown at 250 °C via thermal Atomic Layer Deposition (ALD). Several samples were prepared, where the number of ALD cycles for the Al_2O_3 slab was kept constant at 17 ALD cycles (2nm), while the number for the Y_2O_3 slabs was varied from 1 to 100. An optical model was built and adapted for each sample considering the Cauchy relationship, which was used to simulate the optical response for transparent materials. The thickness obtained from the optical model was in agreement with the thickness of cross-sectional SEM images. The optical band gap, obtained from single-effective-oscillator model, varied from 5.45 to 4.24 eV as a function of the Y_2O_3 slab thickness. The refractive index as well as the optical band gap can be modulated systematically using the Al_2O_3:Y_2O_3 ratio as control parameter. By means of simulated propagation modes it is shown that there is a multimode behavior for thickness around 200 nm at wavelengths between 300 and 1550 nm. This study reveals the possibility of using Al_2O_3-Y_2O_3 nanolaminates as the core of optical waveguides useful in miniature optical circuits.

T60.00273: Probing plasmon-NV0 coupling at the nanometer scale with photons and fast electrons

Hugo Lourenco Martins, Mathieu Kociak, Sophie Meuret, François Treussart, Yih Hong Lee, Xing Yi Ling, Huan-Cheng Chang, Luiz Galvao-Tizei

The local density of optical states governs an emitters' lifetime and quantum yield through the Purcell effect. It can be modified by a surface plasmon electromagnetic field, but such a field has a spatial extension limited to a few hundreds of nanometers, complicating the use of optical methods to spatially probe emitter-plasmon coupling. Here we, show that a combination of electron-based imaging, spectroscopies and photon-based correlation spectroscopy enables measurement of the Purcell effect with nanometer and nanosecond spatio-temporal resolutions. Due to the large variability of radiative lifetimes of emitters in nanoparticles we relied on a statistical approach to probe the coupling between nitrogen-vacancy centers in nanodiamonds and surface plasmons in silver nanocubes. We quantified the Purcell effect by measuring the nitrogen-vacancy excited state lifetimes in a large number of either isolated nanodiamonds or nanodiamond-nanocube dimers and demonstrated a significant lifetime reduction for dimers.

T60.00274: Hybrid QD – Graphene/2DEG Semiconductor Phototransistors: Performance and Gate Tuning

Andrei Sergeev, Kimberly Sablon

Hybrid phototransistors combine solution processed colloidal semiconductor quantum dots (QDs) with graphene or two-dimensional (2D) semiconductor materials. While the outstanding performance of these devices has been already demonstrated, their photoreponse and noise characteristics have not understood yet. We have generalized the traditional "semiconductor" photoresponse model to the weakly degenerate optoelectronic materials. The presented model describes well the responsivity as a function of the electromagnetic power and material parameters. We also calculate and analyze the noise characteristics related to generation-recombination processes. We determine limiting characteristics of hybrid phototransistors and compare the theoretical limitations with available experimental results. We also analyze and compare advantages and disadvantages of graphene and 2D semiconductor materials for use in hybrid phototransistors. Finally, we calculate tradeoff detector characteristics depending on the gate voltage and examine perspectives of these detectors for adaptive sensing with tunable photodetector parameters.

T60.00275: Thermal plasmons and transport coefficients for pseudospin-1 dice lattices

Andrii Iurov, Godfrey Gumbs, Danhong Huang

Closed-form analytic expressions have been derived for the dynamic polarizability of the 2D pseudospin-1 dice lattices with a Berry phase for arbitrary frequency and wave vector. These calculations generalize previously reported results (J. D. Malcolm and E. J. Nicol, Phys. Rev. B { \bf 93}, 165433 (2016)). The plasmon dispersion relations at finite temperature for the dice lattice are compared with those of graphene to determine the role played by the presence of an additional flat

subband. We also calculated the corresponding temeprature-depedent Boltzmann concuctivity in the relaxation-time approximation.

T60.00276: Optical gaps in pristine and heavily doped silicon nanocrystals: TDDFT versus quantum Monte Carlo benchmarks

Rene Derian, Balint Somogyi, Adam Gali, Ivan Stich

We present a time-dependent DFT study of optical gap of light-emitting nanomaterials, the pristine and heavily B and P co-doped silicon crystalline nanoparticles. Twenty DFT exchange-correlation functionals sampled from the best currently available inventory such as hybrids and range-separated hybrids are benchmarked against ultra-accurate quantum Monte Carlo results on small (~1 nm) model Si nanocrystals. Overall, the range-separated hybrids are found to perform best as expected for charge-transfer type transitions. However, even the range-separated hybrids exhibit pronounced quality variation for our limited test set. The quality of TDDFT gaps is correlated with deviation from the Koopmans' theorem as a possible quality guide. In addition to providing a generic test of the TDDFT ability to describe optical properties of silicon crystalline nanoparticles, the results also open up a route to benchmark-quality DFT studies of nanoparticles sizes approaching those studied experimentally.

T60.00277: Spectral response and mapping of plasmonic resonances in nanometric-thick gold nanotriangles using a scanning tunneling microscope

Mario Zapata Herrera, Shuiyan Cao, Eric Le Moal, Dana Codruta Marinica, Sylvie Marguet, Elizabeth A Boer, Javier Aizpurua, Andrei Borisov

The optical response and mapping of the electromagnetic Local Density of States (EMLDOS) of single gold triangle nano-platelets (GTNP) is studied using a scanning tunneling microscope (STM). The GTNP are chemically-synthesized and deposited on a 100nm-thick ITO layer on a glass cover-slip. As the STM tip scans the GTNP, the inelastic tunnel current (ITC) in the biased tip-sample cavity locally excites the sample and the emitted light is collected to generate a position-dependent intensity map. We theoretically describe this process by describing the ITC of the junction as an external point dipole located above the platelet which induces the excitation of its different plasmonic modes. By solving Maxwell's equations under the dipolar junction excitation, dark, bright, edge and breathing plasmonic modes are identified in the energy-filtered plasmonic maps, as well as in the spectral response of the light emission. By comparing theory and experiment, we attempt to demonstrate the effective excitation of edge plasmonic modes and the possibility of using photon mapping with the STM as a characterization tool of dark-modes hardly excitable by optical means. Our goal is to establish electrically driven light emission as an alternative way to access dark modes at the nanoscale.

T60.00278: Power loss of a beam of charged particles to encapsulated graphene

Dipendra Dahal, Godfrey Gumbs

We have calculated the rate of loss of energy for a beam of charged particles to a hybrid structure consisting of a graphene layer and a conducting substrate. The theory involves a determination of the surface response function which we obtain in the random-phase approximation (RPA) in conjunction with a transfer matrix method involving the induced electrostatic potential due to an external electric field. A comparison of the contributions to the power loss due to plasmons and particle-hole excitations is carried out. We analyze the way in which the plasmon losses are influenced by an applied uniaxial strain as well as plasmon-phonon coupling.

T60.00279: Low-Frequency Surface Plasmons in Multicoaxial Negative-Index Metamaterial Cables

Manvir Kushwaha, Bahram Djafari-Rouhani

We employ an elegant response function theory, which does not require matching of the messy boundary conditions, to investigate the surface plasmon excitations in the multicoaxial cylindrical cables made up of negative-index metamaterials. The multicoaxial cables with dispersive metamaterial components exhibit a rather richer (and complex) plasmon spectrum with each interface supporting two modes: one TM and the other TE for $m \neq 0$ (the integer order of the Bessel function). The cables with nondispersive metamaterial components bear a different tale: they do not support simultaneously both TM and TE modes over the whole range of propagation vector. The computed local and total density of states enable us to substantiate spatial positions of the modes in the spectrum. Such quasi-one-dimensional systems as studied here should prove to be the milestones of the emerging optoelectronics and telecommunications systems. [See, e.g., M.S. Kushwaha and B. Djafari-Rouhani, J. Opt. Soc. Am. B 27, 148 (2010); B 27, 605 (2010); Mod. Phys. Lett. B 27, 1330013 (2013).]

T60.00280: Covalent and Noncovalent Functionalization of Single-Walled Carbon Nanotubes: A MD/DFT Study

Braden Weight, Svetlana Kilina

Carbon nanotubes (CNTs) have electronic and optical properties that depend on the chirality of the nanotube and can be tuned via covalent functionalization. The composition of these groups has been proven to affect the optical properties. We hypothesize that the geometric orientation of these groups has a larger impact on the electronic properties. Non-covalent functionalization by conjugated polymers affects the interaction between the CNT and covalently-attached groups, resulting in changes to the absorption and emission properties. Calculations have shown correlations between the tube chiralities and polymer wrapping morphology to pristine CNTs for the purposes of chirality separation. We extend this approach to covalently-functionalized CNTs to explore the CNT-polymer interactions and examine the impact on the optical properties. Our goal is to be able to understand and predict relative band gap values and emission energies for any given functionalization group and orientation. This will be achieved in two ways: (I) classical molecular dynamics to observe trends in binding energy of covalently-attached groups and (II) density functional theory (DFT) and time-dependent DFT to obtain the energy and intensity of optical transitions.

T60.00281: Anomalous quantization trajectory and parity anomaly in Co cluster decorated BiSbTeSe2

Shuai Zhang, Rui Wang, Fengqi Song

Through the application of Co clusters, quantum Hall effect is modulated for the topological insulator BiSbTeSe2, allowing an optimized surface transport. We show the extraction of two sets of converging points in the conductivity tensor space, revealing that the top surface exhibits an anomalous quantization trajectory, while the bottom surface retains the 1/2 quantization. Co clusters are believed to induce a sizeable Zeeman gap through antiferromagnetic exchange coupling, which delays the Landau level hybridization on the top surface for a moderate magnetic field.

T60.00282: Acoustic Metasurfaces for Energy Harvesting

Badreddine ASSOUAR, Shuibao Qi

As a kind of clean, ubiquitous and renewable form of energy, sound/noise may act as a promising sustainable power source for energy production. Due to low power densities in ordinary surroundings, sound/noise generally needs to be focused or confined through effective conversion media for better acoustic energy harvesting (AEH). Intuitively, classical Helmholtz and other chamber resonators could be used to enhance the acoustic confinement and subsequently realize AEH. The strategy based on the resonators suffers from defect of the bulky structures and uncontrolled wave field, thus hampering the applicable energy harvesting. In a different context, the recent emergence of the artificially engineered metamaterials and metasurfaces has significantly broadened the horizon of acoustic wave and wavefront manipulations. In this research, we theoretically and numerically report on innovative and practical acoustic energy harvesters based on acoustic metamaterials and metasurfaces [1, 2]. We will present our recent works on acoustic energy harvesting making use of a metamaterial and multilateral metasurfaces based on the coiling up space geometry and discuss their functionalities.
1. S. Qi, M. B. Assouar et al. APL, 108 (2016) 263501
2. S. Qi, Y. Li & M. B. Assouar. PRAppl, 7 (2017) 054006

T60.00283: Wigner delay times of Frozen Mode Regime in the presence of weak disorder

Zhi Ming Gan, Huanan Li, Tsampikos Kottos

Our ability to control wave transport via dispersion management is one of the greatest achievements of the last thirty years. It offers us the possibility to reduce a wave's group velocity, thereby enhancing wave-matter interaction. One way to achieve this slow wave propagation is through stationary inflection point (SIP) singularities where the relation between frequency and the wavenumber can be approximated as $(w-w_0) \sim (k-k_0)^3$. When an infinite periodic system is studied in the scattering scenario, the SIP gives rise to the so-called frozen mode regime (FMR). We investigate the stability of this FMR in the presence of (weak) disorder and derive scaling expressions (both with respect to the size of the sample and frequency detuning) of Wigner delay time, which provide a measure of time that a particle spends inside the scattering domain.

T60.00284: Reusable Moth-Eye nano-patterned PDMS sticker with a versatile function of coating for photovoltaics

Yong Ghymn, Sungeun Cho, Ahrim Jung, Hongsu Kim, Han Young Lee

Using PDMS, moth-eye nano-patterned anti-reflective coatings(ARCs) which are protuberant, aspect ratio >1 long and truncated corn-like shape are fabricated for both the photovoltaic efficiency enhancement and the device surface protection. Here, the nanostructured PDMS was replicated by soft imprint lithography using Si master prepared through colloidal lithography. We have two novelties in this work. The first, in contrast with the previously reported ARCs which are fixed in the device itself, the moth-eye nano-patterned PDMS ARC of this work is free from the device just like a sticker with the ability both repeatedly attachable and easily detachable. And the second, it is state of the art to make the protuberantly nano-patterned PDMS with high aspect ratio (>1), taking into account the fabrication difficulty attributed to PDMS nanostructures' collapse and clustering while hollow patterns on PDMS are well researched. The PDMS film of this work is expected widely applicable thus useful to such devices as flat panel displays, photodetectors, photovoltaics, etc.

T60.00285: Composition Profile Reconstruction From Simulated X-Ray Diffraction Patterns of Nanometer-Sized Core/Shell Nanoparticles

Wenbin Li, Matthew DeCamp, Karl Unruh

A computation approach to the reconstruction of composition profiles at various stages of diffusional mixing in core/shell nanoparticles has been developed and tested on simulated x-ray diffraction data. The algorithm consists of a two-step approach. In the first step a set of atomic coordinates based on an arbitrary initial composition profile is constructed and relaxed using a Monte Carlo algorithm and realistic Lennard-Jones interaction potentials. In the second step the Debye formula is used to calculate the corresponding diffraction profile which is compared to the target diffraction pattern. An updated concentration profile is then constructed and the entire process repeated with the best concentration profile at each iterative step used as the starting point for the iteration. This approach does not assume that the actual composition profile is a solution to the diffusion equation and, therefore, can be used in the analysis of x-ray diffraction data on nanostructured diffusion couples and at very early diffusion times and/or in the presence of steep composition gradients.

T60.00286: Tunable surface plasmonic property of Au/Au hybrid bullseye nanostructure

Qigeng Yan, Desalegn Debu, Pijush Ghosh, Mourad Benamara, Gregory Salamo, J. B. Herzog, M. E. Ware

Metallic bullseye nanostructures have been widely studied for its enhanced focusing property for electric-field and surface plasmon (SP) excitations. Possible applications include plasmonic lenses, biological sensors, and light-absorption enhancement for solar energy devices. Focused ion beam (FIB), which is widely used as a single-step patterning technique, has been introduced to fabricate bullseye resonators with periodic concentric rings and grooves. We are showing a bullseye nanoresonator fabricated by FIB patterning with tunable plasmonic properties by employing Au/Ag hybrid metallic layers. The use of hybrid metallic structure, consisting of 50 nm Au on the top of 50 nm Ag can increase the sample quality, since Ag bullseye plasmonic lens has an intense surface plasmon resonance and appropriate plasmonic activity, and Au has a good chemical and structural stability. Tunable SP property can be found by using cathodoluminescence (CL) as the characterization technique. The strong background can be seen based on the fabrication method, however, we can investigate the tunable SP signal by controlling the excitation location, size, and the number of grooves.

T60.00287: SURFACES, INTERFACES AND THIN FILMS

T60.00288: *Increasing the Area Capacity of Lithium-Ion Battery Electrodes via Surface engineered Tape-Casting Method*

Tawaddod Alkindi, Rahmat Susantyoko, Saif Al Mheiri, Hamda Al Shibli, Amarsingh Kanagaraj, Boo Hyun An, Daniel Choi

Although Li-ion batteries are very promising for energy storage applications, their areal capacity is quite low (2.09 mAh cm^{-2} for conventional $LiFePO_4$ on aluminum foil). The aim of this work is to enhance the areal capacity of $LiFePO_4$ cathode via Surface-Engineered Tape-Casting (SETC) technique. SETC technique enables fabrication of strong stand-alone structured carbon nanotube (CNT) sheet with tunable thickness and composition. The CNTs form electrically conductive networks that also result in enhancing the charge transport of Li-ions. In addition, areal capacity will be increased by using the following approaches: increasing the thickness of CNT-$LiFePO_4$ sheet and changing the CNT/$LiFePO_4$ ratio. We will determine the optimum thickness and composition of the CNT-$LiFePO_4$ sheet. Batteries will be assembled in a glove box and characterized (CV, charge-discharge, EIS) using a potentiostat/galvanostat. Investigation of the multi-layered CNT-$LiFePO_4$ sheets by scanning electron microscopy, Raman scattering spectroscopy and X-ray diffraction is also in progress. Preliminary results show 0.4 mAh cm^{-2} for 2 layers of CNT-$LiFePO_4$ (CNT:$LiFePO_4$ = 1:1, w/w ratio). Fabrication of the electrodes with more than 10 layers of CNT-LiFePO4 is in progress.

T60.00289: Abnormal Phase Transition Between Two-Dimensional High-Density Liquid Crystal and Low-Density Crystal Phases of Carbon Monoxide on Cu(111)

Wenbin Li, Longjuan Kong, Baojie Feng, Huixia Fu, Hui Li, Xiao Zeng, Kehui Wu, Lan Chen

A few matters in nature show anomalous density change, i.e., their density decreases upon liquid-to-solid transition. Such an anomalous density change can be either attributed to directional intermolecular hydrogen bonds, e.g., in case of liquid water, or to the directional covalent bonds, e.g., in cases of liquid phosphorus, gallium, and silicon. For two-dimensional (2D) matters, e.g., liquid water confined to a nano-slit, a similar anomalous first-order transition between the high density liquid (HDL) and low density amorphous (LDA) ice was predicted based on atomistic molecular simulation. Herein, we report the first direct experimental observation of an entropy-driven phase transition from the 2D high density liquid crystal (HDLC) to low density crystal (LDC) for the carbon monoxide (CO) monolayer adsorbed on Cu(111) surface, in the temperature range of 5~77 K. This anomalous 2D liquid crystal-to-solid transition provides a novel platform for exploring unusual thermodynamics of 2D matters, in addition to the application driven research of copper-based catalysis such as CO oxidation.

T60.00290: Characterization of dielectric mirrors

Michael Milovich-Goff, Lamar Glover, Riccardo DeSalvo, Seth Linker, Lara Daneshgaran

The performance of the mirrors used in the LIGO interferometric system is limited by both thermal noise and light scattering that are a result of the manufacturing process. The study of these scatterers is fundamental in the development of better mirrors. We attempt to measure the distribution of light scatterers within the layers of coating witness samples. Mapping them both depth-wise and laterally using microscopy and fitting procedures. Last year we demonstrated the feasibility of identifying the depth of small features with a few nm precision. Building on that experience we now try to identify the size and location of a scatterers inside real coatings, using CCD microscope camera, 3-axis stepper motor stage and advanced cleaning techniques to eliminate spurious signals by traces of dirt. Currently another feasibility study is being conducted to see if it is possible to determine weather scatters are within 3 microns of each other on a lower magnification microscope. If indeed they are its possible to determine if scatterers reside in the roughly 3 micron thick deposition of a LIGO test mass or witness sample. If successful this may become a standard inspection technique to monitor and guide the development of lower scattering and thermal noise.

T60.00291: Physical Vapor Deposition of Sn Films on Si Substrates

Danica Bergin, Miguel Ochoa, Yize Li

Sn films are grown on Si (100) and Si (111) substrates through physical vapor deposition of solid Sn sources, where ultra-high purity Ar gas serves as the carrier gas. The dependence of the morphology and structure of the Sn film on the surface termination of the Si substrate, the deposition temperature, and the deposition pressure is investigated. The strain of the Sn film, as determined by x-ray diffraction (XRD), is found to be dependent on the deposition temperature.

T60.00292: Adsorption characteristics of a DHTAP molecule on Cu(110)

Walter Malone, Abdelkader Kara, Anthony Thomas, conrad Becker

Using density functional theory we study the adsorption of DHTAP(C18H12N4) on the Cu(110) surface. To account for long range dispersion interactions, we use the van der Waals inclusive functional (vdw-DF), optB88-vdW. We explore a total of 4 adsorption sites with the molecule's plane parallel to the surface for 5 different coverages. We find the most energetically favorable adsorption site occurs when the center of molecule's rings lie over the troughs present on the (110) surface, allowing the molecule's nitrogen atoms that lack hydrogen to bond to the rows present on the (110) surface. We calculate a variety of geometrical properties of the substrate/adsorbate system including adsorption height, buckling of the first layer of the substrate, and buckling of the molecule upon adsorption on the Cu(110) surface. Along with this, we calculate several electronic properties of the system in each unit cell including change in the surface's work function, charge transfer, and change in the width and center of the d-band of the first layer surface atoms upon the adsorption of DHTAP. Comparisons with experimental data show good agreements for adsorptions geometries.

T60.00293: Predictive first-principles modeling of complex inorganic/organic interfaces: PTCDA on Au(111)

Victor Ruiz, Alexandre Tkatchenko

Understanding the properties of hybrid inorganic/organic systems has implications in both fundamental science and technology. An ab-initio modeling of these interfaces require efficient electronic-structure methods that capture accurately covalent and non-covalent interactions and an atomistic model that includes complex adsorption configurations and accurate surface representation. We present a predictive characterization of the structure and stability of perylenetetracarboxylic dianhydride (PTCDA) adsorbed on Au(111) within density-functional theory. Our calculations include collective many-body effects in the modeling of non-covalent interactions and a quantification of the self-interaction error in the adsorption energy of the system. We address effects due to single molecule/monolayer surface coverage and the role of the experimentally observed 22 × √3 surface reconstruction. Our approach yields an adsorption geometry in agreement with experiments within 0.1 Å and explains a difference of ≈ 0.5 eV observed in the adsorption energy of the system between atomic-force microscope and temperature-programmed desorption experiments. Our work shows that the inclusion of all relevant collective effects yields predictive power in the first-principles simulation of complex interfaces.

T60.00294: The Calculation of Surface Plasmon of Ag Nanowire on Quantum Dots Semiconductor

Chin-Sheng Wu

The surface conduction electrons of Ag nanowire and quantum

dots semiconductor provide the collective excitations.

ZnO with wide direct band gap (3.37 eV) is a well-known and

an interesting compound semiconducting material, which have

been used for the fabrication of light emitting diodes and

piezoelectric devices in spontaneous emission amplifiers.

Furthermore the fluorescence emission is enhanced in Ag

nanowire/ZnO quantum dot system.The resonance peak depends

on the shape of the Ag nanowire. The red shift of the peak

becomes more obvious with the increase of Ag nanowire

radius. The localized surface plasmon resonance modes of Ag

nanowires are investigated theoretically by Maxwell's

equations and the usual boundary conditions method. The

introduction of the electronic density directly into the

macroscopic dielectric constant is used as a means of

calculating the plasmon frequency of inhomogeneous

electronic systems. The spectrum, electric field

distribution versus excitation wavelength of Ag nanowires

are simulated. The results show that the Ag nanowires have

peaks.

T60.00295: A Study of the Microstructural Effects on Optical Parameters and Quantum Efficiency in VO_2 Thin Films on TiO_2 and TiO_2:Nb

Jason Creeden, Melissa Beebe, Douglas Beringer, Scott Madaras, Irina Novikova, Rosa Lukaszew

The project goal is to optimize the photosensitivity of VO_2 thin films in the near-UV and UV regions; following the recent demonstration that VO_2 grown on niobium doped TiO_2 (TiO_2:Nb) substrates can push the photoconductive response into the visible spectrum. By controlling the microstructure of the films via deposition parameters and substrate doping, we optimize the VO_2 growth for TiO_2 and TiO_2:Nb substrates. In doping the substrates, we strain the monoclinic structure in the insulating VO_2 phase toward the tetragonal structure in the metallic phase. Using X-ray diffraction, we determine that films grown on TiO_2:Nb structurally exhibit a ~.25^o shift in peak location compared to the undoped films. Under a 405 nm laser, the VO_2 on TiO_2:Nb exhibits sharp and comparatively large optical responses, through the thermally induced insulator to metal transition, to those seen with VO_2 on TiO_2. The films exhibit a photocurrent, upon 405 nm illumination, for both the doped and undoped films with a greater quantum efficiency associated with the optimized doped films. Suggesting that the optimized doping enhances the near-UV optical response and quantum efficiency of the film.

T60.00296: Discontinuity of the Corner-shared Octahedral Network at the Interface of $BiFeO_3/SrTiO_3$

Dianxiang Ji, Min Gu, Chunchen Zhang, Zhengbin Gu, Sebastian Reyes-Lillo, Jeffrey Neaton, Peng Wang, Yuefeng Nie, Xiaoqing Pan

T60.00297: Abstract Withdrawn

Titanium nitride films were grown by a pulsed laser deposition technique using a variety of deposition parameters such as substrate temperature, gas pressure etc.The TiN thin films fabricated at temperatures in the range of 500-800 °C in vacuum are found to be epitaxial with (111) orientation. Low temperature transport properties were systemically studied in TiN films with varying room temperature resistivity (100-500 μOhm cm) under applied magnetic fields of 0 to 5.0 T. The temperature dependence of resistivity ρ(T) shows minima at low temperatures (T < 40 K) under various applied fields. Fittings of ρ(T) data were done by considering both electron-electron (e-e) interaction term μ $T^{1/2}$ and Kondo-like scattering term μ ln T. Hall measurements and their data analysis have shown that the charge carriers are electrons in metallic TiN films. For example, the Hall coefficient and electron density at 300 K were found to be -6.4×10^{-5} cm^3/C and 9.7 × 10^{22}/cm^3, respectively. A renewed interest in research in TiN films stems from the possibility of converting metallic TiN films into semiconducting TiNO films with variable band gaps. The bandgap engineering of TiN/TiNO might open up a new avenue in the photocatalytic splitting of water for fuel cell applications using solar light.

T60.00298: Refractive Index and Bandgap Variation in Al_2O_3-ZnO Ultrathin Multilayers Prepared by Atomic Layer Deposition

Javier Alonso Lopez Medina, Hugo Borbón Nuñez, Eder Lizarraga Medina, Eduardo Murillo Bracamontes, Roberto Machorro, Nicola Nedev, Heriberto Márquez, Mario Farías Sánchez, Gerardo Soto, Hugo Tiznado

This research focuses on the study of the refractive index n(λ) and optical bandgap E_g behavior in ultrathin multilayer films of Al_2O_3-ZnO bilayers grown via atomic layer deposition (ALD) technique on Si(100). The multilayer configuration consists in alternate layers of constant thickness Al_2O_3 (2 nm) and varying thickness ZnO films in order to obtain a total thickness of ~100 nm. A set of 10 samples based on bilayers with various 2:X thickness ratios were prepared, where X refers to the ZnO layer thickness. X is proportional to the number of cycles (N) of the ZnO precursor, varying from 1 to 100. The total thickness, n(λ) and E_g values of each multilayer sample were studied via spectroscopic ellipsometry. Scanning electron microscope images verified the multilayer total thickness and corroborated the accuracy of the optical model used. We observe that the n(λ) values varies between 1.63 and 2.3 for λ ~ 370 nm and the E_g values decreases when the bilayer thickness increases, with a maximum variation for ΔE_g ~1.6 eV. These results reveal that the n(λ) and E_g of this material can be modulated systematically as a function of the bilayer thickness and can been suitable for optoelectronics applications.

T60.00299: Control of II-VI/III-V heterovalent interfaces with light

Kwangwook Park, Kirstin Alberi

In-situ light stimulation can provide an additional parameter to control semiconductor epitaxy along with well-known parameters such as growth temperature and V/III ratio. However, the influence of light on the properties of II-VI/III-V interfaces has not been investigated. Using ZnSe/GaAs as a model system, we probe the mechanisms of light-stimulated heterovalent interface formation by molecular beam epitaxy. X-ray diffraction, scanning electron microscopy, atomic force microscopy, and photoluminescence measurements reveal that UV light irradiation during interface initiation enhances As desorption and promotes additional Ga-Se related bonding at the ZnSe/GaAs interface. In moderation, the Se coverage passivates the interface and improves emission from the GaAs epilayer. Light stimulation also allows the ZnSe epilayer to be grown at lower temperatures to prevent excessive atomic interdiffusion. These results suggest that low temperature growth accompanied by UV light irradiation can be used to control intermixing at the ZnSe/GaAs interface [1].
[1] Kwangwook Park and Kirstin Alberi, Sci. Rep. **7** 8516 (2017).

T60.00300: Nanofabrication of GLAD Structures – A Comparison of Ion and Electron Beam Deposition Techniques

Judy Tran, Rene Feder, Matthew Hilfiker, Eva Schubert

In this work we have grown slanted columnar thin films, by method of glancing angle deposition, from titanium (Ti) on silicon (Si) substrates using ion beam sputtering (IBS) and electron beam evaporation (EBE) to produce a particle flux which hits the substrate at an angle of approximately 85 degrees. Due to mechanisms of atomic shadowing and limited surface diffusion, these films exhibit a high porosity. Particle fluxes created by IBS and EBE show some significant differences regarding the particle energy distribution, flux rate, and flux angle divergence. We show a comparison between the growth rate, porosity, and slanting angles of the films for different growth methods. To achieve this data, the deposited films were optically analyzed by spectroscopic ellipsometry using an RC2. A model containing an ABEMA layer was built and fitted to the experimental data, providing the physical properties of the thin film. The structural properties from the optical analysis were supported by high resolution SEM images.

In conclusion, EBE provides a higher deposition rate than IBS, but the films show a higher porosity and the columnar structures tend to have a more pronounced fanning, limiting the usability and thickness of the film.

T60.00301: Transfer Process of Epitaxial Functional Oxide Thin Films onto Flexible Substrates

Shinji Umatani, Hiroaki Nishikawa

Recently, fabrication of functional materials such as transparent conducting oxides on flexible polymer substrates has been intensively investigated. Because most flexible substrates are not heat resistive, these flexible devices have mainly consisted of amorphous oxides or organic materials showing excellent electric and optical transparency due to their low process temperature. We have proposed to realize flexible devices of functional oxides which show many attractive properties such as ferroelectricity, ferromagnetism. Thin film growth of functional oxides requires relatively high process temperature of several hundreds °C, thus it is difficult to deposit these materials on flexible substrates directly. We focused on acid etching of MgO (100) single-crystal substrates in order to realize flexibilization of epitaxial functional oxide thin films. In this study, we report a result on transfer of ferroelectric/piezoelectric $BaTiO_3$ (BTO) on flexible plastic sheet as a preliminary examination.
BTO thin films were deposited on MgO (100) substrate using pulsed laser deposition. After the deposition of BTO, the sample was soaked into a phosphoric acid solution. Using this process, we succeeded in transfer of *c*-axis oriented BTO thin film onto polymer sheet.

T60.00302: Capillary Wrinkling of Nanocomposite Films

Jooyoung Chang, Thomas Russell

We have investigated morphology and capillary wrinkling of PS-SH M_w 124k chemisorbed on 12 nm (diameter) of Gold Nanoparticles (GNPS) in PS M_w 97k matrices with various weight fractions (0%, 5%, 9% 13%) of the GNPS. The PS chemisorbed GNPS were uniformly dispersed in the PS M_w 97k matrices even if the weight fraction of GNPS increased up to 13%, determined by AFM micrographs. Various thicknesses (30 to 300 nm) of nanocomposites were floated on water. A water droplet was applied on the floating nanocomposite film to induce hoop compression, resulting in the radial wrinkle patterns on the film [1]. As the weight fraction of the GNPS increases, the length of wrinkle increases while the number of wrinkle decreases, regardless of the thickness of the nanocomposite films. This indicates the Young's modulus of the composites increases twice with the addition of GNPS from 0 to 13 wt%.

[1] Science 2007, 317(5838), 650-653

T60.00303: Long-term reliability of Pb-free solder joint between copper interconnect and silicon in photovoltaic solar cell

Marco Fronzi, Omid Mokhtari, Yunjiang Wang, Hiroshi Nishikawa

SnAgCu (SAC) solder, the most common Pb-solder in-use for PV modules, is reported to exhibit formation of crack at the interface of solder and Ag paste, limiting the lifetime of PV devices. This is reported to be as a result of thermal expansion mismatch caused by low coefficient of thermal expansion (CTE) of the Si compared with the metallic elements in this system. However, since the formed IMCs at the interfaces in this system is prone to crack due to their brittle natures, the crack forms at the interface of these IMCs rather than the Si/Ag interface. This is due to the distribution of the generated thermal stress to the other layers in the system.
This study aims to expand the lifetime of the PV solar modules by reducing the possibility of the formation of cracks, by the addition of a minor alloying element. To understand the possible crack formation in the resulting systems, we evaluate:
1) the theoretical CTE of the Ag_3Sn and the newly formed IMC layer by a first-principles investigation.
2) the thermal stress distribution throughout the solder/Ag interface including the interface of the IMC layers by molecular dynamics simulations.
3) the experimental evaluation of possible crack in the joint.

T60.00304: Effects of thickness and substrate properties on cracks in thin films bonded to an elastic substrate

Dong Hyun Kim, Won Bo Lee

Cracks occurring in thin films caused by residual tension can change desired film properties and lead to flaws or failures. Since the geometry of cracks or flaws is governed by the fracture properties of the interface and the substrate, in addition to known effects of film thickness, we investigate crack formations according to the film thicknesses using thermal deposition. Also by using different kinds of substrates and films, the effects of residual stress and elastic moduli on crack formation are investigated. As a result, several dimensionless quantities describing the cracks of thin films can be introduced.

T60.00305: Charge separation by high electronic excited state transition in organic photovoltaics

Shohei Koda, Mikiya Fujii, Koichi Yamashita

Organic photovoltaics (OPVs) are promising alternative energy devices with low cost, flexibility, light weight. Though the power convergence efficiencies (PCEs) of OPVs have reached more than 11%, the PCEs are lower than Silicon solar cells. Therefore, it is indispensable to achieve high PCEs, but one of the reasons for difficulty in improving PCEs is that the charge separation process in OPVs is not clear. In this research, we investigated why hot process and cool process which are currently discussed in the charge separation process differ depending on the molecules.
We investigated the energy profile from exciton states to charge separated states in two kinds of atomistic interface, P3HT/PCBM and PCPDTBT/PCBM. Namely, we prepared bilayer interfaces of P3HT/PCBM and PCPDTBT/PCBM, which were made by conducting molecular dynamics simulations with 48 donor molecules and 144 acceptor molecules. Then, we calculated electronically excited states in those interfaces by applying semi-empirical quantum calculations and then revealed charge separation pathway reaching 4 nm of electron-hole distance. Finally, we discussed critical effects of charge delocalization on the charge separation pathway and charge recombination rate.

T60.00306: Atomic structure of a monolayer of NaCl on Ag (110) surface

khalid Quertite, karima Iasri, Hanna Enriquez, Andrew J. Mayne, Azzedine Bendounan, Gérald Dujardin, Nicolas Trcera, Abdallah El kenz, Abdelilah Benyoussef, Abdelkader Kara, Hamid Oughaddou

Here we report on the adsorption of an NaCl film on Ag (110) under ultra-high vacuum conditions. At room temperature, Low Energy Electron Diffraction and Scanning Tunneling Microscopy show that the NaCl film forms a (4x1) superstructure. At RT, the film consists of small-sized islands that coalesce into larger islands at 410 K. These large islands preserve the (4x1) superstructure and cover the entire surface. A computational study using density functional theory calculations, with and without the inclusion of van der Waals effects confirm the co-existence of two domains in agreement with the observed structure. We report on the calculated change in the work-function and charge transfer for the tow adsorption configurations as well as the geometrical details including adsorption height and corrugation.

T60.00307: PANI and PEDOT:PSS Dip-Coating on CdS/CdTe Solar Cells

Michael Patullo, Nnamdi Ene, Quinn Szanyi, Mehmet Sahiner

The ever-increasing importance of solar energy in today's green initiative creates an immense demand for the continual improvement of photovoltaic technologies, particularly thin film solar cells. The Department of Physics at Seton Hall University wishes to produce a more advanced solar cell by dip-coating high-conductive grade polyaniline (PANI) and poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) onto pulsed laser deposited cadmium sulfide/cadmium telluride substrates. In our previous studies, we have determined that depositing and dip-coating these particular substrates and polymers on indium tin oxide glass improves the photovoltaic conversion efficiency due to a reduction of the Schottky barrier resistance. In this study, we focus on optimizing the application of PANI and PEDOT:PSS solutions by experimenting with dip-coating procedures. The thin films are characterized by scanning electron microscopy, energy dispersive x-ray spectroscopy, and ellipsometry techniques. Electrical conductivity tests are also performed using a Keithley SourceMeter, and structure and efficiency results are going to be discussed.

T60.00308: Numerical Investigation of Topography's Role During Conductive Atomic Force Microscope mapping of Organic Semiconductors

REZA PEJMAN, Yongfeng Liang, Junpin Lin, Congrui Jin

In recent years, conductive atomic force microscopy (C-AFM) has been an indispensable tool for probing the nanoscale electrical properties of organic semiconductor films. It is currently unclear, however, the extent to which local topography impacts the probe-sample contact area, and in turn the measured C-AFM current levels. In this study, we numerically model the adhesive contact between C-AFM probes and organic semiconductor films with experimentally determined film topographies. The adhesive interactions are represented by the Lennard-Jones potential and the surface deformations are coupled by using half-space Green's functions discretized on the surface. We find that classical contact models do not accurately represent the probe-sample contact area. Topography is shown to impact the local contact area in cases when the local root mean squared roughness is greater than a few nanometers. For organic semiconductor films with a local root mean squared roughness under 5 nm, contact area variations from the planar case are less than 10%, indicating that for such samples, topography will have a minimal influence on C-AFM current.

T60.00309: Thermoelectric and Mechanical Characterization of Thinfilms of Bi(Se)Te doped with Gold Nanorods

Alem Teklu, Greg Smith, Jacob Marke, Sam Bleser

We studied thermoelectric and mechanical properties of polymer: topological insulator films composed of PVDF and Bi_2Se_3 nanoplatelets blended with different concentrations of gold nanorods. The surface morphology of the films using scanning electron microscopy and atomic force microscopy were investigated. Both high and low concentration (10% wt. and 67% wt. Bi_2Te_3) show homogenous distribution of polygonal platelets in pristine samples; however, the small size of the topological insulator nanostructures does not allow for facile conduction between ends of the sample. The addition of small quantities of gold nanorods provided conduction pathways between domains of the Bi_2Te_3 platelets, giving rise to a finite sheet resistance. The apparent usage for these devices is in flexible thermoelectric applications so we used the AFM to investigate the mechanical properties of the films as a function of gold nanorods concentration using a technique called nanoindentation.

T60.00310: Inter-diffusion of Hafnium and Silicon as studied by sputter depth profiling and X-ray Photoelectron Spectroscopy

Ritesh Bhakta, Anil Chourasia

The Hf/Si interface has been characterized by x-ray photoelectron spectroscopy. Thin films (thicknesses of about 500 nm) of hafnium were deposited on a silicon substrate. Prior to the sample deposition the silicon substrate was cleaned by HF for one minute and then loaded into the deposition chamber. The e-beam method was used for the deposition. The samples were annealed for 30 min at temperatures of 200 and 300°C. The inter-diffusion of hafnium and silicon was investigated by sequential sputter depth profiling and x-ray photoelectron spectroscopy. The x-ray photoelectron spectral data were recorded in the Hf 4f and Si 2p regions. The areas under the curve were used to determine the atomic concentration of the constituents. The interdiffusion was analyzed by the Matano-Boltzmann's procedure using the Fick's second law. The interdiffusion coefficients as determined from the data have been correlated with the annealing temperature.

T60.00311: Controlling Surface Patterning of Diamond: The Origin of Anisotropy with Electron Beam Induced Etching

Marco Fronzi, James Bishop, Milos Toth, Mike Ford

Diamond is an ideal material for a broad range of current and emerging applications in tribology, quantum photonics, high power electronics and sensing. However, top-down processing is very challenging due to its extreme chemical and physical properties. Gas-mediated electron beam induced etching (EBIE) has recently emerged as a minimally invasive, facile means to dry etch and pattern diamond using oxidizing precursor gases such as O2 and H2O. Here we elucidate the roles of hydrogen and oxygen in EBIE of single crystal diamond and show that oxygen gives rise to rapid isotropic etching, whilst the addition of hydrogen gives rise to anisotropic etching and topographic pattern formation. The anisotropy is attributed to preferential passivation of {110} and {111} planes over {100} planes, which is consistent with adsorbate binding energies calculated by density functional theory. Our findings constitute a comprehensive explanation of anisotropic EBIE and are important for the design and control of new and existing etch processes.

T60.00312: Effects of Dimensional Confinement on the Reactivity of Carboxylic-Acid-Functionalized Molecules

Dominic Goronzy, Erin Avery, Nathan Gallup, Jan Staněk, Jan Macháček, Tomáš Baše, Kendall Houk, Paul Weiss

Self-assembled monolayers (SAMs) provide a system to explore the effects of dimensionality on chemical functional groups. We probed interactions within carboxylic-acid-functionalized carboranethiol SAMs as well as the interactions between the monolayer and the environment. Monolayers composed entirely of *meta*-functionalized carboranethiols were imaged *via* scanning tunneling microscopy (STM). Unlike *para*-functionalized carboranethiols, which adopted the same nearest-neighbor spacing as unfunctionalized carboranes (7.2 Å), *meta*-functionalized carboranethiols have a larger spacing of 8.4 Å. Studies with two isomers of *meta*-carboranethiols yielded similar results. To examine the impact of dimensionality on the carboxylic acid group's acidity, we employed contact angle titration. We found a pK_a shift of nearly four pH units from 3.01-3.23 in solution to approximately 6.95 on the surface. Density functional theory calculations tested the effect of desolvation by two-dimensional (2D) confinement, showing a shift in pK_a consistent with experimental results. STM-observed differences in SAMs deposited in ethanol versus benzene provided further evidence for profound changes in carboxylic acid reactivity when placed in the 2D confinement imposed by the thin-film configuration.

T60.00313: In situ Monitoring Copper-based Oxide/Water Interfacial Reactions by X-ray Photoelectron Spectroscopy

Pitambar Sapkota, Alejandro Cabrera, Sylwia Ptasinska

Current research in material sciences is continuously trying to enhance the efficiency of photoelectrochemical (PEC) cells using various semiconductor photoelectrodes for water splitting. Such photoelectrodes should have good stability in aqueous media with suitable band-edge and band-gap energies to match both the potential for water oxidation-reduction reactions and the solar spectrum, respectively. Copper-based oxide semiconductors are candidates showing a great promise to fulfill these criteria, but little is known about the interfacial properties of these compounds with H_2O under operational conditions. Therefore, knowledge of interfacial reactions on their surface under realistic conditions is essential to improve our understanding of water-splitting mechanisms, as well as to increase the stability and efficacy of PEC devices. To perform chemical characterization of the interfaces under reaction conditions, we used an ambient pressure X-ray photoelectron spectroscopy. In this study, thin films of $CuFeO_2$ and $CuFe_{1-x}Ga_xO_2$ composites were exposure to H_2O. Water interactions with the Cu-based oxide surface and the electronic structures of the surface atoms were evaluated from the Cu 2p, Fe 2p, C 1s and O 1s photoemission spectra to identify surface species newly formed.

T60.00314: Self-Regulated Nanoparticle Assembly at Liquid/Liquid Interfaces: A Route to Adaptive Structuring of Liquids

Caili Huang, Brett Helms, Thomas Russell

The controlled structuring of liquids into arbitrary shapes can be achieved in biphasic liquid media using the interfacial assemblies of nanoparticle surfactants (NP-surfactants), that consist of a polar nanoparticle "head group" bound to one or more hydrophobic polymer "tails". The non-equilibrium shapes of the suspended liquid can be rendered permanent by the jamming of the NP-surfactants formed and assembled at the interface between the liquids as the system attempts to minimize the interfacial area. While critical to the structuring process, little is known of the dynamic mechanical properties of the NP-surfactant monolayer as it is dictated by the characteristics of the components, including NP size and concentration and the molecular weight and concentration of polymers bound to the NPs. A comprehensive study of the dynamic mechanical character of 2-dimensional NP-surfactant assemblies showed that the dynamics of NP-polymer interactions are self-regulated across multiple time scales, and are associated with specific mesoscale interactions between self-similar and cross-complementary components. The mechanical properties of the NP-surfactant monolayer are tunable over a broad range, providing a control over the functional attributes of the to suit specific applications.

T60.00315: Hydrogen atom adsorption on graphene buffer layer grown on SiC(0001) surface: first-principles study

Jun Nara, Takahiro Yamasaki, Takahisa Ohno

Thermal decomposition of SiC substrate is known as high-quality graphene fabrication method, and then has been intensively studied. The C-atom layer grown on SiC substrate is not graphene but so-called buffer layer (BL), which has similar honeycomb structure to graphene but does not have the graphene's characteristic electronic properties due to the lack of the Dirac cone. To utilize BL grown on SiC substrate as graphene, it is necessary to anneal it under hydrogen (H) ambient to intercalate H atoms between BL and SiC substrate to break the covalent bond between BL and SiC surface. However, the lack of knowledge on the intercalation mechanism make it difficult to control this process to obtain high quality graphene. In this study, we investigated the interaction between BL grown on SiC substrate and H atoms by using ab initio density functional calculations. We found that H atoms adsorbed on BL prefer to desorb from BL than penetrate thru BL, because the activation energy of the former process is much lower than that of the latter. It is considered that H atoms enter between BL and SiC substrate from surface steps or some large cracks of BL rather than the honeycomb structures of BL. We used the Earth Simulator of JAMSTEC and the NIMS Numerical Materials Simulator for this study.

T60.00316: Improving the Dilution Factor in Loss Angle Measurements of Optical Coatings Used in Gravitational Wave Detection

Seth Linker, Joshua Neilson, Riccardo Desalvo, Shuih Chao

Thermal noise due to the interaction of optical coatings with their environment is a fundamental source of noise in the current generation of gravitational wave detectors. It is crucial to accurately identify future materials and/or coating methods that possess the largest possible mechanical quality factor (Q). Current methods to find the Q of optical coating candidates suffer in precision due to depositing them onto thick substrates that store a large portion of energy during the measurement. We propose a new experimental approach that will more precisely measure the Q of coatings by depositing them onto 100 nm Silicon Nitride membranes.

T60.00317: Preparation and Characterization of 2D-MoS_2/Cu(111) Decorated with Au Nanoparticles for Photocatalytic Applications

Md Afjal Khan Pathan, Mark Wasuwanich, Mihai Vaida

Nanostructured materials composed of two dimensional (2D) semiconductors decorated with metal nanoparticles are predicted to be efficient photocatalysts for water splitting and CO_2 reduction. In this research, 2D-MoS_2 is prepared on various substrates such as Cu(111), Au(111), Si(111) using a multistep procedure based on Mo evaporation in an H_2S environment under ultrahigh vacuum conditions. Subsequently, the 2D material is decorated with Au nanoparticles via physical vapor deposition. The composition and crystallinity of the 2D-MoS_2 are investigated by Auger electron spectroscopy and low energy electron diffraction, while the electronic structure of the Au particles as well as the band alignment at the Au-MoS_2 junction is investigated by XUV photoemission spectroscopy. Besides the preparation and characterization of Au/2D-MoS_2, this contribution will also provide details about the interaction of CO_2 and H_2O molecules with the Au/2D-MoS_2 photocatalyst, which is investigated via temperature programmed desorption/reaction in the presence and absence of light irradiation and will correlate the catalytic and photocatalytic activity with the Au particle size and 2D-MoS_2 morphology.

T60.00318: Computational study of catalytic activity of high index platinum surfaces

Gabriele Tomaschun, Thorsten Klüner

In heterogeneous catalysis the selectivity and reactivity of the catalyst often depends on the surface shape and structure. To enhance the catalytic performance of a catalyst, improvement of surface structure is of great importance. [1] Pt nanoparticles show for instance different catalytic reactivity by varying surface shape and structure.[2] Surfaces with high density of atomic steps and kinks can lead to more active sites and thus increase their reactivity.

In the present work we analyze the influence of stepped and kinked Pt surfaces on the catalytic reactivity and selectivity of condensation, oxidation reactions of light alcohols and hydrogenation reactions. These calculations are performed using the exchange-correlation functional PBE [3] implemented in the Vienna ab initio simulation package (VASP) [4]. Fundamental mechanistic studies of adsorption sites, adsorption energies and transition states are performed in order to determine favorable reaction pathways and mechanisms on these high index Pt surfaces.

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T60.00319: Effects of Fluorination on the Structural and Electrical Properties of Epitaxial $La_{0.67}Ca_{0.33}MnO_{3-y}$ Thin Films

Joseph Cartelli, Dustin Ullery, Benjamin Storke, Saneyda Hernandez, Francis Walz, Mary Sajini Devadas, Sylwia Ptasinska, Rajeswari Kolagani

We have studied the effects of fluorination (i.e. fluorine incorporation into the material) on the structural and electrical properties of epitaxial thin films of the hole doped rare earth manganese oxide $La_{0.67}Ca_{0.33}MnO_{3-y}$ (LCMO). Flourination is known to alter the electronic properties of other ABO3-y materials such as SrFeO3-y where fluorine occupies the oxygen vacancy sites forming an oxy-fluoride structure. Our preliminary results in LCMO indicate similar changes in the lattice structure and electrical conductivity upon fluorination, the effects being more pronounced in films grown under oxygen-poor conditions using pulsed laser deposition. These changes are highly temperature dependent with the fluorinated samples exhibiting metal insulator transitions that previously were not present.

T60.00320: Hopping conduction of amorphous Carbon film modified by embedded Au nano-particles

You Jiun Chen, SSU-TING LIN, H. W. Yang, Ying Pei Hsu, Nan Si Li, Shih-Jye Sun, Hsiung Chou

Insulated amorphous Carbon with sp3 orbital can be modified into sp2 graphene-like orbital by the interface effect when in contact with Au nanoparticles. When the density of the modified domains exceeds the percolation limit, a hopping conduction via percolation paths becomes possible. In this study, Au nanoparticles generated on the top of quartz or amorphous C film were grown by sputtering technique at liquid nitrogen temperature or dipping in Au nanoparticle solution at room temperature, while the amorphous C films were grown by DC sputtering method at room temperature from a graphite target. The morphology, crystal structure and electric transportation were investigated by using an AFM in a tapping mode, a high resolution TEM and a high resistance meter in a cryostat, respectively. The size of Au nanoparticles was found to vary in a wide range of 40 nm to 300 nm with a height of ~10 nm. TEM images show that the modification for sp2 regions are a very thin layer within adjacent Au nanoparticles. The resistivity as a function of temperature indicates that the film is purely conducting by hopping mechanism.

T60.00321: AMPSIES: A new top-layer selective positron induced electron spectroscopy for studying the surface electronic structure of materials.

Alex Fairchild, Varghese Chirayath, Vincent Callewaert, Randall Gladen, Ali Koymen, Rolando Saniz, Bernardo Barbiellini, Bart Partoens, Alexander Weiss

Research at the University of Texas at Arlington's positron lab has led to the first observations of a positron induced low energy electron emission mechanism, termed Auger mediated positron sticking (AMPS). AMPS is initiated by the energy transfer associated with the positron's transition from a scattering state to a surface bound state. Recent theoretical investigations of the AMPS mechanism have revealed that the emission process is sensitive to surface localized valence electron states near the Fermi level, with minimum contamination from bulk electronic states. This surface selectivity is due to the highly localized character of the screened Columbic potential. A model based on the valence density of states near the Fermi level, the unoccupied density of states above the vacuum level, and the escape probability of emitted electrons has been shown to successfully reproduce the line shape of the AMPS peak for several materials. Therefore, the AMPS mechanism offers a new type of surface selective positron induced electron spectroscopy, which we have termed, AMPS induced electron spectroscopy (AMPSIES). In this report, we present AMPSIES measurements on Cu, Si, and HOPG and their simulated line shapes.

T60.00322: Electronic Structure of Ru(0001)

Patricio Haberle, Valeria del Campo, Julian Correa, Jonathan Correa-Puerta

For a long time Ruthenium has attracted considerable interest due to its applications in catalytic processes. These days a renewed interest in this surface derives from its current use as substrate to grow graphene by low pressure CVD. In this work we used k-resolved inverse photoemission spectroscopy (KRIPES) and an A*b initio* calculations of the electronic structure of Ru(0001), to determine the energy dispersion of the different states and surface resonances. The setup to perform KRIPES measurements mainly consists of an electron gun capable of producing a parallel electron beam with energies up to 30 eV and a Geiger Müller counter filled with iodine as discharge gas capped with a SrF2 window.This configuration allows the detection of optical transitions between unoccupied bands (photons of 9.5 ±0.2 eV). The comparison between IPES features and calculations enabled us to identify several Ru bulk states and surface resonances in the ΓMΓ̄ direction up to 8 eV above the Fermi Energy.

T60.00323: Advancements in Transparent Conducting Oxides: Amorphous IO & ZITO

Timothy Holmes, Brett Freese, Miko Stulajter, Manuel Osorio

In this research project, we set out to discover why the compounds indium oxide (IO) and zinc-indium-tin-oxide (ZITO) are better semiconductors in their amorphous state, just before they become crystalline. A series of IO and ZITO thin films ranging from fully amorphous to fully crystalline were prepared. We analyzed their x-ray pair distribution function data collected at Argonne National Laboratory. We evaluated the films' lateral and depth uniformity by analyzing different sections of the data that were measured at different penetration depths. A variety of software packages were used, including GSAS II, PDFgetX3, and MATLAB. For both IO and ZITO, we found that the in-plane and out-of-plane atomic structures differed suggesting that the films are not laterally homogeneous. Shorter bond lengths correlated with high electron mobility. These results will be compared with molecular dynamic simulations to better understand which local atomic structure produces enhanced electrical properties.

T60.00324: The Effects of Co-catalyst on Water-splitting Photocatalyst: A DFT Analysis

Kaharu Mizuno, Koichi Yamashita

Water splitting photocatalysts are getting a lot of attention due to their ability to produce H_2 by utilizing solar energy. One of the promising way to boost their efficiency is to load co-catalysts such as noble metal nanoparticles on the photocatalysts. Co-catalysts are believed to separate photogenerated electrons and holes by forming a Schottky barrier at the metal-semiconductor interface, at which O_2 and H_2 evolution reaction (OER, HER) are thought to occur. Nevertheless, the details of the reactive sites and the reaction mechanism are still not clear due to the difficulty in detecting OER and HER experimentally.
Thus, in our research, we aimed to elucidate the role of co-catalysts in HER by means of first-principle calculations. We used Pt/$SrTiO_3$ as an example, and found the stable structure of dissociative adsorption of H_2O. The calculations suggested that H^+ moves onto co-catalysts while OH^- stays on the surface around co-

catalysts. We also revealed that co-catalysts donate electrons to their adsorbents. We will also investigate the changes of the charge distribution of transition states during the water splitting reaction on the surface.

T60.00325: Metal / Oxide Interface Control for the Turn-on Voltage Change of Oxide Thin-film Diodes

Jun-Woo Park, Donggun Lee, Youn Sang Kim

As the size of electronic devices has been reduced, there is a growing need for current to flow through an insulating thin-film. Although, due to the inherent energy band properties of most insulating materials, the transport of charge carriers through an insulator remains a limited process window. Recently, we have presented a technique for transferring electrons stably through a thick insulator film (over 100 nm) in metal / insulator / oxide semiconductor / metal (MIOSM) contact structures. Depending on the interface charge state of the oxide semiconductor film, the current passes uni-directionally as a conventional diode. Herein, we propose a method of controlling the turn-on voltage in MIOSM structure, based on the control of the interface contact resistance between the oxide semiconductor and the metal. When Al and Ag were deposited on the IGZO, the turn-on voltage was adjustable from 0V to 14.4V due to a difference in the respective interface contact resistance. We also demonstrated that the turn-on voltage can be precisely controlled by changing the IGZO thickness in contact with Ag.

T60.00326: Structural and spectroscopic view of insulator-metal transition characteristics in epitaxial VO_2 films

Dooyong Lee, DongHyuk Yang, Hyegyeong Kim, Jiwoong Kim, Yunhee Cho, Sehwan Song, Jong-Seong Bae, Kyoung Soon Choi, Jouhahn Lee, Jaekwang Lee, Sungkyun Park

Vanadium dioxide (VO_2) is interesting materials not only for the fundamental aspect owing to the unclear physical origin of the insulator-metal transition (IMT) but also for the numerous device applications such as, Mott field effect transistors, infrared detectors, tunable optical switching. Recently, many studies performed to modify the transition temperatures by doping, varying crystal orientations and strain state. Among them, the strain state is a very effective way to control the IMT characteristics. However, the presence of multivalent vanadium states, which is always in the VO_2, causes the difficulty to control the properties. In this presentation we will demonstrate how the various parameters can tune the IMT characteristic. Using spectroscopic and structural analysis we were able to correlate the variation of multivalent state and strain with IMT characteristics.

T60.00327: Direct Measurement of Phonon Specularity in Silicon membranes using Transient Grating

Navaneetha Krishnan Ravichandran, Hang Zhang, Austin Minnich

Boundary scattering of thermal phonons is an important physical process that remains poorly understood. While a quantitative understanding of the process has long been established for many types of waves, the precise manner in which thermal phonons reflect from atomically rough surfaces remains unclear owing to limited control over THz frequency phonon generation and detection. Here, we report measurements of a key property for these efforts, the specularity parameter, which describes the probability of specular reflection of thermal phonons at a surface, by performing transient grating thermal conductivity measurements on free standing silicon membranes. Our observations demonstrate that thermal phonons coherently reflect from surfaces with Angstrom-scale roughness, and further show that completely diffuse reflections occur with surface imperfections on the scale of only a few atomic planes. Our work provides direct experimental insights into the roughness scattering mechanism for phonons that will inform applications such as the coherent manipulation of thermal phonons and passive cooling of electronics.

T60.00328: First-principles study of topological phase transition in two-dimensional bismuth and its alloys

Hikaru Sawahata, Naoya Yamaguchi, Fumiyuki Ishii

Bulk and thin-film bismuth have attracted wide physical interests since they show the topological insulating phase and anomalous transport properties such as spin-to-charge conversion in Bi/Ag interfaces, originating from its electronic structure with strong spin-orbit coupling. Especially, to explore the possibility of new device applications, it is important to investigate the electric field effect on topological insulating phases in the bismuth. In the previous study, we reported that the one-bilayer Bi(111) shows electric field inducing topological phase transition at $E > 2.1$ V/Å[1].
In this study, to reduce critical electric fields for application in novel devices, we investigate the electric-field and strain dependence of band structure and Z_2 topological invariant on one-bilayer Bi(111) and $Bi_{1-x}M_x$ (M =P, As, Sb) alloy by the first-principle calculation. We will present the phase diagram and discuss the origin of changes in critical electric fields by alloying.
[1] H. Sawahata, N. Yamaguchi, H. Kotaka, and F. Ishii, arXiv:1710.04812.

T60.00329: Surface electronic structure of the HOPG, Au, and 1-Butanethiol films on HOPG under ambient conditions

Indrajith Senevirathne

Investigating semiconductor/metal and their thin film surfaces usually done under UHV conditions. Although the UHV conditions bring inarguable advantages in taking measurements, the systems thus created in many instances must work in the atmosphere. Therefore it would be prudent on some occasions to obtain this information in systems while under normal ambient conditions which would provide a direct reflection of how they work. This is an attempt to investigate the localized surface bands via Scanning Tunneling Spectroscopy (STS) under the ambient conditions. I have used Nanoscience Instruments NAIO Scanning Tunneling Microscope (STM) to investigate and find the surface electronic properties of SPI supplies fresh cleaved Grade V-1 HOPG surfaces and Au magnetron sputter deposited on fresh cleaved HOPG under varying conditions. 1-Butanethiol films were self-assembled on fresh cleaved HOPG. A comparative discussion of the results will follow with the measurement of Localized Density of States (LDoS).

T60.00330: Classification of defects on rutile TiO_2 (110) surface: Hybrid versus Hubbard-U DFT

Jan Brndiar, Yanjun Li, Yasuhiro Sugawara, Ivan Stich

Titanium oxide surfaces are among the most important oxide surfaces with applications as catalytic, anti-bacterial, construction materials, etc. Defects on these surfaces play an important role in their applications. Using two different DFT treatments, hybrid functionals and DFT+U, we have attempted classification of oxygen vacancy, single and double hydrogen defects. In agreement with previous DFT+U modeling we find that electronic signatures of all three defects are very similar. In addition, for each defect we have found dozens of quasi-degenerate minima differing by their position, orbital character, and spin coupling. The estimated migration barriers for some of the minima indicate that they may be thermally populated at finite temperatures. The main result of the study is the coupling between the hybrid DFT solution and the DFT+U maintaining the defect electronic signature. We find that the values of the U so determined are unexpectedly small, around 2.7 eV. We have also addressed the possibility of existence of charged defects. Our calculations indicate that charge defects are not favored.

T60.00331: First-principles Wannier Function Approach to Rashba Effect

Naoya Yamaguchi, Fumiyuki Ishii

In various two-dimensional electronic systems, Rashba effect arises due to the spin-orbit interaction. Rashba coefficients α_R, strength coefficients of Rashba effect, are key ingredients to spintronic applications such as spin-to-charge conversion [1]. However, it is not clear what determines α_R. For example, the trend of α_R for M(111) surfaces (M = Cu, Ag, Au) is Au(111) > Cu(111) > Ag(111), but this trend doesn't coincide with that of atomic SOC strength, that is, the order of atomic number. In this study, we have performed first-principles density functional calculations for typical Rashba systems such as M(111) surfaces, Bi/M surface alloys [2] and oxide interfaces [3], and focused on what dominates α_R in terms of the localization length and Wannier center for Rashba states. We will discuss the correlation between α_R and the localization length or Wannier center of Rashba states.

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[2] N. Yamaguchi, H. Kotaka and F. Ishii, J. Cryst. Growth, **468**, 688 (2017).
[3] N. Yamaguchi and F. Ishii, to be published in Appl. Phys. Express, arXiv:1709.08335.

T60.00332: Highly Mobile Two-Dimensional Electron Gases with Strong Gating Effect at the Amorphous-$LaAlO_3$/$KTaO_3$ Interface

Hui Zhang, Hongrui Zhang, qinghua zhang, Lin Gu, Bang-Gui Liu, Jirong Sun

Two-dimensional electron gas (2DEG) at perovskite oxide interface exhibits a lot of exotic properties, presenting a promising platform for the exploration of emergent phenomena. While most of the previous works focused on $SrTiO_3$-based 2DEG, we demonstrate the fabrication of high quality 2DEGs by growing an amorphous $LaAlO_3$ layer on a (001)-orientated $KTaO_3$ substrate, which is a 5d-metal oxide with a polar surface, at a high temperature that is usually adopted for crystalline $LaAlO_3$. Metallic 2DEGs with the Hall mobility as high as ~2150 cm^2/Vs and the sheet carrier density as low as 2×10^{12} cm^{-2} are obtained. For the first time, gating effect on transport process is studied, and its influence on spin relaxation, inelastic and elastic scattering are determined. Remarkably, the spin relaxation time can be strongly tuned by back gate. It is reduced by a factor of ~69 while sweeping gate voltage from -25 V to 100 V. The mechanism that dominates the spin relaxation is elucidated.

T60.00333: INSTRUMENTATION AND MEASUREMENTS

T60.00334: Is there a resting frame in the universe? A proposed experimental test based on a precise measurement of particle mass

Donald Chang

According to the Special Theory of Relativity, there should be no resting frame in our universe. Such an assumption, however, could be in conflict with the Standard Model of cosmology today, which regards the vacuum not as an empty space. Thus, there is a strong need to experimentally test whether there is a resting frame in our universe or not. We propose that this can be done by precisely measuring the masses of two charged particles moving in opposite directions. If all inertial frames are equivalent, there should be no detectable mass difference between these two particles. If there is a fixed resting frame in the universe, one will observe a mass difference that is dependent on the orientation of the laboratory frame. This can be tested by repeating the experiment at different times of the day (or on different days of the season). The detailed experimental setup is discussed in this paper. Our analysis suggests that, with the existing technological limits, the proposed measurement should have sufficient accuracy to determine if there is a resting frame or not.

T60.00335: Integrating Scanning Tunneling Microscopy with Fourier-Transform Infrared Spectroscopy

Kristopher Barr, Andrew Guttentag, Paul Weiss

The scanning tunneling microscope (STM) has revolutionized our ability to observe surface features at the scale of atoms and molecules on a variety of conductive substrates. Conventional STM images contain limited chemical information, generally related to electronic structural variations of surfaces and adsorbates. We

propose to expand the capabilities of the STM by simultaneously exciting the surface with an evanescent wave of infrared radiation and measuring the changes in apparent conductance with the probe tip. Due to the local nature of scanning probe microscopies, we investigate vibrational structure below the diffraction limit. An interferometer source enables us to probe the surface at a variety of frequencies simultaneously. We are using cyanide monolayers on Au{111}, because of its stability, simple absorption spectra distinct from water and CO_2 absorption spectra, and its theoretical vibronic coupling to the surface electronic states of Au{111}. This methodology will serve as the framework for future experiments on a wide variety of systems.

T60.00336: Quantum and tunneling capacitance in charge and spin qubits

Ryo Mizuta, Andreas Betz, Ruben Otxoa, M Fernando Gonzalez-Zalba

We present a theoretical analysis of the capacitance of a double quantum dot in the charge and spin qubit configurations probed at high frequencies. We find that, in general, the total capacitance of the system consists of two state-dependent terms: the quantum capacitance arising from adiabatic charge motion and the tunneling capacitance that appears when repopulation occurs at a rate comparable or faster than the probing frequency. The analysis of the capacitance lineshape as a function of externally controllable variables offers a way to characterize the qubits' charge and spin state as well as relevant system parameters such as charge and spin relaxation rates, tunnel coupling, electron temperature, and electron g factor. Overall, our analysis provides a formalism to understand dispersive qubit-resonator interactions which can be applied to high-sensitivity and noninvasive quantum-state readout.

T60.00337: Detectors with High Efficiency and Low Noise for Exoplanet Studies and Cosmology

Shouleh Nikzad, John Hennessy, April Jewell, alina kiessling, Michael Hoenk, Rhonda Morgan, Stefan Martin, Samuel Cheng

In preparation for the National Research Council's next Decadal Survey for Astrophysics, NASA is developing concepts for four flagship missions, including the Habitable Exoplanet Imaging Mission (HabEx) and the Large Ultraviolet/Optical/Infrared Survey Mission (LUVOIR). Science and Technology Definition Teams (STDT) have embarked on formulating mission objectives, developing instrument designs and defining technology requirements and technology gaps. This talk focuses on potential solid-state detector options and briefly reviews their performance. The emphasis will be on silicon based detectors with high efficiency from far ultraviolet to near infrared with photon counting capability.

T60.00338: Stratospheric Organisms and Radiation Analyzer (SORA)

Dorian Pena, Steven Oliver, Fre'Etta Brooks

The SORA payload will sample for the existence of microorganisms and bacterial spores in the upper atmosphere. The payload will also analyze different aspects of the surrounding environment such as radiation exposure, temperature, pressure and humidity. The payload has three main scientific objectives. First, design and build a novel system that will isolate surrounding air and sample for cells. Second, onboard sensors will analyze exposure to solar and cosmic radiation that microorganisms may encounter. Finally, monitor the environmental conditions such as temperature, pressure, and humidity. Furthermore, the design will employ additive manufacturing and hobby electronics in its construction to provide an accessible basis for future missions and explore the bounds of the technology available.

T60.00339: Sub-nanometer level vibration detection of a piezo crystal oscillator's surface, using time series tunneling current measurement.

Dibya Sivananda, Amit Banerjee, Satyajit Banerjee

We study the vibration characteristics of a piezo crystal oscillator surface using time series measurement of tunneling currents. We determine the fluctuations in the tunneling current between an STM tip and the surface of a vibrating piezo crystal oscillator. These fluctuations reveal sub-nanometer vibrations on the piezo crystal oscillator's surface with a sensitivity of 10^{-2} A/√Hz. The vibrations on the surface of the oscillator exhibit a resonant response as we vary the excitation frequency. An unconventional sub-nanometer perpendicular vibrations mode excited on the crystal surface is detected. The direction of these vibrations is perpendicular to the surface whereas the conventional vibration mode is in a direction parallel to the crystal surface. We find that this perpendicular mode also has higher harmonics near resonance. We can conveniently call the piezo crystal oscillator together with the time series tunneling current measurements a simultaneous drive and detection system.

T60.00340: Analysis of the line shape of a low energy Auger emission (VVV) initiated by a valence hole to investigate the surface electronic states of graphene, highly oriented pyrolytic graphite (HOPG) and Si (100).

Varghese Anto Chirayath, Alex Fairchild, Vincent Callewaert, Randall Gladen, Ali Koymen, Rolando Saniz, Bernardo Barbiellini, Bart Partoens, Alexander Weiss

Recently, our group reported the direct observation of an Auger electron emission process from single layer graphene (SLG) that is initiated by a hole created by the annihilation of a valence electron with a surface-bound positron (Chirayath et al., Nature Comm. 8, 16116, 2017). The annihilation induced valence hole decays through an intra-band Auger relaxation process and is termed as VVV. The ability to model all the features of the VVV Auger peak using valence and conduction band density of states of a freestanding SLG shows the sensitivity of the process to the surface electronic states. Energy conservation requires that the valence bandwidth be greater than the work function of the sample for electron emission into the vacuum through a VVV Auger process and hence, the VVV peak should be detectable in materials where this condition is satisfied. Here we report on positron annihilation induced Auger electron spectroscopy (PAES) measurements, which shows the presence of VVV Auger peak in Si (100) and HOPG. The VVV Auger peaks from Si (100) and HOPG are compared to the VVV Auger peak from SLG and to the theoretically generated VVV Auger spectrum to understand the ability of VVV-PAES to investigate unoccupied surface states in wideband materials.

T60.00341: Analyzing Copper Etching Dynamics by Hybridizing AFM Controlled SECM with Raman MicroSpectroscopy

Aaron Lewis, Yirmi Bernstein, Yossi Bar-David, Dmitry Lev, Rimma Dechter, Sofia Kokotov, Oleg Fedosyesyev

Local etching of a thin copper film evaporated on silicon was investigated by developing Atomic force microscopy (AFM) regulated scanning electrochemical microscopy (SECM). For this investigation such an AFM controlled SECM was hybridized with in-Situ Raman spectroscopy. This allowed for an understanding of the nanometric controlled etching of the copper coating on the silicon. The design of the instrument and the probe has allowed for spectrochemical analysis in real time. The etching produced a micrometer aperture in the copper film which was characterized, in terms of morphology, by the AFM capabilities of the probe. It was discovered that a time gap occurred between the measured SECM current and the exposure of the Si beneath. This was demonstrated by the in-situ Raman spectrometer. An AFM scan of the etched area using the same SECM probe was demonstrated too. Such an integration has allowed for obtaining the type of real time information of the etching processes for understanding in depth the parameters that control etching. As a result, deeper, well quantified insights have been obtained of diffusion mechanisms in redox reactions. The data also leads to new horizons and insights into etching processes in general.

T60.00342: Advanced Ultraviolet Imaging Spectrometer for Planetary Studies

Alexander Carver, John Hennessy, Daniel Wilson, April Jewell, Pantazis Mouroulis, Shouleh Nikzad

The ultraviolet spectral range is rich with key information that can be utilized to study a variety of scientific targets such as planetary atmospheres, satellites, and primitive bodies. This spectral region is particularly important for sensing the tenuous atmospheres produced by outgassing and internal activity, as well as for probing surface composition. Spectra of active comet-like asteroids can include diagnostic atomic lines (e. g., H, C, O, N, S) and molecular bands (e. g., N_2, OH, CO_2, CO, C_2). Surface reflectance spectra in the UV to visible range can characterize absorption due to solids such as H_2O, CO_2, SO_2, and other ices, characterize the red spectral slope typical of organics, and enable detection of electronic absorption features due to iron oxides, organics, and other compounds. Ultraviolet spectrum is significantly challenging for all aspects of dispersion, imaging, and detection. Using 2D doped detectors developed at JPL plus the electron-beam fabricated convex gratings (flow scattering loss and high efficiency) a high throughput and compact UV imaging spectrometer has been developed. We will discuss the design, results, and application of this advanced UV spectrometer.

T60.00343: A Numerical Analysis of Interaction-free Measurement With a Shot-Noise-Limited Electron Source and Conditional Sample Re-illumination

Akshay Agarwal, Vivek Goyal, Karl Berggren

Interaction-free measurement (IFM) has been proposed as a means of high-resolution, low-damage imaging of radiation-sensitive samples, such as proteins and biomolecules. The basic setup for IFM is a Mach-Zehnder interferometer (MZI). Recent progress in nanofabricated electron diffraction gratings has made it possible to incorporate an MZI in a transmission-electron microscope (TEM). Therefore, analysis of IFM with an MZI and a shot-noise-limited electron source (such as that in a TEM) is of interest. In this work, we numerically compared the error probability and number of scattered electrons for IFM and classical imaging schemes, with and without an additional detector for scattered electrons, for a black and white sample. The additional detector reduced error for the same number of scattered electrons by an order of magnitude, for both IFM and classical schemes. We also investigated a sample re-illumination scheme based on updating priors after each round of illumination until a stopping criterion is met. This scheme further reduced error by a factor of two. Implementation of these methods is likely achievable with existing instrumentation and would result in improved resolution in low-dose electron microscopy.

T60.00344: Characterization of Dynamic Light Scattering Instrumentation to Determine Nanoparticle Size

Bryan Augstein, James Coyne, Anton Wiggins, Brian Sears, Sam Harding, David Schaefer, Jeffrey Simpson

Dynamic Light Scattering (DLS) provides a high-throughput and accurate measurement of particle sizes for monodisperse (MD), spherical nanoparticles (NPs). We report on the characterization of homebuilt DLS instrumentation to measure the size of NPs of gold and polystyrene. HeNe and Ar-ion lasers comprise the excitation sources for the scattering experiment. An avalanche photodiode detects the scattered light and an autocorrelation card analyzes the signal to provide a measurement of the translational diffusion coefficient, which allows for the determination of NP diameter. We have tested our apparatus using commercially-produced gold and polystyrene NPs in the range of 10nm to 250nm. Given the strong temperature-dependence of the viscosity, periodic ambient temperature measurements were used to produce dynamic values for viscosity and hence minimize uncertainty in the determination of NP size. We compared our DLS results to NP size measurements obtained by Atomic Force Microscopy (AFM) and found that DLS provides a facile, high-throughput, and accurate measure of NP size. Additionally, we present DLS measurements of NPs suspended in highly-viscous fluids, *e.g.*, glycerin.

T60.00345: 11-BM Complex Materials Scattering (CMS) - A New SAXS/WAXS Beamline at NSLS II

Masafumi Fukuto, Ruipeng Li, Kevin Yager

The Complex Materials Scattering (CMS) beamline at the National Synchrotron Light Source II (NSLS II) at Brookhaven National Laboratory provides small- and wide-angle x-ray scattering (SAXS/WAXS) capabilities for materials science community, both in transmission and grazing-incidence geometry. With the initial construction phase completed and commissioning work started in 2016, the CMS beamline has been taking general users since June 2017. We will present the current status of the beamline, available techniques and sample environments, as well as our vision for the future development. Topics such as high-throughput sample handling, in situ sample environments, and automating beamline workflow will be discussed.

T60.00346: Optimizing the Direct Visualization of Microgels via Scanning Electron Microscopy

Tony Dobrila, Kiril Streletzky, Petru Fodor

To better understand the dynamics of microgels in solution, their volume phase transition, and to correlate images of individual particles with Dynamic Light Scattering (DLS) data on their diffusion, new imaging techniques were developed using scanning electron microscopy (SEM). Accurate imaging of such systems is challenging as microgel samples lose water content under high vacuum. To address these issues, a controlled environment chamber was developed, allowing the microgels to dry over a longer period of time at higher humidity levels than standard room conditions. Using the controlled humidity environment allowed microgels to better maintain original structure for imaging and produced microgel size distributions more consistent with DLS both below and above the volume phase transition. Another method for microgel imaging was developed by suspending particles in ionic liquids. Low vapor pressures and high ionic concentrations of these suspensions allowed the capture real time dynamics of swollen microgels. Microgels in ionic liquid were observed to be smaller than expected, whilst maintaining size distribution uniformity. Such observations could be due to charge screening or the increased salt concentration due to presence of ionic liquid.

T60.00347: A unified Lagrangian treatment of charge and cantilever dynamics in electric force microscopy

Lee Harrell, Ryan Dwyer, John Marohn

Numerous microcantilever-based electric force microscopy (EFM) protocols have been developed since the invention of scanned probe microscopy. In spite of a common physical basis, a comprehensive formalism for connecting the tip-sample forces to the cantilever dynamics in these experiments is lacking. We present a unified Lagrangian treatment of the EFM, which, significantly, reveals assumptions underlying equations that are widely-used to interpret EFM data. The force is usually stated as $F = (1/2)C'(V - \Phi)^2$, with C the tip-sample capacitance, V the tip voltage, and Φ the surface potential, while the associated frequency shift is stated as $\Delta f = -(f_0 / 4k)\, C''(V - \Phi)^2$, with
f_0 the cantilever resonance frequency and k the cantilever spring constant. We find that these equations imply assumptions about sample charging that are seldom explicitly stated or experimentally checked. We identify the conditions under which they are valid and analyze the cantilever dissipation that arises from finite equilibration times for sample surface charging.

T60.00348: Theoretically and Experimentally Demonstrated Enhanced-Speed Thermoreflectance Imaging

Kyle Allison, Mark Hallman, Johanna Hardin, Ami Radunskaya, Janice Hudgings

Charge coupled device (CCD) -based thermoreflectance imaging using a “4-bucket” algorithm to essentially provide pixel-by-pixel lock-in imaging is a well-established research tool for obtaining two-dimensional thermal maps of optoelectronic, electronic, and MEMs devices with high spatial and thermal resolution [1,2]. However, the technique is relatively slow, limiting broader commercial adoption. In this work, we show that the image acquisition speed is fundamentally limited by an underlying statistical bias in the 4-bucket imaging algorithm. Furthermore, the straightforward extension to an n-bucket technique by faster sampling fails to address this statistical bias and hence does not improve image acquisition time. Instead, we develop a modified “enhanced n-bucket” algorithm that halves the image acquisition time for every doubling of the number of buckets. We derive detailed statistical models of the algorithms and confirm both the models and the resulting speed enhancement experimentally. In addition, we investigate optimizing a stochastic resonance imaging enhancement and explore other, novel avenues to increase the speed of the imaging technique.
[1] M. Farzaneh, et. al, J. Phys. Appl. Phys. **42**, 143001 (2009).
[2] P. M. Mayer, et. al, JOSA A **24**, 1156 (2007).

T60.00349: Stability and size restrictions of trapped objects in acoustic levitation

Anthony DiChiara, Jason Lerch, Kamlesh Suthar, Md Abdul Momen

High intensity ultrasonic waves confined in an acoustic resonator can be used to trap objects a fraction of the wavelength. Objects are completely free from contact with a rigid surface only maintaining contact with the surrounding fluid medium, in this case air. However, trapped objects suffer from spontaneous oscillations in both the longitudinal and transverse directions of the resonator. The tendency of objects to oscillate becomes more pronounced as the object size decreases, thus setting a lower limit on object size. Stability presents an extreme problem for beam-based experiments, i.e. laser or x-ray probe, since the motion of the trapped object couples to measurement noise. We will discuss a sequence of oscillation or ‘jitter’ measurements to characterize the relative noise as a function of object size. A critical parameter to exploit here is the shape of the resonator mode that determines the peak sound intensity as well as the acoustic force gradient on trapped objects. We will discuss our efforts to accurately model and control the acoustic profile in an ultrasonic resonator. Modeling and simulation work has been carried out in COMSOL Multiphysics platform and focusing schemes have been used to optimize the resonator mode for trapping stability.

T60.00350: Stability and size restrictions of trapped objects in acoustic levitation

Anthony DiChiara, Kamlesh Suthar, Md Abdul Momen

High intensity ultrasonic waves confined in an acoustic resonator can be used to trap objects a fraction of the wavelength. Objects are completely free from contact with a rigid surface only maintaining contact with the surrounding fluid medium, in this case air. However, trapped objects suffer from spontaneous oscillations in both the longitudinal and transverse directions of the resonator. The tendency of objects to oscillate becomes more pronounced as the object size decreases, thus setting a lower limit on object size. Stability presents an extreme problem for beam-based experiments, i.e. laser or x-ray probe, since the motion of the trapped object couples to measurement noise. We will discuss a sequence of oscillation or ‘jitter’ measurements to characterize the relative noise as a function of object size. A critical parameter to exploit here is the shape of the resonator mode that determines the peak sound intensity as well as the acoustic force gradient on trapped objects. We will discuss our efforts to accurately model and control the acoustic profile in an ultrasonic resonator. Modeling and simulation work has been carried out in COMSOL Multiphysics platform and focusing schemes have been used to optimize the resonator mode for trapping stability.

T60.00351: Refracto-Vibrometry Visualization of Ultrasonic Wave Fronts Interacting with Bone Mimicking Phantoms and Heel Bones

Matthew Huber, Brent Hoffmeister, Tom Huber

Ultrasonic measurements of the heel bone (calcaneus) are used commonly for osteoporosis screening. Pulses emitted by an ultrasound transducer are incident on the calcaneus, and the transmitted wave fronts are detected with a separate transducer. In the current study, full field videos were obtained using refracto-vibrometry of ultrasonic pulses interacting with bone mimicking phantoms, and human calcaneus samples. Pulses were emitted by a 500 kHz Panametrics V303 transducer. The measurement beam from a Polytec PSV-400 scanning laser Doppler vibrometer laser was directed through a water tank towards a stationary retroreflective surface. Acoustic wave fronts (density variations) which pass through the measurement laser cause variations in the integrated optical path length. The time-varying signals detected by the vibrometer at numerous scan points were used to determine the time evolution of ultrasonic wave fronts. The resulting videos enable visualization of the propagating wave fronts and the backscattered and transmitted wave fronts. These videos enable direct investigation of wave front distortion due to reflection, refraction and diffraction effects.

T60.00352: Molecular beam methods to study real time product chemistry: triglyceride thermal cracking

Ibrahim Alhroob, Mark Sulkes

The pyrolysis product chemistry of triglycerides (TGs) is not well understood, but has important implications for renewable fuel production. In a somewhat modified molecular beam methodology, soft laser photoionization spectroscopies now are used to *identify* numerous products that can appear in time, rather than to study any particular one. Pyrolysis products are analyzed in real time after they are entrained in He gas expansions. Experiments proceed by recording time-of-flight mass spectra (TOFMS), using both 118 nm and 266 nm photoionization, as a function of increasing temperature of the TG sample. Correlations in the growth/diminution of various product mass peaks can be clarified by applying multivariate analysis calculations to the entire experimental set of TOFMS. New observations have emerged using the foregoing methods--results not seen in past gas chromatographic analysis of collected terminal products. Rather large polycyclic aromatic hydrocarbons (PAHs), up to 444 amu, have been detected, at non-trivial relative product fractions. Indeed, a small number of PAHs with MW ≥ 276 amu increasingly dominate the aromatics product distribution. Furthermore, PAH production begins at surprisingly low temperatures, as low as ~260 C.

T60.00353: Transforming the Transmission Electron Microscope into an Electron Interferometer

Gino Carrillo, Rose Marie Haynes

Here we extend electron interferometric capabilities to older model transmission electron microscopes (TEM) which continue to use lower quality thermionic electron sources. Currently, conventional electron interferometry can be done using the Mollenstedt biprism, but the spatial coherence requirements needed to conduct such experiments is demanding as the electron beam must be spatially coherent over much of the electron beam. Instead, we suggest the use of a nanofabricated grating to act as an amplitude-splitting beam splitter. The spatial coherence requirement is less demanding and need only be coherent across two or more grating bars for diffraction to take place. We place the nanofabricated grating in the condenser aperture of the TEM where we can then use the microscopes condenser lens system to form well focused, spatially separated, diffraction orders in the specimen plane. Using post specimen lenses, we are able to interfere the diffraction orders to form an image of the grating, giving rise to a path separated electron interferometer similar to that of the optical Mach Zehnder.

T60.00354: A Compact Uniaxial Pressure Device Based on Piezobender

Zhaoyu Liu, Huiqian Luo, Shiliang Li

A compact uniaxial pressure device based on a commercial piezobender is designed to be used in resistivity measurements on electric anisotropy property. This device can apply force on sample continuously varying from stretching to pressing by precisely controlling the drive voltage in a wide range of temperature from 380 K down to less than 1.4 K. Moreover, via measuring the strain on a $SrTiO_3$ substrate by strain gauge, we show that the uniaxial pressure is almost temperature independent and suitable for measurements near zero pressure, thus we calibrate an effective pressure which is proportional to drive voltage. Furthermore, by comparing with other techniques we give detailed discussions about some issues that may affect the measurement precision and validity of device. So far, the device has been widely utilized in measuring nematic fluctuations in many iron pnictides systems. At last, we suggest some improvements on the device to make it be extensively available in other experimental techniques.

T60.00355: APPLICATIONS

T60.00356: Global WiFi Coverage with a Polar Low-Earth-Orbit Satellite Network

Cole Brown, Matthew Bruno, Dr. Darren Williams

Global communications, such as household high speed internet, mobile data, and cellular networks, are a keystone of today’s society. There is not, however, a single global communications platform that encompasses all three modern systems. Such a platform would revolutionize the telecommunication industry, connect the entire world population in a way impractical with cellular towers and fiber optics, and lay the foundation for installing similar systems for future bases on the Moon or Mars. Today, SpaceX, Boeing, and other corporations are researching the notion of such a communications platform based in low-Earth-orbit satellites. We model the astrodynamics of a polar-orbit variant of this platform that uniformly

distributes high-speed internet across the planet with 1200 satellites. We also analyze the platform's economic feasibility. We show that our satellites have orbital lifetimes that make it practical to cloak Earth in high speed internet. In addition, we show that the expense of installing our global-satellite network is less than 1% of the per capita revenue of existing WIFI systems.

T60.00357: Fourier Analysis and Compression of String based Instrument Signals
Joshua Rabanal

Fourier analysis provides many possibilities in the study of periodic signals' compression. Previous modeling of the normal modes of three weakly coupled strings under small oscillations has provided functions with decaying amplitudes for each of the normal modes. Outside of the small oscillation regime, the periodicity of each mode is found to be dependent on the amplitude. Comparing this model to the instrument's signal can aid in the compression of these signals via a representative output function instead of a representative raw signal. Implementing Fourier synthesis, with a sine cardinal function as a window and linear regression techniques, we simplified the signals into simple functions containing amplitude decay and time dependent periodicity. This was achieved through independent linear regression of the amplitude and the phase. The resulting output functions resulted in a compression ratio of 300 or greater than 95% space savings when deflated. It is the goal of this investigation to provide a proof of concept for future compression techniques.

T60.00358: Fourier Ptychographic Microscopy in the telecommunication wavelength using a femtosecond laser.
Ishtiaque Ahmed, Maged Alotaibi, Sueli Skinner-Ramos, Daniel Dominiguez, Ayrton Bernussi, Luis Grave de Peralta

We report the succesful implementation of Fourier Ptychographic Microsopy (FPM) in the telecomunication wavelength using an ultrafast, low coherence laser. High resolution with reduced (near) speckle (free) images were obtained using the proposed approach. We also demostrate FPM can be used to image periodic structures through a silicon wafer.

T60.00359: GaN based MEMS accelerometer for high temperature application
Boo Hyun An, Mariam Mansouri, Hamda Al Shibli, Tawaddod Alkindi, Hamad Al Yassi, Ji Sung Lee, Mihai Sanduleanu, Daniel Choi

Inertial sensing technologies in high temperature environments over 500°C are in great demand in aerospace, power plants and material processing applications. However, conventional micro-electromechanical systems (MEMS) sensors still cannot be operated at such high temperature area and need to be isolated in controlled environments.
Gallium nitride (GaN) is very promising for high power devices, high temperature electronics and microsystems due to their wide energy bandgap with low intrinsic carrier density at high temperature over 500°C.
Capacitive inertial sensors which consist of two separated electrodes can be operated by detecting capacitance changes between the electrodes upon applied stress. Capacitive inertial sensors have lower thermal drift, high resolution and good noise performance compare to peizoresistive sensors.
In this study, we present a design of MEMS accelerometer using GaN as structure layer, grown epitaxially on aluminum nitride/silicon substrate. The resonance frequency of the designed accelerometer shows 2.235 kHz and bandwidth is around 1.2 kHz. Modeling and simulation results of the GaN accelerometer will be discussed and characterization of the fabricated devices would be presented.

T60.00360: Large-Scale Robust Quantum Dot Microdisk Lasers with Controlled Cavity Modes
Chun Hao Lin, Qingji Zeng, Evan Lafalce, Marcus Smith, Sidney Malak, Jaehan Jung, Youngjun Yoon, Zhiqun Lin, Zeev Valy Vardeny, Vladimir Tsukruk

We report the facile on-chip fabrication of $CdSe/Cd_{1-x}Zn_xSe_{1-y}S_y$ quantum dots microdisk lasers and their large-area arrays via a pattern-assisted layer-by-layer assembly process. This approach combines the versatility of colloidal semiconducting nanoparticles (bright emission, solubility, and high stability) with the spatial precision of optical lithography to create robust large-area optical lasing arrays (up to a few thousand disks). Specifically, microdisk lasers with high quality factors (within 1000-2000) were fabricated with predefined size and shape (as controlled by master templates) with high consistency and throughput, essentially providing a new approach to fabricate difficult-to-control on-chip optical cavities in a low-cost and effective manner. Notably, the number of longitudinal cavity modes in the microdisk laser can be precisely controlled by varying the microdisks' diameter, allowing for either near-single mode or multimode operation while preserving high quality factors. As such, these quantum dot microdisk laser arrays are promising candidates for advancing the development of large-area, low-cost on-chip photonic structures with controlled lasing modes.

T60.00361: Graphene-based Metasurfaces for Multimode Tunable Terahertz Modulators
ERIN STRICKLAND, Thomas Searles, Mehdi Rezaee, Amir Hassan Ansari, Tina Brower-Thomas, Gary Harris, Riad Yahiaoui

Metamaterials are artificial structures with engineered electromagnetic properties derived from the arrangement of metallic unit cells (or meta-atoms). The feature size of the unit cell is directly proportional to the wavelength of interest. Therefore, large gains in research and development of metamaterials have been made in longer wavelengths due to well-established microfabrication techniques. Graphene metastructures have several advantages over traditional metallic structures including, but not limited to high carrier mobility, flexibility and tunability through application of a gate voltage or external field. Therefore, the objective of this research is to fabricate the theoretically proposed tunable graphene metamaterial terahertz (THz) devices with high amplitude modulation (up to ~80%) and tunability (up to 400 GHz). The active surface of the fabricated devices is 2.5 x 2.5 mm2 and measurements to monitor the ability to modulate THz waves were made using a high resolution terahertz time-domain spectrometer. We aim integrate these devices into systems for sensing and quantum electronics applications.

T60.00362: Using Multiple Ground-based LiDAR Scanners to Digitize Trim Castle in Trim, Ireland
Alex Tuong

3D laser scanning is becoming more prominent in fields such as autonomous vehicles, forensics, and 3D modeling in architecture, construction, and historic preservation. The research being presented involves the methodology of implementing two Leica 3D laser scanners simultaneously. The fieldwork focused on the digital historic preservation of Trim Castle in Trim, Ireland. A method for using both scanners simultaneously and efficiently was used in which small scan teams were proven to be more efficient. Creating a local grid allows the scanners to share a grid system. To move a scanner within the grid we must create a new station at the next location. Then, the scanner must be able to record the new location by scanning in a target placed at that location. Lastly, the scanner and the target switch position and the scanner will scan the target again to orient itself in the grid system. When using two 3D laser scanners, each scanner has its own set of coordinates in the grid system. Tying both the scanners into a local grid system allows them to share coordinates.

T60.00363: First-order Phase Transitions in the polarization switchings of vertical-cavity surface-emitting lasers
Tsu-Chiang Yen

The geometry of the laser cavity of vertical-cavity surface-emitting lasers (VCSELs) is a flat cylinder, which gives an intrinsically two-dimensional isotropic freedom to the polarization states of VCSEL's emitted light. This symmetry can be broken by some residual stresses created in the manufacture processes, resulting in a linearly polarized output. Experimentally, it is often to observe the occurrence of the VCSEL's Polarization Switching (VPS) in which the polarization direction of VCSEL's output switches with the laser's current. The investigations of VPS is important for the understanding of strong photon-carrier interactions in quantum wells. Earlier studies suggested that VPS is a second-order phase transition based on some criticalities observed in the experiments. However, conventional experiments were carried out with a tuning of laser's current. Therefore, those experiments cannot clarify whether VPS is conducted by the thermal effect or by the field effect of the laser's current. This research try to distinguish VPS caused by these two effects. Experiments discovered that some VPS exhibited features of the first-order phase transitions. More results will be represented in the conference.

T60.00364: Linewidth Narrowing of Surface Plasmon Polaritons Mode in Au Hollow Nanodome Lattices
Jinlin Zhang, Woo Ri Ko, Fei Long, Min Hyung Lee, Jae Yong Suh

Au hollow nanodomes arranged in continuous and hierarchical hexagonal lattices support surface plasmon polaritons (SPPs) propagating at air-Au interface. The cross-sectional heights of the both hexagonal nanodome arrays can be altered by a simple thermal treatment. We report that the change of nanodome size leads to a significant linewidth narrowing of SPP modes because of reduced scattering loss. Furthermore, the optimized surface modulation depth is found to be around 100 nm for achieving a longer propagation length of SPP. Quantitative evaluation of the linewidths and integrated intensities of SPP resonances, in correlation with material's surface morphology, suggests two size regimes where the initial SPP excitation strength varies differently depending on the surface modulation depth.

T60.00365: A single-X-ray photon detector with possible energy resolution based on superconducting W0.8Si0.2 stripes
Xiaofu Zhang, Andreas Schilling, Qiang Wang

We fabricated a superconducting single X-ray photon detector based on W0.8Si0.2 and the basic detection performance for keV-photons was measured. The detector has a critical temperature of 4.97 K and it is able to work just below the critical temperature with negligible dark counts. We measured the detection efficiency at different temperatures and bias currents, and a saturated detection characteristics on bias current was observed at all temperatures. The signal pulse amplitude histograms show three distinct peaks, similar to the characteristic peaks from the used tungsten target. This demonstrates a possible energy resolution for superconducting X-ray detectors based on the current biased two dimensional stripes.

T60.00366: Size-based Sorting of Magnetic Microparticles using Patterned Circular Arrays in Variable Magnetic Fields
Edward Cullom, Noah Sanchez, Robert Raulston, Gregory Vieira

The controlled locomotion of superparamagnetic microparticles is useful for lab-on-chip biomedical devices and sorting heterogeneous particle populations. We have built and refined a low-cost system capable of applying tunable magnetic forces and moving particles of varying sizes. Controlled locomotion is made possible by patterning micro-sized circular NiFe arrays onto a 1 cm^2 silicon chip, generating magnetic traps at the circles' peripheries when external fields are present. The direction of particle motion is determined by pre-programmed sequences of changing magnetic field and input from a joystick, allowing the user to manipulate the particles in real-time. Particles of varying sizes were used, ranging from 2μm − 4μm in diameter. For given field sequences, we have found that each particle has a maximum velocity, dependent on its size and selected features of the platform, at which it can travel across the array. At higher velocities, microparticles of differing sizes transverse the circular array at different rates. The particles posess an intrinsic cut-off velocity, dependent on diameter, at which they can no longer transverse the array. This allows the user to selectively manipulate particles of a particular size, potentially allowing for sorting of the microparticles.

T60.00367: Electrostatically Gated p-n Junctions based on Encapsulated Few Atomic Layers of InSe
Shahriar Memaran, Wenkai Zheng, Luis Balicas

InSe, similar to Transition Metal Dichalcogenides (TMDs), has a layered crystallographic structure and can be exfoliated down to a single unit cell. It has been shown that InSe is a good candidate for photodetectors, covering the visible to the near-infrared region, with high photoresponsivities that are superior to those of other recently reported two-dimensional (2D) crystal based photodetectors. It has also been proved to be a promising candidate for field effect transistors (FET), with

carrier mobilities exceeding 1000 cm^2/V.s at room temperature. Here we evaluate the performance of p-n junctions that are based on few atomic layers of InSe encapsulated between h-BN on two separate back gates. The thickness of the InSe crystal ranges between 7 to 10 atomic layers with a near direct band gap φ of 1.3<φ<1.4 eV, which makes them a good candidate for photovoltaic applications. Moreover, due to smaller badgap of about 1.25 eV for bulkier crystals the devices are potential candidates for near infrared detection.

T60.00368: Laser Patterned Graphene Electronic Devices on Graphene Oxide Films Derived from Natural Carbon Feedstocks

Michael Seas, Joseph Murphy, William Rice, John Ackerman, Patrick Johnson

Recent research has shown that laser irradiation of graphene oxide (GO) films produces a significant change in the lattice structure of the material resulting in greater sp^2 hybridization and causes the precursor, GO, to become conductive. This technique has been exploited to design transparent, flexible electrode arrays for touch screen and supercapacitor applications promising a new, low-cost alternative to methods involving more expensive exotic compounds such as indium tin oxide (ITO). One challenge this process has faced is lower than expected conductivities, on the order of 10^4 S/m, observed in the patterned material as compared to bulk graphite (10^5 S/m) and epitaxially grown graphene (10^8 S/m). We utilize carbon phase change data derived from annealing of natural carbon feed stocks to understand optimized conditions for patterning. We then show that these conditions produce electrode arrays of superior conductivity through laser patterning in a controlled atmosphere laser annealing chamber. Phase change data is also employed to relate graphene oxide to natural carbon feed stocks to demonstrate a proof of concept for low cost electronics.

T60.00369: Degenerate Four-Wave Mixing of Surface Plasmon Polaritons and Volume Waves in Au/VO2

Nardeep Kumar, Armando Rúa, Jennifer Aldama, Karla Echeverria, Félix Fernández, Sergiy Lysenko

We investigate experimentally the nonlinear degenerate four-wave mixing process with excitation of surface-plasmon polaritons (SPPs) in Au/VO2 composite structure. The ultrafast formation of transient grating in VO2 layer is accompanied by nonlinear wave interaction with SPPs excited by attenuated total reflection (ATR) coupler at Au/VO2 interface. Optical mixing of waves with same and different linear polarizations gives rise to surface plasmon wave by inducing a nonlinear polarization. Photoinduced diffraction grating in photorefractive layer is also used to decouple the SPPs from surface and to convert SPPs to volume optical wave, which was then directly detected by a photodetector. It is demonstrated a possibility of efficient tuning of enhancement, reflection and diffraction of optical waves in photorefractive Au/VO2 structure via excitation of surface plasmons within visible and near-infrared region. Nonlinear energy transfer between different types of waves with the ability to manipulate and decouple SPPs from the surface opens new possibilities for future plasmonics devices.

T60.00370: Decoupling of IMT and SPT for Mott Transition in Strained VO2 Films on AlN/Si

Jin-Cheol Cho, Tetiana Slusar, Hyun-Tak Kim

Insulator-to-metal transition (IMT) in a strongly correlated material VO$_{\mathrm{2}}$ is under the gaze of scientists, attempting to obtain the solely electronic Mott transition without any structural intervention in the vicinity of room temperature. It would open up the numerous prospects for application, for example, Mott field effect transistor able to overcome the size and switching speed limitations of the Si-based transistors Moreover, synergy of VO$_{\mathrm{2}}$ and existing silicon technology can provide inexpensive mass production of the new generation switching devices. In this work, using the high-quality epitaxial VO$_{\mathrm{2}}$ films, successfully integrated with Si, we were able to delay IMT and structural phase transition (SPT) by strain engineering and to decouple this two processes. In particular, through simultaneous monitoring of evolution of the IMT and SPT with temperature we obtained the evidence of the electron-correlation-driven Mott transition in VO$_{\mathrm{2}}$ (IMT precedes SPT for up to 10 K!) occurring in the same monoclinic crystalline structure.

T60.00371: Magnetic Critical Fluctuations Of Ising-like Antiferromagnet DyScO3

Liusuo Wu, S. E. Nikitin, Matthias Frontzek, Alexander Kolesnikov, Georg Ehlers, Mark Lumsden, Er-Jia Guo, Andrei Savici, Zheng Gai, Athena Sefat, Andrei Podlesnyak

Orthorhombic perovskites provide a perfect playground for investigations of novel magnetic phenomena. We here report on detailed low temperature magnetic properties of the DyScO3 by means of single crystal and powder neutron scattering, and magnetization measurements. We show that Dy3$+$ has an Ising-like anisotropy with easy axis of magnetization lying in ab plane, consistent with the calculated wave functions of the ground doublets, which is mostly contributed from \textbar ±15/2\textgreater . Below TN $=$3.2 K, Dy3$+$ ising moments orders antiferromagnetically, with the ground state configuration AxGy, selected by the dipole-dipole interaction. Magnetic diffuse scattering in the elastic channel were observed over a wide temperature range, indicating the existence of strong critical fluctuations associated with the Ising ground states. The ground state wave function indicates that conventional transverse fluctuations like magnons are strongly suppressed. In addition, the longitudinal fluctuations are `hidden' to neutrons, restricted by the selection rules $\Delta S=$1.

T60.00372: Extraction and characterization of cellulose nanocrystals from Puerto Rico's Bambusa vulgaris

Nicole Ramos Solis, Nelson Granda Paz, Josee Vedrine-Pauleus, Mariana I. Leon Berrios, Wilfredo Otano

Cellulose nanocrystals (CNCs) were extracted and characterized from \textit{Bambusa vulgaris Schrad. ex Wendl}, a species of bamboo found in Puerto Rico. The CNCs extraction process was based on the acidic hydrolysis of delignified and bleached bamboo pulp, removing phenolic compounds and chromophoric molecules in lignin and degrading hemicellulose and lignin components within the bamboo fibers. A pure form of bamboo CNCs were isolated as colloidal suspension and characterized using Fourier transform infrared (FTIR), X-ray diffraction (XRD), spectroscopies scanning electron and atomic force microscopies. FTIR analysis of freeze-dried CNCs indicated that hemicellulose and lignin were efficiently removed. Atomic force microscope images of polydispersed CNCs depicted rod-shaped structures with average distribution in dimensions of 480 nm and 120 nm, in length and diameter, respectively, and aspect ratio of 4.

T60.00373: Synthesis of Transparent and Flexible Supporting Films from Cellulose Acetate

Kevin Diaz Aponte, Nicole Ramos Solis, Josee Vedrine-Pauleus

In this work, we developed a method to fabricate transparent substrate films derived from cellulose acetate. We combined blends of cellulose acetate with organic solvents such as DMSO, SMF, THF, acetone and glycerol, taking into consideration the mechanical and optical properties of the resulting films. In the first stage of investigation, we studied the concentrations of cellulose acetate with acetone or glycerol solvents, and determined the appropriate concentration of cellulose acetate with Acetone (CA/A); we then performed further studies with DMSO, DMF, and THF solvents using a 10 wt% stock solution, and decreased the concentration with dilution factor of 2. The solutions were deposited on silicon wafers using spin coating and drop-cast processes. UV-Vis analysis was used to measure film transmission from 200 to 750 nm. In addition, we used AFM to reveal surface topography of film substructures.