2013 Annual Fall Meeting of the APS Prairie Section

Columbia, Missouri

http://meetings.aps.org/Meeting/PSF13/

Program updates:

New posters:

F1.02a - Studying TGE's Using Fixed Land-Based Detectors; E. Bell, A. Keller, Z. Monti, B. Shannon, C. Turner, R. Williams and C. Fasano; Monmouth College. Work is supported by NSF-AGS1232594.

F1.02b - Calibration of Neutrino Detector Via the Decay of Cosmic Muons; Emily Bell; Monmouth College. Work is supported by NSF-AGS1232594.

Thursday, November 7, 2013 7:00PM - 8:00PM –

Session A1 Public Lecture Life Sciences Center Monsanto Auditorium - Carlos Wexler, University of Missouri

7:00PM A1.00001 Higgs Boson and Beyond: The Big Questions in Particle Physics MARK NEUBAUER, University of Illinois at Urbana-Champaign — This year's Nobel Prize in physics was awarded to two theorists that predicted the existence of the long-sought Higgs boson particle, which was discovered by teams of physicists at the Large Hadron Collider. This is no ordinary particle—it gives mass to other particles and completes our best theory of nature called the "standard model." Is this end of the story? Far from it, as the standard model is an incomplete description of Nature even with a Higgs boson now observed. In this talk, I will discuss what we know about this new particle and the open questions in particle physics, the pursuit of which might lead to big discoveries on the horizon.

Friday, November 8, 2013 8:30AM - 9:54AM –

Session B1 Particle Physics I Memorial Union Benton Bingham - Bahram Mashhoon, University of Missouri

8:30AM B1.00001 Higgs Boson Properties and Prospects , MARK NEUBAUER, University of Illinois at Urbana-Champaign — In this talk, I will present what is known about the Higgs boson from measurements at the Large Hadron Collider. I will also discuss searches for other Higgs bosons and prospects for improved understanding of the Higgs boson properties.

9:06AM B1.00002 Observation of a Z boson produced in association with a charm quark at the Fermilab Tevatron , JESSICA SECKLER, Wheaton College, KEITH MATERA, KEVIN PITTS, University of Illinois at Urbana-Champaign, CDF COLLABORATION — The production of W and Z bosons in conjunction with heavy quarks has been the object of study at the Tevatron and LHC. In addition to testing the standard model, understanding these processes is relevant to studies of the Higgs boson as well as searches for new physics. We present a new analysis of Z boson plus charm production with the CDF detector at the Fermilab Tevatron using fully reconstructed D* decays.

9:18AM B1.00003 Particle Assignment in the ttH Production Channel of the Higgs Boson[1] , EMMA MOLDEN, University of Illinois at Urbana-Champaign, NEUBAUER TEAM — Even though the Large Hadron Collider has been shut down for improvements since February 2013, there is still an abundance of data to investigate. We focused on looking for the Higgs boson in a production channel where it is produced in association with two top quarks. When searching for the Higgs boson in a collision it is necessary to reconstruct the mass of the Higgs boson to improve the signal-to-noise ratio, which requires correct particle assignment. I present a method of particle assignment for the ttH production channel, used on simulated data from the ATLAS detector. This production channel could reveal information about this newly-discovered particle that has potential to open new doors in the search for new physics beyond our current understanding.

[1]National Science Foundation Grant No. 1062690

9:30AM B1.00004 The Complete Test Results of 1800 Multi-Anode Photomultiplier Tubes for CMS-HF Calorimeter Upgrade , EMRAH TIRAS, None, CMS-HCAL COLLABORATION — The Compact Muon Solenoid (CMS) is one of the two large general-purpose particle detectors used with the Large Hadron Collider (LHC) project at CERN. The Hadronic Forward (HF) calorimeters cover the polar angles from 0.78° to 5.70° with respect to the beam direction at each end of the CMS detector. The HF plays important roles in identifying tagging jets, measuring the luminosity and determining the missing transverse energy. Currently, the HF undergoes upgrades (2013 and 2014) to deal with larger beam currents and higher center-of-mass energy collisions expected in the LHC Run-II starting in 2015. The High Energy Physics (HEP) group at the University of Iowa is responsible for characterization and installation of 1800 multi-anode photo-multiplier tubes (PMT), testing of readout boxes and light guide systems and the replacement of the front-end electronics. We are also participating in simulation studies to understand the expected performance of the upgraded HF. In this talk, the complete test results of multi-anode PMTs for several different parameters are presented. These results can provide insights about the expected performance of the upgraded CMS-HF detector.

9:42AM B1.00005 Proposal to search for $D^0 \to \mu^+\mu^-$ decay at CMS , SULEYMAN DURGUT, None — We propose to use $D^0 \to \varphi\rho$ as the normalization for search of $D^0 \to \mu^+\mu^-$ at CMS. The branching fraction of flavor changing natural current decay (FCNC) $D^0 \to \mu^+\mu^-$ is about 10^{-13} by SM. They decay via box diagrams in the short distance limit, but SUSY quarks and wino can contribute to the box diagrams can significantly enhance it. The charm meson decays are constraining couplings to up-type quarks not necessarily constrained by B decays, thus presents and immaculate and unexplored region to search for new physics. The current BF limit is 6×10^{-9} at 90% confidence level by LHCb. CMS PAS paper (BPH-11-017) sets limit to 5×10^{-7} at 90% confidence limit based on $90pb^{-1}$ of data. This is certainly an important channel to search for new physics.

Friday, November 8, 2013 8:30AM - 9:54AM –

Session B2 Condensed Matter Physics I Memorial Union Stotler I&II - Tom Heitmann, University of Missouri Research Reactor

8:30AM B2.00001 $Tb_2Mo_2O_7$: Spin glass, spin ice and possible candidate for magnetic monopoles exploration , DEEPAK SINGH, University of Missouri, Columbia — The frustrated pyrochlore compound $Tb_2Mo_2O_7$ stands at an interesting crossroads, being a representative of both the Mo-based family $R_2Mo_2O_7$ (R = rare earth) and other Tb-based compounds $Tb_2X_2O_7$ (X = metal). As a function of the R-site radius, $R_2Mo_2O_7$ compounds exhibit a metal-insulator transition between the ferromagnetic metal states and the spin glass insulators. $Tb_2Mo_2O_7$ exhibits the spin-glass behavior, $T_G \sim 24$ K, despite the apparent lack of chemical disorder. This compound crystallizes in a cubic space group in which both the Tb and Mo atoms form three-dimensional networks of corner-sharing tetrahedra. Thus, each magnetic ion resides on a highly frustrated pyrochlore lattice. Neutron scattering measurements on single crystal specimens of $Tb_2Mo_2O_7$ revealed the short-ranged spin arrangements resembling the "spin ice" structure with Tb moments slightly tilted off the local <111> -direction. Detailed analysis of a.c. and nonlinear susceptibilities suggest that $Tb_2Mo_2O_7$ is not sufficiently frozen below glass transition, rather finite spin dynamics persists to the lowest measurement temperature. Such nonconventional glassy behavior is also reflected in thermodynamic scaling of the nonlinear susceptibilities. In addition to the spin ice configuration and a nonconventional spin glass transition, $Tb_2Mo_2O_7$ also exhibits **Q**-independent temperature dependent background. Similar experimental observations in an isostructural pyrochlore, $Ho_2Ti_2O_7$, were identified as distinct signatures of Dirac's effective magnetic monopoles. Thus $Tb_2Mo_2O_7$ provides a new frontier to extend this noble quest.

9:06AM B2.00002 Structural and Magnetic Transitions in $Ca_{10}(Fe_{1.996}Pt_{0.004}As_2)_5(Pt_3As_8)$ studied by neutron and x-ray diffraction[1] , AASHISH SAPKOTA, ANDREAS KREYSSIG, GREGORY TUCKER, MEHMET RAMAZANOGLU, Iowa State University (ames lab), DOUGLAS ROBINSON, Argonne National Laboratory, NI NI, University of California, Los Angeles, ALAN GOLDMAN, ROBERT MCQUEENEY, Iowa State University (ames lab) — $Ca_{10}(Fe_{1.996}Pt_{0.004}As_2)_5(Pt_3As_8)$ compound is a member of the Fe-based high-temperature superconductor family. Recent work showed that instead of being tetragonal as most of the pnictide superconductors are, this compound exhibits only a pseudo-tetragonal structure. We studied the structure and magnetic properties of $Ca_{10}(Fe_{1.996}Pt_{0.004}As_2)_5(Pt_3As_8)$ single crystal by x-ray and neutron diffraction at the station 6-ID-D, Advanced Photon Source, Argonne, and at the instrument HB-1A, High-Flux Isotope Reactor, Oak Ridge, respectively. We found a lattice distortion from pseudo-tetragonal to pseudo-orthorhombic below T_s = 110 K and stripe-like antiferromagnetic order below T_N = 96 K. Both phase transitions are 2^{nd} order in nature. Though the structure is pseudo-tetragonal with a complex superstructure rather than being common tetragonal, the magnetic order and lattice distortion are similar to most other pnictide superconductors demonstrating these ordering phenomena extremely robust against deviations from simple structure motifs and against chemical disorder.

[1]This research was supported by the U.S. DoE, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering. Ames Laboratory is operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358.

9:18AM B2.00003 Magnetic Order in $CeGe_{1.76}$ studied by neutron diffraction on single crystals[1] , W. JAYASEKARA, Ames Laboratory and Dep. of Physics and Astronomy, Iowa State University, AmesAmes Laboratory and Dep. of Physics and Astronomy, Iowa State University, W. TIAN, HFIR, Oak Ridge National Laboratory, A. KREYSSIG, S.L. BUD'KO, P.C. CANFIELD, R.J. MCQUEENEY, A.I. GOLDMAN, Ames Laboratory and Dep. of Physics and Astronomy, Iowa State University, AmesAmes Laboratory and Dep. of Physics and Astronomy, Iowa State University — The $CeGe_{1.76}$ compound shows a very interesting magnetic behavior with a rich set of features in magnetization measurements indicative for several antiferromagnetic and ferromagnetic transitions at low temperatures. In this report we will present our recent neutron diffraction studies on a $CeGe_{1.76}$ single crystal performed at the instrument HB-1A, High-Flux Isotope Reactor, Oak Ridge. We revealed a complex magnetic phase diagram: Below approx. 7 K, the magnetic Ce moments order in an antiferromagnetic structure with an incommensurate propagation along the c direction. The major component of the ordered moment is aligned along the b direction. Detailed temperature-dependent scans along the c direction show a lock-in to a commensurate antiferromagnetic order around 5.5 K connected with a squaring up of the ordered moments indicated by the occurrence of higher harmonic satellite Bragg peaks. Below 4 K additional Bragg peaks occur indicative of a second coexisting type of magnetic order with small moments aligned along the a or c direction. Further experiments are necessary to conclude the determination of this complex magnetic ordering in the $CeGe_{1.76}$ compound.

[1]This research was supported by the U.S. Department of Energy, Office of Basic Energy Sciences, DMSE through contract No. DE-AC02-07CH11358.

9:30AM B2.00004 On the wetting, phase transitions, and diffusion of water on supported bilayer lipid membranes[1] , ZACHARY BUCK, ANDREW MISKOWIEC, MIA BROWN, MENGJUN BAI, JASON COOLEY, RENEE JIJI, HASKELL TAUB, University of Missouri - Columbia, FLEMMING HANSEN, Technical University of Denmark, HELMUT KAISER, MU Research Reactor, MADHUSUDAN TYAGI, NIST Center for Neutron Research, SOULEYMANE DIALLO, EUGENE MAMONTOV, KENNETH HERWIG, Oak Ridge National Laboratory — Temperature-dependent elastic incoherent neutron scattering shows qualitatively different freezing behavior for water associated with single bilayers of the charge-neutral DMPC (dimyristoylphosphocholine) lipid and for the anionic DMPG (dimyristoylphosphoglycerol) bilayer membrane supported on a silicon substrate. While water in the vicinity of the neutral DMPC membrane shows a major freezing transition slightly below the bulk freezing point, water near DMPG is characterized by continuous freezing to lower temperatures. Water remains mobile in the DMPG system down to 210 K in contrast to water associated with the DMPC membrane, which freezes completely at 255 K. We suggest that this behavior may be related to a film-like water structure in the DMPG case owing to the hydrophilic nature of the substrate, while most of the water in the DMPC system is bulk-like and dewets from the hydrophobic surface. Analysis of the quasielastic spectra of the DMPC system yields a diffusion constant of the membrane-associated water that decreases in a step-like fashion on cooling, indicating a second freezing transition below the one attributed to bulk-like water.

[1]Supported by NSF IGERT Grant No. DGE-1069091.

9:42AM B2.00005 Magnetic diffraction at MURR and possible magnetic ordering in magnetoelectric $HoAl_3(BO_3)_4$, TOM HEITMANN, University of Missouri Research Reactor, QIANG ZHANG, Ames Laboratory, U.S. DOE, K.C. LIANG, Texas Center of Superconductivity and the Department of Physics, University of Houston, L.M. BEZMATERNYKH, V.L. TEMEROV, Institute of Physics, Siberian Division, Russian Academy of Sciences, Krasnoyarsk, 66036, Russia, B. LORENZ, Texas Center of Superconductivity and the Department of Physics, University of Houston, DAVID VAKNIN, Ames Laboratory, U.S. DOE — We report on single-crystal diffraction studies of $HoAl_3(BO_3)_4$ we have performed to unravel its magnetic properties. $HoAl_3(BO_3)_4$ is among a number of compounds with the trigonal huntite crystal structure (R32, No. 155) that display magnetoelectric (ME) coupling and is notable as having one of the strongest ME effects [Liang et a. PRB 83, 180417(R) (2001)]. To test for any putative magnetic ordering, we have performed single-crystal neutron diffraction measurements on flux grown $HoAl_3(BO_3)_4$ crystals. We report preliminary results on the appearance of a crystallographic reflection that is forbidden in the huntite structure at a temperature that is consistent with the appearance of the ME effect. We associate this reflection with the emergence of antiferromagnetic ordering of the Ho^{3+} moments that establishes a broken time-reversal symmetry, the prerequisite condition for the ME effect. These experiments will be placed in the context of the burgeoning collaborative effort between MURR and the neutron scattering group at the Ames Laboratory.

Friday, November 8, 2013 10:30AM - 11:54AM –

Session C1 Particle Physics II Memorial Union Benton Bingham - Mark Neubauer, University of Illinois

10:30AM C1.00001 Studies of the CMS HF "aging" effect at the High-luminosity LHC , KAMURAN DILSIZ, None, CMS COLLABORATION — The Hadronic Forward Calorimeters (HF) at the CMS are instrumented to have a pseudorapidity coverage from 3.0 to 5.0 in the CMS laboratory frame. It plays a key role in identifying forward jets to study the Higgs boson produced in vector boson fusion (VBF) processes. After the proposed high-luminosity LHC upgrade, during the course of running the quartz fibres used in the HF readout are expected to receive significant radiation dose and the performance of the forward jet reconstruction could be degraded, an "aging" effect. This could degrade the performance of the Higgs studies in VBF channels. In this talk, we present a study of this "aging" effect using CMS fast Monte-Carlo simulations in the context of VBF Higgs decaying into taus. Preliminary results show that the VBF signal is not significantly diminished by the "aging" effect in the HF.

10:42AM C1.00002 J/ψ photo-production at the Relativistic Heavy Ion Collider with STAR. , L. CHANAKA DE SILVA, Creighton University, STAR COLLABORATION — Ultra-peripheral collision events are effectively photo-production on nuclear targets. Relativistic heavy ions carry strong transverse electromagnetic fields that can be treated as sources of quasi-real virtual photons. The ions interact through photon-pomeron and photon-photon collisions at impact parameters more than twice the nuclear radius, so hadronic interactions are suppressed. These events also provide an ideal proving ground for new programs in e+A physics. We present recent results from the J/ψ photo-production measurement using 200GeV Au+Au collisions in the STAR experiment at RHIC. The p_T distribution of the J/ψ mesons peaks at very low p_T, consistent with expectations for coherent photo-production. Because of its heavy mass, the J/ψ meson has sufficient virtuality to probe the Au wave function deeply enough to discern the possible presence of gluon shadowing. We will present the measurement of J/ψ cross section in 200GeV Au+Au collisions, as well as a distribution of J/ψ rapidity within $|y| < 1$. Possible theory comparisons are also discussed.

10:54AM C1.00003 Evidence of Narrow Structure in the J/$\psi\phi$ Mass Spectrum in Exclusive $B^+ \to J/\psi\phi K^+$ decay at CMS , MAKSAT HAYTMYRADOV, CMS, CMS COLLABORATION — Analysis of heavy quarkonium states provides an effective method to test QCD predictions. Recent studies on these mesons show that there are states which have decay modes similar to charmonium, but are difficult to put in a charmonium system. There have been several proposals explaining these states as hybrid($q\bar{q}g$) or four-quark ($q\bar{q}q\bar{q}$) exotic mesons. Discoveries such as the X(3872) and Y(3940) motivated examination of other VV states. Observation of Y(4140) at CDF detector further inspired to search for the same structure at CMS detector. In this analysis the $J/\psi\phi$ channel was studied through the exclusive decay of $B^{\pm} \to J/\psi\phi K^{\pm}$, where $J/\psi \to \mu^-\mu^+$ and $\phi \to K^+K^-$. The analysis was conducted on pp collision data at $\sqrt(s) = 7$TeV collected by the CMS detector. We report on two narrow structures with masses around 4148 and 4317 GeV in $J/\psi\phi$ mass spectrum which are well above the threshold for $c\bar{c}$ charmonium decays.

11:06AM C1.00004 Optimizing the Monte Carlo Simulation for the DarkSide Detector[1] , MATTHEW SMALLCOMB, ANDREW ALTON, Augustana Coll - Sioux Falls, DARKSIDE COLLABORATION — My goal was to test and help optimize the new Monte Carlo simulator being developed by Davide Franco of the DarkSide collaboration. Developing a robust optical simulation of the Darkside-50 detector is essential for understanding the behavior of background events and is necessary for showing proof of concepts in order to procure funding for the project. I spent the summer looking at reproducing event positions from simulation data and comparing detector data and simulation results of the ratio between light detected on the top and bottom photomultiplier tubes. Testing showed that there were some critical changes that need to be implemented in the simulation.

[1]SD Space Grant, National Science Foundation, Augustana College, State of South Dakota, Davide Franco, DarkSide Collaboration

11:18AM C1.00005 The Muon Charge Asymmetry Measurement in Inclusive pp→W+X production at $\sqrt{s}$=7 TeV , HASAN OGUL, The University of Iowa, CMS COLLABORATION — Measurements of the muon charge asymmetry in inclusive pp→W+X production at $\sqrt{s}$=7 TeV are presented. The data sample corresponds to an integrated luminosity of 4.7 fb^{-1} recorded by the CMS detector at the LHC. With a sample of more than 20 million $\mathrm{W} \to \mu\nu$ events, the statistical precision is greatly improved in comparison to previous measurements. These new results provide additional constraints on the parton distribution functions of the proton in the Bjorken parameter x range from 0.001 to 0.1.

11:30AM C1.00006 Comparative study of nonperturbative heavy quarks in the nucleon , TIMOTHY HOBBS, JOHN LONDERGAN, Indiana University, WALLY MELNITCHOUK, Jefferson Lab — We perform an analysis of the role of nonperturbative (or intrinsic) charm in the nucleon. Charm is generated nonperturbatively through Fock state expansions of the nucleon wave function to include five-quark virtual states involving charmed mesons and baryons. We consider contributions from a variety of charmed meson-baryon states and find surprisingly dominant effects from the $\bar{D}^{*0}\,\Lambda_c^+$ configuration. Particular attention is paid to the existence and persistence of high-x structure for intrinsic charm, and the x dependence of the $c - \bar{c}$ asymmetry predicted in meson-baryon models. We also discuss efforts to constrain intrinsic charm via a forthcoming global QCD analysis, and the possibility of extracting intrinsic strangeness using a similar approach.

11:42AM C1.00007 Searches for possible T-odd and P-odd short range interactions using polarized nuclei , RAKSHYA KHATIWADA, Indiana University, PINGHAN CHU, Duke University, ALEC DENNIS, Indiana University, CHANGBO FU, Shanghai Jiaotong University, HAIYAN GAO, GEORGIOS LASKARIS, Duke University, KE LI, ERICK SMITH, WILLIAM SNOW, HAIYANG YAN, Indiana University, WANGZHI ZHENG, Duke University — Various theories predict the possible existence of T-odd and P-odd short-range forces between spin-1/2 fermions, proportional to $\mathbf{S} \cdot \mathbf{r}$ where $\mathbf{S}$ is the fermion spin and $\mathbf{r}$ is the separation between particles. We use ensembles of polarized nuclei and an unpolarized mass to search for such a force over sub-mm ranges. We established an improved upper bound on the product $g_s g_p^n$ of the scalar coupling to particles in the unpolarized mass and the pseudo-scalar coupling of polarized neutrons for force ranges from 10^{-4} to 10^{-2} m, corresponding to a mass range of $2 \cdot 10^{-3}$ to $2 \cdot 10^{-5}$ eV for the exchange boson.

Friday, November 8, 2013 10:30AM - 12:06PM –

Session C2 Condensed Matter Physics II Memorial Union Stotler I&II - Helmut Kaiser, University of Missouri Research Reactor

10:30AM C2.00001 Site-inversion versus frustration in the $CoAl_2O_4$ spinel: A neutron diffraction study at MURR[1] , DAVID VAKNIN[2], Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames IA 50011 — Neutron diffraction studies of a well defined $CoAl_2O_4$ polycrystalline sample reveal the role that site-inversion plays in determining the magnetic properties of this system. The A-B site-inversion in the spinel system is a long standing issue. In this regard $CoAl_2O_4$ is notorious as Co-Al site-inversion can exceed 20% and, so far, could not be totally eliminated. In this talk, I will review previous reports including more recent ones that emphasize Co-Co next-nearest-neighbor coupling in the diamond-like Co sublattice that is claimed to lead to exotic spin-liquid structure or to be on the boundary of a recently predicted phase diagram between a collinear antiferromagnetic and a spiral magnetic structure. I will present the various views on the phase diagram of $CoAl_2O_4$ as a function of Co-Al site inversion parameter and contrast them with our neutron diffraction studies.

[1]Ames Laboratory is supported by the U.S. Department of Energy, Office of Basic Sciences and Engineering. under Contract No. DE-AC02-07CH11358.

[2] In collaboration with Q. Zhang, T. W. Heitmann, B. Roy, A. Pandey, D. C. Johnston, and Y. Furukawa

11:06AM C2.00002 Adsorption-Induced Conformational Changes in Porous Materials , MATTHEW CONNOLLY, CARLOS WEXLER, University of Missouri — In physisorption it is normally assumed that the adsorbent is structurally inert, its porous conformation unchanged by the adsorption; this assumption underlies most conceptual/theoretical framework used for characterization of porous solids. Recently, the mechanical response of the material has come under scrutiny: when a gas enters pores with sizes comparable with the range of the van der Walls forces an excess pressure/tension is created. Here we present a theoretical, computational and experimental demonstration of conformational expansion (breathing) of graphene-like adsorbents upon adsorption: Molecular dynamics simulations show the potential for supercritical hydrogen to open new pores in carbons. Grand Canonical Monte Carlo perturbative calculations demonstrate a reduction of the free energy of strip-shaped pores with gas loading upon a conformational change that increases the net size of micropores. Experimentally, reversible pore expansion during adsorption was measured by x-ray scattering for graphene oxide frameworks. These breathing modes have significant consequences for medium- to high-pressure adsorption, with modified adsorption isotherms that may require re-interpretation of standard models. Supported by DOE DE-FG02-07ER46411, ACS-PRF 52696-ND5, and NSF 1069091.

11:18AM C2.00003 Diffusion of Squalene in n-alkanes and squalane , BRUCE KOWERT, St. Louis University — Squalene, an intermediate in the biosynthesis of cholesterol, has a 24-carbon backbone with six methyl groups and six isolated double bonds. Capillary flow techniques have been used to determine the translational diffusion constant, D, of squalene at room temperature in several nonpolar solvents; they include squalane, n-hexadecane, and three n-octane-squalane mixtures. Values of r, squalene's hydrodynamic radius, are calculated from the Stokes-Einstein relation and decrease as the viscosity increases. These solvent-dependent r values are a consequence of the relative sizes of squalene and the solvents. The Stokes-Einstein limit assumes the solute is much larger than the solvent; this is not the case for our solutions. A number of n-alkane solutes diffusing in n-alkane solvents also have r values that decrease as the viscosity increases. The r values for squalene and these n-alkanes have a common dependence on the ratio of the solvent's van der Waals volume to that of the solute probe. The translational motion of squalene appears to be similar to that of n-alkane solutes with similar chain lengths diffusing in n-alkane solvents; n-tetracosane is an example.

11:30AM C2.00004 Emergence of coherence in the charge density wave state of intercalated 2H-NbSe2.[1] , S. ROSENKRANZ, Argonne National Laboratory — Charge density waves (CDWs) are ubiquitous in condensed matter and associated with many exotic phenomena of great interest. This symmetry breaking state is described by a complex order parameter with an amplitude and a phase. In the conventional view of CDW formation, based on clean, weak-coupling systems, finite amplitude and long-range phase coherence set in simultaneously at a single temperature, the CDW transition temperature, but the situation may be dramatically different at strong coupling or in the presence of disorder. We have studied in detail the CDW formation in pristine and intercalated samples of 2H-NbSe2, a CDW material with strong electron-phonon coupling, combining structural (X-ray), spectroscopic (photoemission and scanning tunneling microscopy) and transport probes. In contrast to the conventional view, we find two separate characteristic temperature scales that can be widely separated. The higher crossover scale marks the onset of short-range CDW correlations, with non-zero amplitude and associated gap in the electronic spectra, but with an incoherent phase of the order parameter. The lower scale is a phase transition that marks the onset of global phase coherence and long-range CDW order. The observation of a persistent gap in the absence of long-range order and the absence of coherent excitations are strikingly similar to the characteristics of the pseudogap state observed in cuprate superconductors and other systems. Our observations thus emphasize the importance of phase fluctuations in strongly coupled CDW systems and provide new insights into the significance of phase incoherence in the realization of pseudogap phases.

[1]Work supported by US DOE BES-DMS DE-AC02-06CH11357

Friday, November 8, 2013 2:00PM - 3:24PM –

Session D1 Astrophysics, Space Physics and Cosmology Memorial Union Benton Bingham - Angela Speck, University of Missouri

2:00PM D1.00001 Thermodynamic modifications to spectral analysis and radiative transfer models of dust: Implications for asteroids, circumstellar dust, and gravitational collapse , ANNE HOFMEISTER, Washingtion University — Radiative transfer of light under diffusive conditions is important to astronomy, engineering, and planetary interiors. Three different errors exist in models, arising from failure to incorporate thermodynamic constraints. 1) Emissions have been mistaken for emissivity in analyzing spectra because the effect of thermal gradients in partially transparent solids was ignored. Applying the correct form of Kirchhoff's law to surfaces of large asteroids indicates mineralogies commonly found in meteorites. 2) Refraction across interfaces has been modeled as conical emanations of a point source, but the 2^{nd} law of thermodynamics only permits heat to flow down the thermal gradient. We revise formula for the effective thermal conductivity and discuss heat flow in Earth's mantle and in dusty nebulae. 3) Because light speed is 5 orders of magnitude larger than speeds of most physical processes, quasi-radiative equilibrium is generally maintained. Specifically, dust clouds cannot heat up during gravitational contraction. We correct stability criteria. Formation of the solar system did not produce heat because the current rotational energy of the objects nearly equals their gravitational potential energy. For young dwarfs, the balance is exact. These examples indicate that substantial corrections are needed in radiative transfer models and data processing in astronomy and planetary science.

2:36PM D1.00002 Using Spatially-Resolved Spectroscopy to Study Stardust , LACEY DANIELS, SPECK ANGELA, NELSON DESOUZA, SUKLIMA GUHA NIYOGI, Univ of Missouri - Columbia, STARDUST COLLABORATION — We present a study of spatial distribution of different dusty spectral features in the Oxygen-rich Asymptotic Giant Branch star SW-Vir. We have spectral data for 8-14μm from Michelle at Gemini North, covering a 10x10 grid centered on the star to yield a set of 100 spectra cover (4 x 4 arcseconds of sky). We analyzed each spectrum by eliminating the continuum and the measuring the parameters (full width at half maximum, peak position, and strength) of the remaining spectral features. To assess the precision of the measurements, we chose to eliminate the continuum in two different ways – dividing and subtracting a fitted power law. We compared the resulting measurements to each other in order to find correlations. We sought correlations between the parameters of the spectral feature as well as between different spectral features and with apparent radial distance from the central star. We did not find any correlation between the equivalent properties when comparing subtracted and divided spectra or between any parameters, even when the parameters of a single continuum-elimination technique were compared. Our results suggest that the standard model for dust formation and/or our attributions of specific compounds to specific spectra features are far too simple.

2:48PM D1.00003 A Newtonian bias embedded within the Schwarzschild metric , JOHN LAUBENSTEIN, Northern Illinois University — Karl Schwarzschild never suggested the existence of the event horizon. What we refer to as the Schwarzschild radius is the result of work done by David Hilbert after Schwarzschild's death. Albert Einstein never accepted what would later come to be known as the black hole. He was heavily criticized for his stubbornness in not accepting what his own theory predicted. Is it possible that both Einstein and Schwarzschild were on the right path all along? This paper explores the Equivalence Principle (EP) and suggests the need for a subtle revision. Specifically, the notion that acceleration may be held constant over a tiny interval within a homogeneous gravitational field. It is not my intent to challenge the mathematics of infinitesimal intervals. I suggest that there is nothing wrong with the mathematics of the Schwarzschild metric, but rather that this flawless mathematics results in modeling something that physically cannot occur from gravitation. My research provides an analysis of gravitational redshift and documents an inequality in the Equivalence Principle. The EP remains a critically important concept in understanding gravitation, yet it must be grounded within the correct correlation between acceleration and gravitation. This paper attempts to establish that correlation and further provides a mathematical proof of a Newtonian bias in the gravitational redshift equation that ultimately challenges the physical basis of the event horizon.

3:00PM D1.00004 Single Pulsar Timing and Gravitational Waves , ADAM HELFER, Univ of Missouri - Columbia — The possibility that gravitational waves might be detected by their effects on pulsar signals has been considered for some time. For studies of single pulsars, however, it has been thought that cancellations in the gravitational-radiation contributions made the effects disappointingly small. It turns out, though, that a plausible assumption in those analyses is incorrect, and the effects, though still very small, might be within the reach of observation. The most promising candidate systems would be pulsars close to rapidly-orbiting binaries. (MNRAS 430 (2013) 305)

3:12PM D1.00005 Gravitational Anomalies: An Attribute of Every Planetary and Satellite Body: A Natural Law , STEWART BREKKE, Northeastern Illinois University(former grad student) — Lateral variations in gravity in a planet or satellite are related to anomalous density distributions are gravitational anomalies. Variations in gravity have been found on Earth,the Moon and Mars. These are mountain ranges, canyons and basins such as mascons on Mars, Argyre and Utopia, and mascons on the Moon such as Imbrium and Orentale. Hawaii is a mascon on Earth. These anomalies result from the evolution in the geology of the planet or moon. Gaseous planets and satellites may have gravitational anomalies in their solid or semi solid cores, if they exist. Gaseous planets and satellites may have density concentrations of gases forming gravitational anomalies. Since gravitational anomalies are found on the Earth, the Moon and Mars, by induction gravitational anomalies will be found on all planets and satellites.

Friday, November 8, 2013 2:00PM - 3:36PM –

Session D2 Biological Physics Memorial Union Stotler I&II - Ioan Kosztin, University of Missouri

2:00PM D2.00001 Predictive modeling of the fusion of uneven multi-cellular aggregates using Cellular Particle Dynamics simulations[1] , MATTHEW MCCUNE, ASHKAN SHAFIEE, GABOR FORGACS, IOAN KOSZTIN, University of Missouri — Cellular Particle Dynamics (CPD) is an effective computational method for describing and predicting the time evolution of passive biomechanical relaxation processes of multi-cellular aggregates. A typical such relaxation process is the fusion of spheroidal bioink particles during post bioprinting structure formation. In CPD cells are modeled as an ensemble of cellular particles (CPs) that interact via short-range contact interactions, characterized by an attractive (adhesive interaction) and a repulsive (excluded volume interaction) component. The time evolution of the spatial conformation of the multicellular system is determined by following the trajectories of all CPs through integration of their equations of motion. CPD was successfully applied to describe and predict the fusion of 3D tissue construct involving identical spherical aggregates. Here, we demonstrate that CPD can also predict tissue formation involving uneven spherical aggregates whose volumes decreases during the fusion process.

[1]Work supported by NSF [PHY-0957914]. Computer time provided by the University of Missouri Bioinformatics Consortium.

2:12PM D2.00002 Investigation of SHAPE mechanism with RNA 3D structure modeling , PEINAN ZHAO, TRAVIS HURST, XIAOJUN XU, Department of Physics and Department of Biochemistry, University of Missouri, Columbia, MO 65211, KEVIN WEEKS, Department of Chemistry, University of North Carolina, Chapel Hill, NC 27599-3290, SHIJIE CHEN, Department of Physics and Department of Biochemistry, University of Missouri, Columbia, MO 65211, SHIJIE TEAM — Selective 2′-hydroxyl acylation by primer extension (SHAPE) chemical probing method for RNA reflects local structural dynamics, which is intrinsically related to RNA three-dimensional structure. To gain quantitative insights into the relationship between RNA three-dimensional structure and SHAPE reactivity, we develop an algorithm to rebuild the SHAPE profile from the three-dimensional structure. The algorithm starts from RNA structures and combines nucleotide interaction strength and conformational flexibility, ligand (SHAPE reagent) accessibility and base-pairing pattern through a composite function. Comparisons between the predicted SHAPE profile and experimental SHAPE data show high correlation, suggesting the validity of the extracted analytical function. The validity of the theory supports the model for the key factors that determine SHAPE reactivity profile. Furthermore, the theory offers an effective method to select viable RNA three-dimensional structures from an ensemble of decoy structure models.

2:24PM D2.00003 ABSTRACT WITHDRAWN –

2:36PM D2.00004 A Physics Approach to the Repositioning of DNA Damage , SARAH LEGRESLEY, MATTHEW ANTONIK, University of Kansas — An open question in genome maintenance is how DNA repair proteins find lesions at rates that seem to exceed diffusion limited search rates. We propose a phenomenon where DNA damage induces nucleosomal rearrangements which move lesions to potential rendezvous points which are more likely to be accessible by repair proteins engaged in a random search. The feasibility of this mechanism is tested by considering the statistical mechanics of DNA containing a single lesion wrapped onto the nucleosome. We consider lesions which make the DNA either more rigid or more flexible. This can be modeled as an increase or decrease in the bending energy in a partition function of nucleosome breathing. Our results indicate that the steady state for a breathing nucleosome will most likely position the lesion at the dyad or in the linker DNA, depending on the energy of the lesion. We speculate that these positions potentially serve as rendezvous points where DNA lesions may be encountered by repair proteins which may be sterically hindered from searching the rest of the nucleosomal DNA. A more sophisticated evaluation of this proposed mechanism will require detailed information about breathing dynamics, the structure of partially wrapped nucleosomes, and the structural properties of damaged DNA.

2:48PM D2.00005 Calculating free energy profiles in systems with memory effects from bi-directional pulling processes , JIONG ZHANG, IOAN KOSZTIN, University of Missouri-Columbia, Department of Physics and Astronomy — In biomolecules, in order to calculate kinetic quantities along a relevant reaction coordinate (RC), besides the corresponding free energy profile (potential of mean force or PMF), one also needs to properly identify the underlying stochastic model that best describes the dynamics along the RC. While there exist several methods for determining the PMF from fast non-equilibrium pulling processes, for simplicity reasons, it is generally assumed that the dynamics along the RC is that of a simple overdamped Brownian particle with known diffusion coefficient. Here we show that both the PDF and the features of the underlying non-Markov stochastic model (with memory effects), described by a generalized Langevin equation, can be determined simultaneously from properly designed bi-directional (forward and time-reversed) pulling processes. Besides the PMF, the proposed method determines the corresponding friction memory kernel, and identifies whether the diffusion along the RC is normal or anomalous (e.g., subdiffusion). The proposed method provides a novel way to analyze fast pulling data from molecular dynamics simulations and single molecule force microscopy.

3:00PM D2.00006 Glass is a viable substrate for atomic force microscopy of membrane proteins , NAGARAJU CHADA, KRISHNA SIGDEL, TINA MATIN, RAGHAVENDAR REDDY SANGANNA GARI, CHUNFENG MAO, LINDA RANDALL, GAVIN KING, University of Missouri, Columbia, MO — Since its invention in the mid-1980s, the atomic force microscope (AFM) has become an invaluable complementary tool for studying membrane proteins in near-native environments. Historically, mica is the most common substrate utilized for biological AFM. Glass being amorphous, transparent, and optically homogeneous has its own set of advantages over mica and has the potential to broaden the use the AFM into fields that require high quality non-birefringent optical access. The use of silanized glass as AFM substrates has been reported as a means to fine tune surface chemistry. However, such coatings usually require hours of additional preparation time and can lead to increased surface roughness. In this work, we present a simple technique for preparing borosilicate glass as a substrate for two membrane systems: non-crystalline translocons (SecYEG) of the general secretary system from *E. coli*, and bacteriorhodopsin (BR) from *H. salinarum*. For both these membrane proteins, quantitative comparisons of the measured protein structures on glass versus mica substrates show agreement. An additional advantage of glass is that lipid coverage is rapid ($<$ 10 minutes) and complete (occupying the entire surface). A goal is to study the bacterial export system using recently developed precision measurement techniques such as ultra-stable AFM.

3:12PM D2.00007 A calibration error revealed via local tip position detection in atomic force microscopy , KRISHNA SIGDEL, GAVIN KING, Department of Physics and Astronomy, University of Missouri-Columbia — Atomic Force Microscopy (AFM) is a versatile tool in nanoscience. In conventional AFM, knowledge of the local 3D tip position is not accessible and tip trajectories are extrapolated from the cantilever deflection (ΔZ) which provides data of reduced dimensionality. The sensitivity (nm/V) of ΔZ is calibrated by taking slope of ΔZcurve when the tip makes contact to a surface. Using a focused laser beam directly focused on the apex of the AFM tip, we have measured 3D positions of the tip as it interacts with a sample surface in fluid. We have observed a significant difference between the slope of (ΔZ) and that of the Z-tip position. This implies an erroneous calibration of sensitivity of ΔZ detection which we can now correct. Also, we have observed significant lateral slipping of tip as it touches the surface. These observations provide a comparison between tip and cantilever dynamics.

3:24PM D2.00008 A novel approach to modeling photon propagation in biological tissue using the scattering signatures of spheroidal particles , VERN HART, William Woods University, TIMOTHY DOYLE, Utah Valley University — Clinical applications of diffuse tomography require a Monte Carlo algorithm to model optical diffusion in turbid media. Of the existing algorithms, random-walk and phase function techniques are the most common. However, these approaches do not include histological information in determining subsequent photon paths. A significant amount of the optical scattering which occurs in cells has been attributed to intracellular structures, such as mitochondria, which are typically spheroidal in shape. The sphere-like cell nucleus can also become elongated during the early stages of certain cancers. The presented research introduces a novel Monte Carlo algorithm in which the scattering solution for light incident on a spheroidal particle is used to determine photon scattering directions. This technique is suggested to be a more physical description due to the inclusion of cellular properties. Diffusion profiles were generated using additional techniques for comparative purposes and significant differences were observed, indicating that the included scattering mechanism has a significant effect on the resulting diffusion. The ability to distinguish structural types in a scattered signal could potentially be used as an early diagnostic tool.

Friday, November 8, 2013 4:00PM - 5:36PM –

Session E1 Physics Education Memorial Union Benton Bingham - Meera Chandrasekhar, University of Missouri

4:00PM E1.00001 Flipping Introductory Physics at the University of Illinois , TIM STELZER, University of Illinois — Students' unprecedented access to content on the web is providing a unique opportunity to transform the role of lectures in education, moving the focus from content delivery to helping students synthesize the content into knowledge. We have introduced a variety of activities to facilitate this transformation at the University of Illinois, including web-based preflight assessments of student understanding before lecture, peer instruction (clickers) to assess and facilitate student understanding during lecture, and web-based multimedia pre-lectures designed to provide students with content before lecture. In this talk I will discuss the pedagogical motivation for introducing these activities, and the impact they have had at the University of Illinois.

4:36PM E1.00002 Tomorrow's Outstanding Physics Teachers at the University of Missouri , KAREN KING, DOUG STEINHOFF, Univ of Missouri - Columbia — The University of Missouri's TOP Teacher Program aims to recruit and prepare Tomorrow's Outstanding Physics Teachers. With support from the Physics Teacher Education Coalition, we have implemented multiple new recruiting tactics and made improvements to coursework and networking opportunities for pre-service physics teachers. Our most successful strategy has been a unique new high school based "Learning Assistant" program. Selected physics, physics education, and engineering majors help out in local high school physics classrooms, working with the same class $\sim$ 5 hours per week. At the end of the first year of the program, at least 67% of LA's reported being "interested" or "very interested" in high school teaching. This result is coupled by a dramatic (>1000%) increase in the number of students pursuing a BS in physics education.

4:48PM E1.00003 Barriers to Developing Physics Faculty Knowledge for Teaching: Identifying Gaps through Critical Review of the Literature , DEEPIKA MENON, University of Missouri, Columbia — In light of bringing reforms in STEM teaching at all educational levels to increase STEM workforce, The National Research Council (1999, 2003) and the Next Generation of Science Standards (NGSS, 2013) emphasize that STEM faculty should shift from traditional teaching to learner-centered instruction. Despite the call and significant efforts to encourage STEM faculty bring changes in their undergraduate instruction through the use of research-based instructional strategies, evidence suggest that only a small percentage of faculty members utilize the most of the pool available. This presentation will summarize the current literature on the barriers and common constraints which the physics faculties face to change their existing practices and use of research-based instructional strategies, and their perceptions of and about teaching. The findings are presented as five themes: a) mismatch between the thought processes of educational researchers and science faculty; b) dilemma to balance the time between research and teaching; c) personal beliefs about teaching and learning; d) graduate students preparation for the professoriate role in the science departments; and e) lack of pedagogical content knowledge. The potential solutions to such problems are discussed by providing existing exemplary programs and workshops that continue to prove successful in bringing desired changes in undergraduate teaching.

5:00PM E1.00004 Facilitating Transfer of Learning and Problem Solving in Physics[1] , N. SANJAY REBELLO, Kansas State University — Transfer of learning – the ability to apply what one has learned in one context to a different context – is an important aspect of problem solving physics. In this talk, I will briefly review contemporary perspectives on transfer of learning and discuss how these perspectives inform a theoretical framework that underpins our research over the past few years. I will present results of studies that demonstrate how instructional strategies based on this framework can facilitate problem solving in a calculus-based physics class. I will also discuss how our perspectives on transfer of learning inform our ongoing research on visual cognition and its application to developing visual cues that facilitate conceptual problem solving in physics.

[1]Supported in part by U.S. National Science Foundation grants 0816207 and 1138697.

Friday, November 8, 2013 4:00PM - 5:36PM –

Session E2 Condensed Matter Physics III Memorial Union Stotler I&II - Sashi Satpathy, University of Missouri

4:00PM E2.00001 Superconductivity in Topological Insulators[1] , YEW SAN HOR, Missouri Univ of Sci & Tech — Topological phases of matter such as three-dimensional topological insulators have been discovered and found to exhibit fascinating quantum phenomena. These materials have shown robust quantized properties i.e. bulk insulating phase but surface conducting phase with Dirac excitations. Three-dimensional topological superconductors have been theoretically proposed recently. These hypothetical topological superconductors (TSCs) are predicted to possess itinerant massless Majorana fermions which are charge neutral and spin 1/2 quasiparticles that only emerge and propagate on the surface. The Bogoliubov-de Gennes (BdG) Hamiltonian for the quasiparticles of a TSC is analogous to the Hamiltonian of a TI, with the superconducting gap corresponding to the band insulating gap. However, TSCs and the associated Majorana quasiparticles have not been conclusively established in real materials so far. Hence, this presentation will show by chemical doping, a TI can change into a bulk superconductor which could be a TSC. The first example i.e. $Cu_xBi_2Se_3$ was discovered few years ago to be a promising TSC. Several other promising candidates of TSCs will also be shown.

[1]YSH gratefully acknowledges support from US National Science Foundation grant DMR-1255607.

4:36PM E2.00002 The lifetime of Dirac plasmons in graphene[1] , ALESSANDRO PRINCIPI, GIOVANNI VIGNALE, Department of Physics and Astronomy, University of Missouri, Columbia, Missouri 65211, USA, MATTEO CARREGA, MARCO POLINI, NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56126 Pisa, Italy — Dirac plasmons in a doped graphene sheet have recently been shown to enable confinement of light to ultrasmall volumes. In this work we calculate the intrinsic lifetime of a Dirac plasmon in a doped graphene sheet by analyzing the role of electron-electron interactions beyond the random phase approximation. The damping mechanism at work is intrinsic since it operates also in disorder-free samples and in the absence of lattice vibrations. We demonstrate that graphene's sublattice-pseudospin degree of freedom suppresses intrinsic plasmon losses with respect to those that occur in ordinary two-dimensional electron liquids. We relate our findings to a microscopic calculation of the homogeneous dynamical conductivity at energies below the single-particle absorption threshold. Finally, we compute the impact of disorder on Dirac plasmon losses and then show that a very reasonable concentration of charged impurities yields a plasmon damping rate which is in good agreement with s-SNOM experimental results.

[1]BES Grant DE-FG02-05ER46203

4:48PM E2.00003 Density-Functional Theory of Thermoelectric Phenomena[1] , FLORIAN G. EICH, GIOVANNI VIGNALE, Department of Physics, University of Missouri-Columbia, Columbia, Missouri 65211, MASSIMILIANO DI VENTRA, University of California - San Diego, La Jolla, CA 92093 — Thermoelectric phenomena play an important role in the development of sustainable energy sources. We have introduced a non-equilibrium density-functional theory of local temperature and associated energy density that is particularly suited for the study of thermoelectric phenomena from first principles [1]. This theory rests on a local temperature field coupled to the energy-density operator. We identify the excess energy density, in addition to the charge density, as fundamental variable. These densities are obtained from an effective non-interacting Kohn-Sham system. We show that the Schrödinger equation for the Kohn-Sham system features a spatially varying mass representing the effect of local temperature variations. Furthermore we discuss strategies to approximate the Kohn-Sham potential and the spatially varying mass emerging in the Kohn-Sham equation.

[1] arXiv:1308.2311

[1]We gratefully acknowledge support from DOE under Grants No. DE-FG02-05ER46203 (GV,FGE) and DE-FG02-05ER46204 (MD).

5:00PM E2.00004 Magnetism in iron-based high-temperature superconductors and its effect on lattice and superconductivity[1] , ANDREAS KREYSSIG, Ames Laboratory, and Department of Physics and Astronomy, Iowa State University, Ames, IA — Shortly after the discovery of iron-based high-temperature superconductors in 2008, extensive studies using neutron and x-ray scattering techniques have revealed a strong interconnection of magnetism, lattice and superconductivity. In this presentation I will give an overview of the complex interplay between these phenomena and will bring it into context with other unusual superconductors. I will illustrate the phase relations exemplarily on the family of $A\mathrm{Fe_2As_2}$-based material (A = Ba, Sr, Ca) where a stripe-like antiferromagnetic order is coupled to a lattice distortion implying a strong coupling between magnetism and structure. Partial chemical element substitution suppresses these transitions and superconductivity occurs.

The study was performed in collaboration with M. G. Kim*, G. S. Tucker*, D. K. Pratt*, S. Nandi*, W. Tian#, J. Zarestky*, J.-W. Kim+, G. E. Granroth*, K. Marty#, M. D. Lumsden#, T. Heitmann=, A. Thaler*, N. Ni*, S. L. Bud'ko*, P. C. Canfield*, R. M. Fernandes*, J. Schmalian*, R. J. McQueeney*, and A. I. Goldman*; *Ames Laboratory, and Iowa State University; +APS, Argonne; #HFIR, Oak Ridge; =MURR, University of Missouri.

[1]The work at the Ames Laboratory was supported by US DOE, BES, DMSE, through contract DE-AC02-07CH11358.

5:40PM - 5:40PM –

Session F1 Poster Session (5:40 - 7:00 PM) Memorial Union Mark Twain - Carlos Wexler, University of Missouri

F1.00001 Detection of Rare Molecular Transitions in a Sample of Massive Star Forming Regions , LI LEE, ESTEBAN D. ARAYA, Western Illinois University — The study of molecular transitions is key to characterize the medium where massive stars form. Several molecular species have been used to study star formation, e.g., CH3OH and H2O. Molecular line studies at mm/submm wavelength are difficult due to confusion of blending spectral lines and atmospheric opacity. In contrast, observations at $\sim$ 6 GHz are not affected by the atmosphere, and blending of bright spectral lines is unusual. Thus, molecular lines in the $\sim$ 6 GHz range could become new probes to study massive star formation. We report a project aimed to detect rare molecular transitions toward 12 massive star forming regions. The observations were conducted with the 305m Arecibo Telescope. We detected four rare molecular transitions, including the second ever detection of 6.28 GHz H2CS. We also report tentative detections of 6.85 GHz and 7.28 GHz transitions of CH3OH, and 7.35 GHz CH emission toward the massive star forming region IRAS18566+0408. These tentative detections are weak but their velocities agree with the velocities of other molecular lines in IRAS18566+0408. We recently submitted an Arecibo proposal to re-observe these lines. If confirmed, we would have discovered three new astrophysical maser transitions.

F1.00002 ~~ABSTRACT WITHDRAWN~~ – Replaced by F1.02a and F1.02b see below

F1.00003 Optical absorption properties of Neodymium ions (Nd^{3+}) doped lead boro tellurite glasses , KINNARY PATEL, P.K. BABU, SAISUDHA MALLUR, Western Illinois University — The optical absorption properties of Nd^{3+} ions in PbO-TeO_2-B_2O_3 glasses were studied as a function of PbO content varying from 30 to 70 mol%. Glasses were prepared by the usual melt quench technique. Glasses were annealed at 400°C for 3 hours to remove thermal strains. Annealed glass samples were then polished. In order to understand the effect of host glass on the absorption properties of Nd^{3+} ions in these glasses, oscillator strength, intensity parameters and radiative transition probabilities of Nd^{3+} ions were calculated using the Judd-Ofelt theory. The variation of the intensity parameters Ω_t (t=2,4,6) with PbO content has been attributed to the changes in the asymmetry of the ligand field at the rare-earth (R) site (due to the structural changes) and to changes in R-O covalency.

F1.00004 Direct calculation of exciton binding energies with time-dependent density-functional theory[1] , ZENGHUI YANG, CARSTEN ULLRICH, University of Missouri - Columbia — Excitons are coupled electron-hole pairs below the band gap in bulk semiconductors. They are vital to photovoltaics, but they are hard to obtain in a TDDFT calculation, due to usually employed exchange-correlation kernels lacking the long-range part. Another difficulty comes from the usual method of applying TDDFT on bulk materials which calculate the spectrum - though suitable for continuum excitations, this approach does not upfront yield the binding energy of the discrete excitonic excitations. We develop a method in analog with the Casida equation formalism, in which exciton binding energies are obtained directly. We calculate exciton binding energies for both small- and large-gap semiconductors with this method. We study the recently published "bootstrap" exchange-kernel within our method, and we extend the formalism to treat triplet excitons.

[1]This work is supported by National Science Foundation Grant No. DMR-1005651.

F1.02a - Studying TGE's Using Fixed Land-Based Detectors; E. Bell, A. Keller, Z. Monti, B. Shannon, C. Turner, R. Williams and C. Fasano; Monmouth College. Work is supported by NSF-AGS1232594.

F1.02b - Calibration of Neutrino Detector Via the Decay of Cosmic Muons; Emily Bell; Monmouth College. Work is supported by NSF-AGS1232594.

F1.00005 Molecular Dynamics Simulations of Melting of Nitromethane Initiated at Crystal-Rare Gas Interfaces

, GANESH KAMATH, University of Missouri-Columbia, ALI SIAVOSH-HAGHIGHI, University of North Texas, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — The melting of nitromethane initiated at the (100), (010), and (001) crystallographic faces in contact with rare gases at pressures over the interval 1 kbar to 16 kbar has been investigated using molecular dynamics simulations with an all atom force field. Simulations were performed to evaluate the melting point of nitromethane crystal in contact with He, Ar, and Kr. The calculated melting curve is in good agreement with experiment and previous simulation results. The molecular-level mechanism of melting initiated at a crystal surface in contact with rare gas was compared with that for melting at the bare crystal surface and void-nucleated melting. Orientational disordering of the molecules at the melt front precedes the onset of translational freedom of molecules both at the crystal-fluid interface and in the core of the crystal. There is an increase of the time gap between the occurence of molecular reorientation and translational mobility in the nitromethane molecules. The predicted melting points for nitromethane in contact with He, Ar, and Kr are within 20 K of each other for all state points and can be correlated to the diffusion of the rare gas atoms into the nitromethane crystal. The diffusion of rare gas atoms into the crystalline solid eliminates the dependence of melting temperature on the crystallographic orientation reported previously for melting at bare surfaces.

F1.00006 Generalized Stacking Fault Energies in the Basal Plane of Triclinic Molecular Crystal 1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)

, NITHIN MATHEW, THOMAS SEWELL, University of Missouri-Columbia — Molecular dynamics and molecular mechanics simulations were used in conjunction with a fully flexible force field to calculate the generalized stacking fault energies in the basal plane (that is, the $a-b$ plane, where a, b, and c define the edge vectors of the primitive unit cell) of the triclinic molecular crystal 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Crystal symmetry and molecular stacking arrangement result in two glide plane types for the same glide plane normal vector. The unstable stacking fault energies are found to be less than 10 mJ/m^2 at 0 K and atmospheric pressure, indicating easy dislocation glide. Glide in the a and $a-b$ directions are favored to that in the b direction. Asymmetric unstable stacking fault energies indicate an asymmetric barrier to dislocation glide. Stable stacking faults with energies less than 1 mJ/m^2 are predicted for the a and $a-b$ directions. A compound twin is observed in the a direction with energy of 2.52 mJ/m^2. Nitro (NO_2) groups on the molecules undergo out-of-plane rotations during glide. The extremely small barriers to twinning and dislocation glide might be sources for observed second harmonic generation in the nominally centrosymmetric crystal.

F1.00007 Radial distribution function of liquid argon in modified hard sphere model[1]

, MICHAEL KORTH, SAESUN KIM, Univ of Minn - Morris, UMP TEAM — We begin with a geometric model of colliding hard spheres and calculate probability densities in an iterative sequence of calculations that lead to the pair correlation function. The model is based on a kinetic theory approach developed by Shinomoto [Phys. Lett A, 89, 19 (1982)]. We added a weak attractive interatomic potential for argon based on the work of Aziz [J. Chem. Phys. 99, 4518 (1993)] in order to find radial distribution function of liquid argon. Results are in partial agreement with experiment. We are exploring additional modifications to the model.

[1]Morris Academic Partnership

F1.00008 Effects of Annealing on the Structure and Properties of $Mn_{5-x}Fe_xSi_3$

, ZACHARY SPENCE, CODY DAWSON, PEGGY HILL, Department of Physics & Engineering Physics, Southeast Missouri State University, IGOR DUBENKO, ABDIEL QUETZ, NAUSHAD ALI, Department of Physics, Southern Illinois University-Carbondale — Materials forming with the Mn_5Si_3 crystal structure have been found to exhibit interesting magnetic, magnetocaloric, and spin polarization properties. In particular, alloys of $Mn_{5-x}T_xSi_3$ (T = transition metal) have been investigated as possible magnetocaloric materials. Previous research has shown that $Mn_{5-x}Fe_xSi_3$, with x = 4, exhibits the largest magnetic entropy of the system (4 J/kgK) and orders ferromagnetically just below 300 K, making it a possible candidate for room temperature magnetic refrigeration applications.[1] Our work aims to study changes in the magnetic and magnetocaloric properties of $MnFe_4Si_3$ as a result of substitution at the silicon site. The effect of annealing, without quenching, on crystal structure homogeneity was investigated for the parent compounds Fe_5Si_3 and Mn_5Si_3 and for Mn_4FeSi_3 by x-ray diffraction. A reduction in x-ray diffraction peaks due to impurities was observed after annealing the Mn_5Si_3 and Mn_4FeSi_3 samples. The x-ray profile of Fe_5Si_3 was greatly improved by annealing and it adopted the proper Mn_5Si_3 $D8_8$ hexagonal crystal structure without quenching.

[1]Songlin, et al., J. of Alloys and Compounds. **334** (2002) 249

F1.00009 Missing Material At The Buried Interface For Ag/Si(111)7x7 Thin Films Deposited at Glancing Angle[1]

, S.T. HAYDEN, YIYAO CHEN, University of Missouri - Columbia, M.W. GRAMLICH, University of Massachusetts - Amherst, R.S. GARI, G.M. KING, P.F. MICELI, University of Missouri - Columbia — Missing material (vacancies) below the exposed surface has not been widely investigated during film growth because conventional surface science experiments do not probe below the surface (STM, LEED, etc.). X-ray scattering techniques, however, can uniquely explore the role of buried defects in epitaxial crystal growth, owing to its sensitivity to both the surface and the subsurface. Our prior work has shown the presence of vacancies in homoepitaxial film growth (Kim et al., Appl. Phys. Lett. 91, 093131 (2007) and Phys. Rev. B 86, 155446 (2012)). In the present study of heteroepitaxial Ag/Si grown at glancing angles, X-ray reflectivity and atomic force microscopy (AFM) measurements each yield the same surface height distribution. However, there is a significant portion of sub-surface missing material that is concealed to the AFM, but, which is revealed by the X-ray reflectivity measurements that detect the electron density profile. This missing material is determined to be concentrated at the buried film-substrate interface for deposition-angle-dependent grown Ag/Si(111)7x7.

[1]Support from the National Science Foundation under grants DMR-0706278 and DGE-1069091 is gratefully acknowledged. The Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory is supported by the US-DOE under Contract No. W-31-109-Eng-38.

F1.00010 Boron Doping of Activated Carbon

, MATTHEW CONNOLLY, ALEXANDER ST. JOHN, MATTHEW BECKNER, PETER PFEIFER, CARLOS WEXLER, University of Missouri — Efficient storage of hydrogen is one of the challenges to be solved for the H2-based fuelling systems. Carbon-based materials show promise, given their light weight, large surface areas and low cost. Unfortunately, the interaction of H2 and carbon, 5kJ/mol, is insufficient for room-temperature operation, the interaction energy for optimal delivery being ¿15kJ/mol. It has been proposed that boron doping of carbon materials could raise the binding energy of H2 to 12kJ/mol. However, the nature of the incorporation of boron into a carbon structure has not been studied in detail. Here, we address the energetics of boron incorporation into a carbon matrix via adsorption and decomposition of decaborane. First principles calculations demonstrate: (1) A strong adsorption of decaborane to carbon (70-80kJ/mol) resulting in easy incorporation of decaborane, sufficient for up to 10-20% B:C at low decaborane vapour pressures. (2) Identification that boron acts as an electron acceptor when incorporated substitutionally into a graphene-like material, as expected due to its valence. (3) The electrostatic field near the molecule is responsible for ca. 2/3 of the enhancement of the H2-adsorbent interaction. Supported by DOE DE-FG36-08GO18142, ACS-PRF 52696-ND5, and NSF 1069091.

F1.00011 Fabrication and characterization of single-supported bilayer membranes of anionic lipids.[1]

, ANDREW MISKOWIEC, MENGJUN BAI, HASKELL TAUB, University of Missouri - Columbia, FLEMMING HANSEN, Technical University of Denmark — We report the fabrication of bilayer membranes of the anionic lipid DMPG (1,2-dimyristoyl-*sn*-glycero3-phosphoglycerol) deposited on a silicon substrate. Due to electrostatic effects associated with the DMPG molecule, traditional vesicle fusion methods for producing supported bilayers must be modified to encourage rupture. In particular, high divalent salt concentrations in the buffer solution are necessary to "prime" the substrate for vesicle adsorption; furthermore, lower DMPG concentrations are required than for the neutral analogue DMPC (1,2-dimyristoyl-*sn*-glycero3-phosphocholine). We speculate that lower DMPG concentrations allow neutralization of the bilayer with hydrogen ions, increasing the membrane fluidity. We also investigated the temperature dependence of the bilayer thickness in order to monitor the gel-to-fluid phase transition of the DMPG and DMPC membranes. Both show a higher transition temperature than found for spherical vesicles. However, the effect is greater for the DMPG bilayer for which the phase transition is shifted to 70 °C, 45 °C above the free-vesicle value.

[1]Supported by NSF IGERT Grant No. DGE-1069091.

F1.00012 Interfacial structure and morphology of nano-crystalline Ag on Si(111)7x7: an in-situ x-ray scattering study[1]

, YIYAO CHEN, M.W. GRAMLICH, S.T. HAYDEN, University of Missouri, M.C. TRINGIDES, Iowa State University, P.F. MICELI, University of Missouri — There is intense interest to understand the factors that control the growth of nano-scale metals on supported substrates and, although the Ag/Si(111) system has been extensively studied for this purpose, little is known about the buried interface of the Ag nano-islands because most experimental probes only detect the top surface. Here, we present the results of in situ synchrotron x-ray scattering studies that reveal previously unknown and unexpected features of the buried nano-island/substrate interface. It is found that the incommensurate FCC Ag nano-islands consume the wetting layer upon which they grow and the islands extend to the reconstructed 7x7 Si surface. Consequently, the Ag island height distribution is one monolayer thicker than previously assumed, with a trilayer being the most stable island height at low coverage. Moreover, the lattice spacing of the islands is determined to be the same as bulk Ag, contrary to several prior STM measurements. These results are discussed in terms of the competition between electron confinement effects versus the role of interfacial energy, both of which are important for determining the growth morphology of nano-scale metals on supported substrates.

[1]Support is acknowledged from NSF grants DMR-0706278 and DGE-1069091. The Advanced Photon Source & Sector 6 beam-line at Argonne National Lab is supported by US-DOE contract W-31-109-Eng-38.

F1.00013 Spin-Orbit Interaction and Rashba Effect in the 2D metal dichalcogenides

, MOHAMMAD MAHDI VALIZADEH, SHANAVAS K. VEEDU, SASHI SATPATHY, Department of Physics, University of Missouri, Columbia, MO 65211 — The monolayer metal dichalcogenides such as MoS_2 and WS_2 are currently an emerging class of 2D materials owing to their possible applications in 2D electronics including spintronics. The Rashba effect which describes the momentum-dependent spin-splitting of the band structure originates from the spin-orbit interaction and inversion symmetry breaking. The effect is expected to be much stronger in the dichalcogenides with high-Z elements such as WS_2, WO_2, etc. Here, we study the Rashba effect in WS_2 from a tight-binding model as well as from density-functional calculations. We find a strong Rashba effect leading to the possibility of applications in spintronics such as spin-valves.

F1.00014 Magnetic and Magnetocaloric Properties of $MnFe_4Si_{3-x}In_x$

, CODY DAWSON, ZACHARY SPENCE, P. HILL, Southeast Missouri State University Department of Physics and Engineering Physics, IGOR DUBENKO, ABDIEL QUETZ, NAUSHAD ALI, Southern Illinois University - Carbondale Department of Physics — The magnetocaloric effect has attracted pressing curiosity for its application in magnetic refrigeration because it presents an alternative to current refrigeration technology that is more efficient and environmentally friendly. Previous research on the $Mn_{5-x}Fe_xSi_3$ system has shown that magnetic entropy changes are enhanced in the $MnFe_4Si_3$ compound [1]. We have prepared samples of $MnFe_4Si_{3-x}In_x$ in order to investigate how In substitution for Si affects the properties of this system. Samples were prepared by arc melting and annealed for 5 days at 900°C and the crystal structure of each sample was systematically studied through X-ray diffraction techniques to determine phase purity. Then the system was investigated by measuring magnetization as a function of temperature and magnetic field. Here we report on the magnetic and magnetocaloric properties of the pseudo ternary $MnFe_4Si_{3-x}In_x$ system for x = 0, 0.5, 1, and 1.5, and discuss its applicability in magnetic refrigeration.

[1] Songlin, Dagula, O. Tegus, E. Brück, J.C.P. Klaasse, F.R. de Boer, K.H.J. Buschow, J. Alloys Compd. 334 (2002) 249.

F1.00015 Forbidden Reflections and Interference Effects in X-ray Reflectivity from Si(111)7x7[1]

, J.W. KREMENAK, YIYAO CHEN, S.T. HAYDEN, University of Missouri, M.W. GRAMLICH, University of Massachusetts Amherst, P.F. MICELI, University of Missouri — In diffraction, X-ray reflections from diamond crystal structures with Miller indices that satisfy h+k+l = 4n+2, where n is an integer, are considered to be forbidden by crystal symmetry. However, these "forbidden reflections" have been observed experimentally, starting with W.H. Bragg over 90 years ago. Asymmetric charge distributions and anharmonic vibrations break the crystal symmetry and result in weak, but non-zero, intensities for these reflections. In the present work, we investigate the forbidden reflections in x-ray reflectivity and crystal truncation rods where we have discovered that the interference between bulk and surface waves can distinguish between the charge and vibrational origins of the reflections. Synchrotron x-ray scattering results, as well as a model, are presented. Understanding the properties of the forbidden reflections in diamond crystal structures not only provides greater insight into the crystal bonding and vibrations, but will also lead to better models for surface structures.

[1]Support from the National Science Foundation under grants DMR-0706278 and DGE-1069091 is gratefully acknowledged. The Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory is supported by the US-DOE under Contract No. W-31-109-Eng-38.

F1.00016 Scaling analysis of the magnetic field-tuned quantum phase transition in superconducting amorphous Pb films

, NICHOLAS OLSON, Monmouth College, IL, ASHWANI KUMAR, Monmouth College, Monmouth, IL — Quantum phase transitions are the transitions (QPTs) that take place at absolute zero, where the crossing of the phase boundary changes the quantum mechanical ground state. Superconductor to insulator transitions is the prime examples of the QPTs. In these transitions the phase boundary can be crossed using various parameters such as disorder, magnetic field, charge carrier density etc. In this presentation we will talk about the scaling analysis of the magnetic field tuned superconductor to insulator quantum phase transition.

F1.00017 Probing charge transfer complex (CTC) states in organic solar cells using photocurrent spectroscopy , DHANASHREE MOGHE, PING YU, University of Missouri-Columbia, CATHERINE KANIMOZHI, SATISH PATIL, Indian Institute of Science, Bangalore, India, SUCHISMITA GUHA, University of Missouri-Columbia — Diketopyrrolopyrrole (DPP) containing copolymers have generated considerable amount of interest in bulk heterojunction organic photovoltaics due their high power conversion efficiency (above 10 percent) and mobility. Within a bulk heterojunction solar cell, the combination of a donor and acceptor chromophores facilitates charge transfer from the donor to the acceptor and may result in the formation of interfacial electronic state at the donor-acceptor interface. Here, we present photocurrent studies to identify the interfacial charge complex states in five DPP based copolymer (donor): fullerene devices using Fourier transform photocurrent spectroscopy (FTPS) and monochromatic photocurrent spectroscopy. The optical band gap of DPP based copolymer ranges from 1.4-1.7eV. Our studies show that a larger optical band gap difference between the donor and the acceptor prohibit the formation of a stable charge transfer complex state. Further, we also observe that devices in which no charge transfer state was observed show a better efficiency than devices in which charge transfer state is observed.

F1.00018 Single Molecule Relaxation in Crystalline Nitromethane , LUIS RIVERA-RIVERA, University of Missouri-Columbia, ALI SIAVOSH-HAGHIGHI, University of North Texas, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Classical molecular dynamics simulation results for the relaxation of a single molecule in perfect crystalline nitromethane (CH_3NO_2) at 250 K and 1 atm hydrostatic pressure will be presented. The molecule was instantaneously excited by statistically distributing excitation energy between 25.0 kcal/mol and 125.0 kcal/mol, initially all in the form of kinetic energy, among the 21 degrees of freedom. Following a subpicosecond interval dominated by intramolecular reequilibration of kinetic and potential energy, loss of kinetic energy from the excited molecule is approximately exponential, with time constants between 11.7 ps and 13.7 ps. A non-linear and non-monotonic correlation between the exponential relaxation time constant and excitation energy is predicted. Energy transfer from the excited molecule to surrounding quasi-spherical shells of molecules occurs concurrently to the first and second shells, but with more energy per molecule transferred more rapidly to the first shell.

F1.00019 Theoretical determination of anisotropic thermal conductivity for crystalline 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) , MATTHEW KROONBLAWD, THOMAS SEWELL, University of Missouri-Columbia — Bond stretching and three-center angle bending potentials have been developed to extend an existing rigid-bond TATB molecular dynamics force field [D. Bedrov, O. Borodin, G. D. Smith, T. D. Sewell, D. M. Dattelbaum, and L. L. Stevens, J. Chem. Phys. **131**, 224703 (2009)] for simulations requiring fully-flexible molecules. The potentials were fit to experimental vibrational spectra and electronic structure predictions of vibrational normal modes using a combination of zero kelvin eigenmode analysis for the isolated molecule and power spectra for the isolated molecule and crystal. A reverse non-equilibrium molecular dynamics method [F. Müller-Plathe, J. Chem. Phys. **106**, 6082 (1997)] was used to obtain the room temperature, atmospheric pressure thermal conductivity along three directions in a well-defined, non-orthogonal basis. The thermal conductivity was found to be significantly anisotropic with values 1.13, 1.07, and 0.65 $W{\cdot}m^{-1}{\cdot}K^{-1}$ for directions nominally parallel to the **a**, **b**, and **c** lattice vectors, respectively.

F1.00020 Concentration-dependent embedded atom method potential for Al-Cu system , SULEIMAN OLORIEGBE, SEWELL THOMAS, THOMPSON DONALD, ZHEN CHEN, SHAN JIANG, University of Missouri-Columbia, YONG GAN, Zhejiang University, Zhejiang, China — A concentration-dependent interatomic potential for Al-Cu alloys has been carefully constructed in the framework of embedded atom method (EAM) refer to here as CDEAM potential. The interatomic interaction terms for the pure components Al and Cu were adapted from a previously published EAM work. The new potential incorporate interactions between Cu and Al using a pair potential function that is augmented with a fourth order polynomial function to account for concentration dependence. The potential was optimized using experimental heat of mixing for liquid Al-Cu alloys at 1467 K, second-order elastic constants and zero Kelvin formation energies from DFT for various alloy configurations and compositions. The resulting potential is able to reasonably reproduce the heat of formation across the entire composition. The heat of formation at zero Kelvin and mixing enthalpy at 1467 K as well as the second-order elastic constants are compared with existing Al-Cu potentials in the literature. Our potential reasonably reproduces the alloy mixing enthalpies at 1467 K. As a further test, we computed properties not included in the fit, such as liquid structures, self-diffusion coefficient, liquid densities, enthalpies and heat capacities as a function of temperature. The results of these properties computed using CDEAM potential are in good agreement with experimental data.

F1.00021 Rotational -Vibrational Energy Transfer in OH(v,J)+ Ar at High Pressures , REZVAN CHITSAZI, DONALD THOMPSON, University of Missouri-Columbia — The exchange of energy in collisions of atoms, molecules and radicals has attracted interest since the introduction of kinetic theory and its subsequent applications in chemistry. We have studied the effects of pressure on the relaxation of excited OH radical. In most modeling of gas phase chemistry it is assumed that it occurs via isolated elementary bimolecular collisions; that is, the fundamental energy transfer and reactions occur between pairs of species. Our interest is to explore the relaxation of an internally excited radical at pressures for which the bimolecular collision assumption breaks down. We will present results for molecular dynamics simulations of the rotational-vibrational energy transfer for OH(v,J) in an Ar bath for internal energies up to the dissociation limit and over pressure and temperature ranges that include and exceed those achievable in the laboratory.

F1.00022 A Study of the Effects of Basis Functions in Interpolating Moving Least Squares Methods for Fitting Potential Energy Surfaces , YI SHI, DONALD THOMPSON, University of Missouri-Columbia — The interpolating moving least-squares (IMLS) method is an efficient means for potential energy surface fitting [R. Dawes, D. L. Thompson, A. F. Wagner, M. Minkoff, J. Chem. Phys., **128**, 084107 (2008)]. To date no studies have been carried out on the effects of basis functions on the accuracy and fidelity of IMLS. Power functions are the only basis functions that have been used in IMLS. In our study, different basis functions have been used to fit different dimensional potential energy surfaces with IMLS. The efficiencies of various basis functions have been compared. The potential energy surfaces selected to fit are the Morse potential and an accurate analytical H_2O_2 potential energy surface. Our results show that other functions can be more efficient than power functions.

F1.00023 Super-resolved Microscopy via Coherent Population Oscillations , KISHOR KAPALE, Western Illinois University, GIRISH AGARWAL, Oklahoma State University — We present a microscopy scheme to attain sub-nanoscale resolution based on the phenomena of coherent population oscillation (CPO). We build on the success of our earlier super-resolution methods based the phenomena of coherent population trapping (CPT). For microscopy applications it is crucial to make sure the effect being employed for super-resolution is attainable in a large class of materials. In this context, it becomes necessary to resort to a phenomena-which is similar to CPT but can be potentially observed in a larger class of materials including gases, liquids, and room-temperature solids–such as CPO. The CPO based schemes involve two-level atoms coupled to two optical fields slightly different in frequency. The CPT-like nonlinear effects such as group velocity manipulations within the CPO schemes have been observed in room temperature solids and biological samples as opposed to in atomic vapors and cold atomic gases in the case of CPT. This parallel allows us to extend our CPT-based work to CPO-based microscopy schemes and makes them attainable in much larger class of materials including solids and biological samples. We show that the CPO-based schemes offer similar resolution as the CPT-based schemes and are attainable in a larger class of materials.

F1.00024 A DFT and *Ab Initio* Study of the Thermal Decomposition of 1,3,3-Trinitroazetidine (TNAZ)

, JEFFREY VEALS, DONALD THOMPSON, University of Missouri-Columbia — Density functional theory (DFT) and *ab initio* methods are employed to investigate unimolecular decomposition pathways of 1,3,3-trinitroazetidine (TNAZ) initiated by loss of NO_2 or HONO. Geometry optimizations are performed using M06/cc-pVTZ for all species commonly included in the initial decomposition mechanisms. Coupled-cluster (CC) theory with single, double, and perturbative triple excitations [CCSD(T)], is used to calculate more accurate single point energies at the M06/cc-pVTZ geometries. The CCSD(T)/cc-pVTZ energies for NO_2 elimination by N-N and C-N bond fission are 43.21 kcal/mol and 50.46 kcal/mol, respectively. The decomposition route initiated by *trans*-HONO elimination can occur by a concerted H-atom and nitramine NO_2 elimination or by loss of an alkyl NO_2 group and H-atom with energy barriers calculated using CCSD(T)/cc-pVTZ, respectively, 47.0 kcal/mol and 48.27 kcal/mol. At the CCSD(T)/cc-pVTZ level, the energy ordering of these four decomposition steps from most favored to least favored is as follows: N-N bond fission (43.21 kcal/mol), HONO elimination involving the nitramine NO_2 group (47.0 kcal/mol), HONO elimination involving the alkyl NO_2 group (48.27 kcal/mol), and finally C-N bond fission (50.46kcal/mol). Therefore the most likely initial decomposition route of TNAZ is predicted to be N-N bond fission.

F1.00025 Controlled Focusing Properties with Cylindrical Vector Beams[1]

, MAOJIN YUN, 1 Department of Physics, Astronomy, and Materials Science, Missouri State University, 2 College of Physics Science, Qingda, LIFENG DONG, Department of Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897, USA, WEI LV, College of Physics Science, Qingda University, Qingdao, 266071, China — The rapid increase of interest in cylindrical vector beams was driven largely by the unique focusing properties of such beams discovered recently. Particularly, it was found that radially polarized light can be forced into a tighter spot than those of spatially homogeneous polarization. In addition, the longitudinal component experiences an apodization effect that is different from the transverse component and is spatially separated from the transverse focal field. These effects enable three-dimensional tailoring of the focus shape. Focusing properties of cylindrical vector beams have attracted great attention and quickly became the subject of extensive worldwide research due to their applications in lithography, optical storage, and optical tweezers. In this study, pure phase plate was used to modulate phase distribution of the cylindrical vector beams to investigate their focusing properties. By using the Richards-Wolf vector diffraction theory, the simulation results show that two optical bubbles of stronger light intensity around dark spots can be obtained with the incoming cylindrical vector.

[1]This work was supported by the National Natural Science Foundation of China (Nos. 10904080, 11144007, and 11274188), the Distinguished Middle-aged and Young Scientist Encourage and Reward Foundation of Shandong Province, China (No. BS2011DX007).

F1.00026 ABSTRACT WITHDRAWN —

F1.00027 Effect of Potentiator VX-770 on the Kinetics of Disease-Associated Mutant CFTR Channels

, ZULEYHA YUKSEK, ZOIA KOPEIKIN, SILVIA BOMPADRE, University of Missouri — CFTR (Cystic Fibrosis Transmembrane Conductance Regulator) is a Cl- channel whose malfunction results in the genetic disease CF. One of the most common CF-associated mutations is the deletion of Phe 508 (ΔF508) resulting in channels with poor membrane expression and impaired function. Several functional abnormalities were demonstrated: infrequent openings, shorter locked-open time, reduced resident-time for the ATP molecule bound in the first nucleotide binding domain NBD1. Recently, the drug VX-770 was approved for clinical use, which increases the activity of ΔF508-CFTR. We studied the effect of VX-770 on the functional defects associated with ΔF508-CFTR: the Po of the channels is increased 12x due to the increase of opening rate and open time. Response to ATP analogues is decreased when channels are treated in conjunction with VX-770, suggesting that the potentiator by itself repairs gating defects. The potentiation effect was observed for temperature-corrected channels as well as channels treated with corrector VX-809. The shorter locked-open time of hydrolysis-deficient mutants is prolonged by VX-770 suggesting a stabilizing effect on the NBD dimer. The ATP resident time at NBD1, reflecting a partial NBD dimer configuration, is not affected by VX-770.

F1.00028 The Isolated Nucleotide Binding Domains of CFTR Form Bipartate ATPase To Regulate ATP Consumption

, MARK PALMIER, SILVIA BOMPADRE, University of Missouri — The CFTR Cl- channel belongs to the ATP binding cassette (ABC) family. Contains 2 transmembrane domains that form the channel pore, 2 nucleotide-binding domains (NBDs) and a regulatory domain. Channel opening is primed by ATP binding to NBDs and their dimerization. The stable dimer forms a bipartite ATPase. With ATP at its center hydrolysis occurs, leading to dimer separation and channel closure. Progress has been achieved in the characterization of CFTR gating. But conformational changes behind the gating transitions can only be inferred on structural data from other ABC transporters. The structural dynamics governing CFTR mechanisms are still unknown. Advancements in purification technology make it possible to address the question of dynamics. Our goal is to investigate the dynamics of NBD dimer formation and separation using Single Molecule Fluorescence. Here we show our progress: that dimerization is a tight binding event ($Kd \sim 1\mu$M), hydrolysis competence only when dimerized and FRET demonstrating the association of the two isolated domains in presence of ATP. The goal of this project is to discern the molecular mechanisms governing the CFTR function. When completed, our findings will increase the overall understanding of the relationship between function and dynamics.

F1.00029 Monitoring the uniformity of alpha helices in lipophilic environments[1]

, ANAHITA ZARE, JIAN XIONG, JASON COOLEY, RENEE JIJI, University of Missouri — It is known that membrane-embedded alpha helices are more uniform structurally than their aqueous counterparts. Despite this uniformity, protein dynamics are thought to be common in these proteins in order for them to conduct their cellular tasks. However, how amino acid sequence facilitates these dynamics remains unknown as methods for investigating structural heterogeneity in transmembrane proteins are limited. Circular dichroism (CD) is often used to characterize the secondary structure of the protein, but its sensitivity to specific non-helical structural configurations is low. Deep-ultraviolet resonance Raman spectroscopy (DUVRR) is a structurally sensitive spectroscopy technique emerging for analyzing membrane protein structures. A set of *de novo* designed peptides have been constructed that contain varying contents of helix breaking residues (HBR) in order to test their role helical instability in lipophilic environments. The secondary structure of each peptide was monitored through the measured by DUVRR spectroscopy, where changes in the Amide III and S modes indicate that HBRs actually cause the "unwinding" or the helix when solubilized in detergent environments. This observation has implications towards the role of water presentation in membrane protein dynamics.

[1]Funding provided by the NSF and the University of Missouri-Columbia

F1.00030 Structured mRNA induces the ribosome into a hyper-rotated state[1] , PETER CORNISH, PEIWU QIN, DONGMEI YU, University of Missouri, XIAOBING ZUO, Argonne National Laboratory — During protein synthesis, mRNA and tRNA are moved through the ribosome by the process of translocation. The small diameter of the mRNA entrance tunnel only permits unstructured mRNA to pass through. However, there are structured elements within mRNA that present a barrier for translocation that must be unwound. The ribosome has been shown to unwind RNA in the absence of additional factors, but the mechanism remains unclear. Here, we show using single molecule Förster resonance energy transfer and small angle X-ray scattering experiments a new global conformational state of the ribosome. In the presence of the frameshift inducing dnaX hairpin, we observed that the ribosomal subunits were driven into a hyper-rotated state and the L1 stalk was predominantly in an open conformation. This previously unobserved conformational state provides structural insight into the helicase activity of the ribosome and may have important implications for understanding the mechanism of reading frame maintenance.

[1]NSF CAREER award MCB-115343 and Pew Charitable Trust

F1.00031 Single molecule studies of the protein export system , RAGHAVENDAR REDDY SANGANNA GARI, NATHAN FREY, LINDA RANDALL, GAVIN KING, University of Missouri-Columbia, MEMBRANE GROUP AT UNIVERSITY OF MISSOURI COLLABORATION — Numerous proteins are exported across or into cell membranes to carry out critical cellular functions. In *Escherichia coli,* pathway through the membrane is provided by the translocon SecYEG, which is highly conserved and has homologs across the kingdoms of life. At the cytoplasmic membrane SecA binds SecYEG and provides energy for protein translocation through the cycle of binding and hydrolysis of ATP. SecA makes large surface area contact ($\sim$ 6,800 Å^2) with cytoplasmic loops spanning TM helices 6-7 and 8-9 of SecY. Despite their functional significance, measurements of these flexible and disordered protein regions remain a significant experimental challenge. Major challenges in protein export system include: determining the oligomeric state of SecYEG and SecA during protein export, and elucidating the mechanism of SecA driving precursor through translocon. Structural details at single molecule level in near native conditions can address these major questions. Recently, atomic force microscopy (AFM) has emerged as an important complementary tool to study membrane proteins. In contrast to other techniques AFM can directly monitor conformational changes and dynamics of bio-molecules. In this work we present the structural details of major components of protein export system at single molecule level in native conditions determined via AFM.

F1.00032 Development of quantum mechanics laboratory for undergraduate teaching[1] , HARRISON KNOLL, PAUL MICELI, PING YU, Univ of Missouri - Columbia — We present our recent development of a quantum mechanics laboratory for undergraduate instruction. The experiments are based on detecting entangled photon pairs from the spontaneous down conversion in a beta-barium borate (BBO) crystal using low level light detection techniques. We address two issues in this work: (1) a demonstration of low level light detection by using a sensitive CCD camera to show the down conversion photon pairs from the BBO crystal and the statistics of photons in a slow time scale. (2) Experiments to show the transitions from classical states, semi-classical states, and quantum states. The wave nature of light is described by Maxwell's equations of electromagnetic fields as well as classical statistics. The construction of a Hanbury-Brown and Twiss interferometer gives an opportunity to examine wave nature of light in non-classical statistics. The quantum nature of light, proposed by Einstein, has been used to explain the phenomena of the photoelectric effect. A detection of second-order correlation for photons through a beam-splitter using their entangled photons as a gate provides experimental proof of quantum nature of photons. We offer this laboratory for the first time in the Department of Physics and Astronomy, University of Missouri during the fall semester 2013.

[1]This work was supported by the research incentive grants from the Arts and Science Alumni Organization at the University of Missouri.

F1.00033 Opposite Thought Experiment , FLORENTIN SMARANDACHE, University of New Mexico — Let's consider the opposite case: when we have the astronaut measures the elapse interval time of the event on the earth. It is alike the rocket stands still and the Earth is moving in the opposite direction with speed v. The observer on earth measures the elapsed proper time of the event on earth, $\Delta t'_E$ The elapsed non-proper time of the event on earth as measured by the astronaut is Δt_E. Using the same calculations, with $\Delta t'_E$ and Δt_Eas the elapsed proper and respectively non-proper time of the event on earth as measured by the observer on earth and respectively by the astronaut, we get: $\Delta t_E = \frac{\Delta t'_E}{\sqrt{1-\frac{v^2}{c^2}}}$. Therefore the time dilation is measured by the astronaut in the rocket. This result is contradictory with the time dilation on the earth from the previous thought experiment. But, according to Einstein's Thought Experiment with the Light Clocks, one has: $\Delta t = \frac{\Delta t'}{\sqrt{1-\frac{v^2}{c^2}}}$, where Δt is the elapsed time interval in the rocket as measured by the observer on earth, and $\Delta t'$ is the elapsed time interval in the rocket, as measured by the astronaut. Then who is right, the observer on earth or the astronaut? Where is really the time dilation: on earth or in the rocket? The advocates of special theory of relativity say that there is no answer to this question. They pretend that's okay. But what kind of theories are those that have undecidable propositions? Incomplete or inconsistent ones!

F1.00034 Hierarchical micro/nanostructure effect on the thermal performance of oscillating heat pipes[1] , FENG ZHANG, ROBERT WINHOLTZ, VITALY GRUZDEV, HONGBIN MA, Univ of Missouri - Columbia — Oscillating heat pipes (OHPs) are a promising new technology for electronics cooling. When hierarchical micro/nanostructures are introduced within the OHP, the overall thermal performance is expected to improve due to the enhancement of thin film evaporation on the interior channel surfaces. Such structures, consisting of hierarchical micron sized waves and nanometer sized pores, were fabricated using a femtosecond laser at different scanning speeds and angles of incidence. Differences in surface topography were characterized with SEM. Contact angle measurements for the hierarchical structured surfaces were conducted with water and ethanol to determine the wettability of these working fluids. Experimental comparisons of the thermal performance of micro/nanostructured OHPs and conventional OHPs will be assessed.

[1]Support from the National Science Foundation under grant number DGE-1069091 is gratefully acknowledged.

F1.00035 Photovoltaic Properties of Electrochemical Deposited Cu2O/ZnO p-n Heterojunction[1]

, MINGWEI SHANG, LIFENG DONG, 1 College of Materials Science and Engineering, Qingdao University of Science and Technology, China 2 Department of Physics, Astronomy, and Materials — In order to fabricate a Cu2O/ZnO heterojunction, single-crystal n-type zinc oxide (ZnO) nanorod arrays and p-type cuprous oxide (Cu2O) thin film were deposited on FTO glass respectively by electrochemical deposition method using an electrochemical workstation. The Cu2O/ZnO heterjunctions were also deposited by electrochemical deposition method. A series of characterization and measurements were taken to indicate its properties. It was found that the diameter of ZnO nanorods increased with the increase of the concentration of ZnCl2 during the deposition of ZnO nanorod arrays. Formation of a p-n junction between Cu2O film and ZnO nanorod arrays were demonstrated through electrical properties measurements. The efficiency of this solar cell was also calculated. The higher external quantum efficiency of the Cu2O/ZnO heterojunctions than that of ZnO nanorod arrays and Cu2O film also indicates the formation of a p-n junction, which can efficiently facilitate the separation and transport of charge carriers for applications in solar cells. But some evidence shows that a weak contact/interface between ZnO nanorods and Cu2O film resulted from solution corrosion may affect its photovoltaic properties.

[1]This work was partially supported by the National Natural Science Foundation of China (51172113), the Shandong Natural Science Foundation for Distinguished Young Scholars (JQ201118), the Taishan Scholar Overseas Distinguished Professorship program (tshw20

F1.00036 Realization of one-way electromagnetic modes at the interface of two lossless metals[1]

, MEHUL DIXIT, University of Missouri Columbia, DAVID STROUD, The Ohio State University Columbus — One-way electromagnetic waveguides are of special interest because of complete suppression of back-scattering by disorder. Such waveguides support a unique class of photonic modes that completely forbid propagation in the opposite direction. We show that a one-way electromagnetic waveguide can be realized at the interface of two dissimilar lossless metals in an external magnetic field parallel to the interface. Electromagnetic surface plasmon modes bound to the interface of the two metals and propagating parallel to it and normal to the direction of the external magnetic field, with the electric field polarized normal to the plane of the interface, support one-way electromagnetic propagation in a range of frequencies. Increasing the magnetic field increases the window of frequencies for one-way propagation. Adding damping reduces the range of frequencies. Details of the calculation and plots showing the dispersion relation will be presented.

[1]Work supported by DOE grant 60011493

F1.00037 The Paradox of Special vs. General Theory of Relativity

, FLORENTIN SMARANDACHE, University of New Mexico — Two clocks *C1* and *C2* are synchronized on the earth. Then clock *C2* is flying with a uniform speed at an altitude $h > 0$ above the earth.

1. According to the Special Theory of Relativity there is symmetry of time dilation between *C1* and *C2*

2. But, according to the General Theory of Relativity, there is an asymmetry of time between *C1* and *C2*, since the clock *C1* is running slower down in the gravitational field than the clock *C2* which is running faster at a higher altitude

F1.00038 Crustal Structure Beneath the Ozark Plateau and Illinois Basin using the OIINK Flexible Array

, JOSHUA RUSSELL, Univ of Missouri - Columbia, HERSH GILBERT, Purdue University, GARY PAVLIS, Indiana University — The Ozarks Illinois INdiana Kentucky (OIINK) FlexArray seismic deployment provides an opportunity to learn more about the assembly and evolution of North America by comparing tectonic boundaries to variations in crustal thickness. We analyze P-to-S receiver functions to measure crustal thickness across eastern Missouri and southern Illinois. These observations indicate that crustal thickness across the region ranges from 55km at its thickest along the eastern part of the Ozark Plateau, to 43km beneath the southern portion of the Illinois Basin. The crust thins from the Ozark Plateau southeastward into Illinois where the thinnest crust in the Illinois Basin is found beneath the region where the basin reaches its greatest depth. By examining how the arrival times of converted phases of receiver functions vary as a function of incidence angle, we identify that complications resulting from the reverberation of converted waves within the low velocity sediments of the Illinois Basin influence our crustal thickness measurements. Incorporating the low velocity, shallow sedimentary layers into the velocity model used to migrate receiver function arrival times to depth reduces the crustal thickness by 3-4 km compared to depths calculated without considering basin effects. By understanding how the basin geometry effects crustal arrivals, we can more accurately estimate crustal thickness and determine how it relates to the evolution of structures in the mid-continent.

F1.00039 Neutron Diffraction of Li-Ion Battery Electrode Materials[1]

, TYLER FEARS, Missouri University of Science and Technology, HELMUT KAISER, University of Missouri Research Reactor, HASKELL TAUB, University of Missouri - Columbia — The performance characteristics of Li-ion batteries are largely dependent upon the crystalline structure of the intercalation electrodes. Li insertion and de-insertion modify the crystal structure cyclically during charging and discharging; this process also induces irreversible changes to the structure which lead to capacity fade. Significant advancements have been made with synchrotron radiation which allow diffraction during electrochemical cycling. Unfortunately, Li (a very important component of Li intercalation materials) is transparent to x-rays. Neutron diffraction is sensitive to Li atoms but has its own drawbacks. Unlike intense synchrotron radiation, neutron characterizations are flux-limited and require large sample sizes and/or long data collection times. Additionally, while the transition metal electrode materials are often the strongest x-ray scatterers in typical electrochemical cells, neutrons interact strongly with other cell components, necessitating the use of non-traditional materials for in-situ experiments. In this presentation, we will discuss the advantages of neutron diffraction with in-situ electrochemical cycling, the hurdles that must be overcome for high-resolution pattern collection, and the various strategies for the next phase of the project.

[1]This work is supported by NSF Grant No. DGE-1069091.

F1.00040 The Nuts and Bolts of Running a Graduate Student-Led Science Outreach Program

, MATTHEW MCCUNE, University of Missouri - Department of Physics and Astronomy, DEEPIKA MENON, University of Missouri - Department of Learning, Teaching and Curriculum, KEVIN TARWATER, CHRISTOPHER OWENS, University of Missouri - Department of Physics and Astronomy — The Public Outreach Committee of the MU Physics and Astronomy Graduate Student Association (PAGSA) was founded in 2012 to increase involvement of its members in science outreach in the community. The committee's goal was to increase the acceptance and understanding of science by the general public while also inspiring the next generation of scientists. Over the past two years the committee has managed events for the Missouri Science Olympiad State Tournament, manned booths at NSTA Science Matter's Night, entertained students at the Mizzou Adventures in Graduate Education event, judged a Junior High and High School Science Fair for the CCAA Conference, as well as helped Smithton Middle School students prepare for the Science Olympiad. The committee's dedication and hard work has been recognized the past two years with the 2012 and 2013 Chancellor's Award in Public Outreach. This poster will show how graduate students can acquire funding, organize volunteers, plan and carry out a successful science outreach program by effective use of department and university resources.

F1.00041 Generation of N-particle Dicke-Class States and their Application to Quantum Information Processing , DANIEL DEYOUNG, KISHOR KAPALE, Western Illinois Univ — Dicke class states are maximally entangled states of atoms or atom-like two-state entities involving a small number of excitations (much less that the total number of atoms). It has been shown in the literature [Z.H. Peng, J. Zou, X.J. Liu, Eur. Phys. J. D 58, 403-407 (2010)] that the so-called asymmetric Dicke states, which carry different relative phases for different permutations corresponding to different atomic entity being in the excited state, are more useful for quantum information processing tasks than the symmetric Dicke states. We have devised a practical conceptual proposal for generation of asymmetric Dicke states based on a proposal to generate symmetric Dicke states [Thiel et al. Phys. Rev. Lett. 99, 193602 (2007)]. We shot that the asymmetric Dicke-class states can be used for perfect teleportation [Agrawal and Pati, Phys. Rev. A 74 062320 (2006)] and dense coding.

F1.00042 Kitchen inspired nanochemistry: dispersive, exfoliation and hybridization of functional MoS_2 nanosheets using culinary hydrocolloids[1] , SUDHIR RAVULA, JEREMY B. ESSNER, GARY A. BAKER, University of Missouri-Columbia — As a material, molybdenum disulfide (MoS_2) has drawn wide attention due to its broad applications and fascinating properties. In order to access its valuable properties, however, van der Waals interactions between the sheets within the bulk crystalline material must be overcome in order to produce stable single- or few-layer nanosheets (S/FLNS). Previous methods to exfoliate MoS_2 into nanoscale sheets were time consuming, employed expensive, environmentally unfriendly methods, or produced poorly stabilized nanosheets (yielding sheet aggregation). Known exfoliation methods also suffer poor scalability and reproducibility, making them ill-suited for the development of large scale devices and nanocomposites. In light of these facts, a simple and efficient approach to exfoliate bulk MoS_2 and generate stable S/FLNS using approaches that embrace the principles of green chemistry is long-awaited. We present results on the sonication-assisted aqueous phase exfoliation of bulk MoS_2 into dispersed S/FLNS using popular culinary agents, including guar gum, tannic acid, and xanthan gum. Subsequent decoration of the sterically-stabilized nanosheets with gold nanoparticles via in situ reduction by the sorbed culinary agent gave a plasmonic nanocatalyst hybrid exhibiting excellent activity toward 4-nitrophenol reduction using sodium borohydride. These agents are green and inexpensively available commercially, opening up interesting possibilities that will be discussed.

[1]ACS PRF grant (51865-DNI)

Saturday, November 9, 2013 8:30AM - 10:06AM –

Session H1 Atomic, Molecular and Optical Physics; Industrial Physics Physics Building 120 - Ping Yu, University of Missouri

8:30AM H1.00001 Classical Trajectory Studies of the Hydrogen Peroxyl Radical HO_2 , JAMIN PERRY, University of Missouri-Columbia, ALBERT WAGNER, Argonne National Laboratory, DONALD THOMPSON, University of Missouri-Columbia — The intramolecular dynamics, intramolecular vibrational redistribution of energy (IVR), isomerization and unimolecular dissociation of the hydrogen peroxyl radical, $HO_2^* \rightarrow H + O_2$ have been studied using classical trajectories. Mode specific effects are found to affect the IVR, isomerization and the rate of dissociation. Exchange of the hydrogen atom between the oxygen atoms increases the rate of energy transfer between the vibrational modes of the radical. The relaxation mechanism of the vibrationally excited radical embedded in a dense gas environment is also presented.

8:42AM H1.00002 Experimental Evidence for a non-Globally Trace-Preserving POVM , RAYMOND JENSEN, Northern State University — A well-known experiment from 1986 involving entangled photon pairs is examined. The data, which until now have not been modeled quantitatively, are shown to be in agreement with quantum theory upon application of a positive operator valued measure (POVM). The POVM has a peculiarity: it is not complete (trace-preserving) on the entire Hilbert space but on a proper subset although they are positive semidefinite observables on the entire space. In spite of this, the state vector of the aforementioned experiment is in the subset where completeness holds.

8:54AM H1.00003 Channelling radiation from a 4 MeV electron beam interaction with a diamond crystal[1] , WADE RUSH[2], JACK SHI[3], Dept. of Physics, University of Kansas, FERMILAB A0 TEAM — Fermilab is conducting experiments with a round 4 MeV electron beam bunch interacting with a diamond crystal. If the crystal is oriented such that one of its (hkl) planes are parallel to the beams ideal trajectory, some of the beam would essentially channel through the diamond and emit coherent soft X-ray radiation instead of the weaker bremsstrahlung radiation. We are attempting to simulate the expected spectral brilliance and replicate some of the primary linewidth contributors which could emerge from this channelling radiation experiment.

[1]A0 Fermilab
[2]PhD Graduate Student
[3]Professor of Physics

9:06AM H1.00004 Graphene Synthesization by Direct Sonication Exfoliation[1] , DANIEL R. SODEN, JINCHENG BAI, LIFENG DONG, Department of Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897 — The emergence of graphene in the scientific community over the last several years has been the cause of much excitement among material scientists and physicists due to its many unusual physical and photovoltaic properties. However, the much sought after monolayer graphene has proven to be difficult to produce in sufficient quantities, with most processes outputting high layer or even defect ridden graphene instead. This experiment aims to correct some of these problems, concerning itself with the synthesis of high quality graphene through continuous sonication with surfactant added throughout, as well as the issue of graphene quality as a function of sonication time. This was accomplished through the creation and addition of a Triton X-100 surfactant solution to a graphite suspension during sonication lasting for 50, 80, 110, 140, 170, and 200 minutes. The resulting suspension was then filtrated to separate out the graphene, before being tested for quality through Raman spectroscopy and SEM microscopy. This completely physical method of graphene synthesis provides a much simpler and more environmentally safe way to achieve the highly desired few layer graphene, and will hopefully allow for greater use of the substance in industry.

[1]L. F. Dong acknowledges the support of the National Science Foundation (DMR-1126375 and DMR-1126375), the Faculty Research Grant and the Sabbatical Leave Award from Missouri State University.

9:18AM H1.00005 Investigation of nitrogen-doped graphene as catalyst and catalyst support for oxygen reduction in both acidic and alkaline solutions[1] , JINCHENG BAI, 1 College of Materials Science and Engineering, Qingdao University of Science and Technology, China 2 Department of Physics, Astronomy, LIFENG DONG, Department of Physics, Astronomy, and Materials Science, Missouri State University, Springfield, MO 65897 — Fuel cells are promising energy devices with low pollutant emission and high energy conversion efficiency. However, the performance of fuel cells depends on oxygen reduction reaction. In order to solve the slow kinetics of oxygen reduction reaction, carbon materials have been utilized as catalyst supports for fuel cells. In this study, graphene and nitrogen-doped graphene were synthesized through a solvothermal method and investigated as catalysts for oxygen reduction reactions. Electrochemical measurements demonstrated that N-doped graphene possessed higher electrocatalytic activity than graphene in both acidic and alkaline solutions. N-doped graphene can directly act as a catalyst to facilitate four-electron oxygen reductions in alkaline solution but two-electron reductions in acidic solution. On the other hand, when employed as catalyst supports for platinum and Pt-ruthenium nanoparticles, N-doped graphene can contribute to four-electron oxygen reductions in acidic solution, yet in alkaline solution the kinetics of reduction reaction is slow. So N-doped graphene can work as an efficient catalyst for oxygen reductions to substitute the precious Pt catalysts in alkaline solution and and Pt-Ru catalysts in acidic solution.

[1]This work was partially supported by the National Natural Science Foundation of China (51172113), the Shandong Natural Science Foundation for Distinguished Young Scholars (JQ201118), the Taishan Scholar Overseas Distinguished Professorship program (tshw20

9:30AM H1.00006 PLD growth of multilayered MgO/Ag(001)/MgO photocathode , DANIEL VELAZQUEZ, ZIKRI YUSOF, LINDA SPENTZOURIS, JEFF TERRY, Illinois Institute of Technology — Films of of Ag, MgO and multilayers of these were grown via pulsed laser deposition on clean Si(111) 7x7 substrates. The films were studied using reflection high-energy electron diffraction, Kelvin probe and ellipsometry. Information about crystalline and atomic structure as well as surface condition, work function and film thickness was obtained using these techniques. Deposition at various substrate temperatures and partial oxygen pressures was performed in order to understand the parameter settings that lead to higher quality crystalline films. Epitaxial films of Ag(111) were found to grow at an optimal substrate temperature of 256 °C (fig 1.). The superstructure Ag(111) $\sqrt{3} \times \sqrt{3}$ occurs when deposition takes place at a substrate temperature of 620 °C. In addition, MgO films were found to grow with small grain size on both, Si(111) 7x7 and Ag(111)/Si(111) at room temperature with a partial oxygen pressure of $5\text{x}10^{-5}$ Torr (fig. 2). Highly-oriented, polycrystalline growth of MgO films is evidenced by their RHEED pattern. In addition, the obliquely-shaped diffraction spots indicate the growth of secondary phase precipitates, most likely due to oxygen deficit. Measurements of the work function of these multilayers indicate that the Ag(111) work function (4.75 eV) is sharply suppressed with the first few MgO shots and has a quasi-linear increase for the first few monolayers (fig. 3). As the thickness of MgO increases (a few nanometers) the work function drops again and stabilizes at the level of MgO ($\sim$4.2 eV).

9:42AM H1.00007 Improved laser heating technique for melting dusty plasma crystals[1] , ZACH HARALSON, JOHN GOREE, Dept. of Physics & Astronomy, The University of Iowa — A dusty plasma is a mixture of polymer microspheres, electrons, positive ions and neutral gas atoms. The microspheres acquire an electric charge as large as many thousands of elementary charges, so that a single layer of thousands of microspheres can be electrically levitated by a vertical electric field. Due to the mutual repulsion among these microspheres, they develop such a large interparticle electric potential energy that they arrange themselves with a uniform spacing, analogous to atoms in a crystalline lattice. This so called "dust crystal" can then be melted by using laser heating to give the microspheres more kinetic energy. Movies of the particle motion, shown in this talk, are recorded using video microscopy. We describe experiments to optimize the sweeping of the laser beam during this heating. By tracking the random motion of the individual microspheres, we can explore the relationship between microscopic particle motions and macroscopic phenomena and calculate transport coefficients, such as the diffusion constant.

[1]Supported by NSF and NASA.

9:54AM H1.00008 Experimental test of the Fluctuation Theorem using a microsphere in a rarefied gas[1] , CHUN-SHANG WONG, JOHN GOREE, BIN LIU, Dept. of Physics and Astronomy, The University of Iowa — The Second Law of Thermodynamics can be violated on short time and distance scales. The extent of the violation is quantified by the Fluctuation Theorem, which was the subject of the 2004 Boltzmann Medal. A variation of the theorem, the Work Fluctuation Theorem, can be tested experimentally [G.M. Wang, PRL 2002], but these experimental tests are still few. We have devised a test using Brownian motion of a 5 μm polymer sphere in a rarefied gas while pushing the sphere with a constant force applied by the radiation pressure of an incident laser beam. To avoid friction with solid surfaces, the microsphere is electrically charged and levitated by a vertical electric field, which is provided by partially ionizing the argon gas to make a plasma. A time series of the microsphere's position is measured using video microscopy with a high speed camera (400 fps), yielding a measure of the fluctuating work done. For various time intervals, τ, the work done on the particle, W_τ, can be calculated by integrating $\mathbf{F}_{\text{laser}} \cdot \mathbf{v}$ over $d\tau$. Finally, a histogram of observed W_τ values is used to test the Fluctuation Theorem prediction $P(W_\tau > 0)/P(W_\tau < 0) = \langle \exp(W_\tau) \rangle$, where P is a probability.

[1]Supported by NSF and NASA

Saturday, November 9, 2013 8:30AM - 10:06AM –

Session H2 Condensed Matter Physics IV Physics Building 126 - Carseten Ullrich, University of Missouri

8:30AM H2.00001 A look at graphene's atomistic geometry and electronic properties from the perspective of discrete differential geometry , SALVADOR BARRAZA-LOPEZ, University of Arkansas — A host of amazing properties of graphene originate from *geometry*. A prime example being actively pursued nowadays is the creation of gauge fields on graphene's conduction electrons, solely from mechanical strain [1-5]. This perspective is remarkable: Indeed, from an applied point of view, and just as an example, strain can help furnish large (pseudo-)magnetic fields, in excess of the $\sim$100 Tesla limit reached so far in state-of-the-art facilities [4]. From a fundamental perspective, graphene is a medium for discussion of (effective) relativistic Dirac-fermion Physics, so curved membranes make it necessary to uncover and revise our understanding of the Physics of Dirac fermions on curved spaces [2]. The theory (References [1-3] and a larger host of work) has been expressed in terms of an effective continuum media. Since graphene is an atomic membrane, our group is realizing a complementary and unique route [6-9] to study the relations among Dirac electrons and graphene's geometry, by applying concepts of Discrete Differential Geometry [10] to graphene. Essentially, the idea is to build the theory for electronic properties up from unit cells and atoms, so that the atomistic conformation is never lost, and no continuum limit is to be applied. The insight gained from this new perspective enters into basic checks of theory [1-3], the furnishing of electronic 'mass,' [7] and other geometrical aspects [9]. An extensive discussion of this approach and salient results will be given on this talk.

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9:06AM H2.00002 Electrical Transport Properties In Large Area Boron-Nitrogen-Carbon Layers , BALEESWARAIAH MUCHHARLA, ARJUN PATHAK, Southern Illinois University Carbondale, ZHENG LIU, LI SONG, Rice University, THUSHARI JAYASEKERA, Southern Illinois University Carbondale, SWASTIK KAR, Northeastern University, ROBERT VAJTAI, Rice University, LUIS BALICAS, National High Magnetic Field Laboratory, Florida State University, PULICKEL M. AJAYAN, Rice University, SAIKAT TALAPATRA, NAUSHAD ALI, Southern Illinois University Carbondale — In this work, we present a detailed investigation of the temperature dependence of transport in thin layers of Boron Nitrogen and Carbon (BNC) and compare it with electrical transport in large area graphene. We find that the temperature dependence of resistance ($5K < T < 400$ K) of pure graphene shows a metallic behavior, whereas the BNC samples display an increasingly semiconducting behavior with increasing B and N concentrations. Density Functional Theory (DFT) calculations performed on pure graphene and BNC structures were in good agreement with this experimental observations. The observed temperature dependence of the electrical resistivity of BNC samples can be classified into two regimes. At higher temperatures ($50K < T < 400$ K), the BNC samples showed a band-gap dominated Arrhenius-like temperature dependence. At the lowest temperatures ($5K < T < 50$ K), the temperature dependence deviates from an activated behavior, and presents evidence for a conduction mechanism that is consistent with Mott's 2D-Variable Range Hopping (2D-VRH).

9:18AM H2.00003 Structural and electronic properties of $SrTiO_3/LaNIO_3$ slabs with and without oxygen vacancies , PABLO RIVERO, SALVADOR BARRAZA-LOPEZ, JAK TCHAKALIAN, SRIMANTA SMIDDEY, University of Arkansas — Perovskite oxide heterostructures with transition metal ions exhibit interfacial electronic states completely different to the bulk [1]. Theoretical and experimental researchers are reaching the conclusion that this new behavior emerge as a result of charge redistribution at the interface as a consequence of the polar discontinuity between materials. The creation of Oxygen vacancies [2] is one of the mechanisms known to avoid the electric field divergence, resulting in some cases in high mobility carriers at interfaces. Studying the structural and electronic properties of these compounds with and without Oxygen vacancies could shed more light on the interesting physical phenomena originating at the interface. We use first principle DFT calculations with the LDA exchange-correlation functional to study the formation energy of oxygen vacancies of (5,n) $SrTiO_3/LaNiO_3$ multilayer slab systems, containing $n = 1$, 2 and 5 layers of LNO. Systems slabs were oriented in the strongly polar (111) direction. We also studied the electronic properties through the electronic density of states (DOS) and the projected full band structure onto the two-oxide interface. We acknowledge computer support from NSF-XSEDE (Project TG-PHY090002. Stampede Supercomputer at TACC). [1] J. Chakhalian, A. J. Millis and J. Rondinelli, Nature Mater. **11**, 92 (2012). [2] G. Herranz, M. Basleti, M. Bibes, C. Carrétéro, E. Tafra, E. Jacquet, K. Bouzehouane, C. Deranlot, A. Hamzi, J.-M. Broto, A. Barthélémy, and A. Fert, Phys. Rev. Lett. **98**, 216803 (2007).

9:30AM H2.00004 Electric Field Tuning of the Rashba Effect , SHANAVAS VEEDU, SASHI SATPATHY, Univ of Missouri - Columbia — The Rashba effect describes the momentum-dependent spin splitting of the electron states at a surface or interface. The control of the Rashba effect by an applied electric field is at the heart of the proposed Rashba-effect-based spintronics devices for manipulating the electron spin. We studied how the Rashba SOI at the polar perovskite surfaces and interfaces can be tuned by manipulating the two-dimensional electron gas (2DEG) by an applied electric field. We saw that the Rashba SOI originates from the first few layers near the surface and it therefore can be altered by drawing the 2DEG to the surface or by pushing the 2DEG deeper into the bulk with an applied electric field. We carried out a comprehensive density-functional study of the recently-discovered polar $KTaO_3$ surface both with and without an applied electric field. y-discovered polar $KTaO_3$ surface both with and without an applied electric field. The strength of the Rashba effect depends intricately on the surface induced asymmetry of the Ta(d) states as well as the strength of the spin-orbit interaction, which is unraveled from the study of a tight-binding model Hamiltonian to describe the Rashba effect.

9:42AM H2.00005 Theoretical studies of terahertz spectra of crystalline energetic materials using molecular dynamics , ANDREY PEREVERZEV, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Terahertz infrared (THz IR) absorption spectra of crystalline pentaerythritol tetranitrate (PETN) and the α and γ polymorphs of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX) were calculated at 300 K for pressures between 0 and 7 GPa using two different theoretical approaches based on molecular dynamics (MD). Beyond the choice of force field, neither method entails the specification of adjustable parameters. In the first approach spectral line frequencies and intensities were calculated using normal mode analysis of three-dimensionally periodic crystal supercells, while spectral line widths were calculated using relaxation times obtained from MD simulations of energy loss from selectively excited THz-region IR-active modes. The IR spectrum was then generated as a superposition of Lorentzian functions completely specified by the calculated frequencies, intensities, and line widths. In the second approach spectra were calculated from equilibrium MD simulations using the Fourier transform of the dipole autocorrelation function of the crystal. Spectra obtained using the two methods are similar and agree reasonably well with experimental results.

9:54AM H2.00006 Time-dependent transition density matrix for visualizing charge-transfer excitations in photoexcited organic donor-acceptor systems[1] , YONGHUI LI, CARSTEN ULLRICH, University of Missouri — The time-dependent transition density matrix (TDM) is a useful tool to visualize and interpret the induced charges and electron-hole coherences of excitonic processes in large molecules. Combined with time-dependent density functional theory on a real-space grid (as implemented in the octopus code), the TDM is a computationally viable visualization tool for optical excitation processes in molecules. It provides real-time maps of particles and holes which gives information on excitations, in particular those that have charge-transfer character, that cannot be obtained from the density alone. Some illustration of the TDM and comparison with standard density difference plots will be shown for photoexcited organic donor-acceptor molecules.

[1]This work is supported by NSF Grant DMR-1005651

Saturday, November 9, 2013 10:30AM - 12:18PM –

Session I1 Condensed Matter Physics V Physics Building 120 - Paul Miceli, University of Missouri

10:30AM I1.00001 QSE growth and super-diffusive liquid-like motion in Pb/Si(111) at low temperature , MICHAEL TRINGIDES, Iowa State University Ames Laboratory — QSE are responsible for the formation of uniform height metal islands at low temperatures [1]. For Pb/Si the islands form unusually fast, within a few minutes as low as T $\sim$ 150K. With STM [1] X-ray scattering [2] and LEEM [3] it was found that this is due to the superdiffusive "liquid-like" motion of the dense wetting layer that moves collectively with constant speed. Unstable islands transform into stable islands as seen in STM movies with the wetting layer climbing the sides of the unstable islands to complete the next layer. X-ray scattering experiments have shown anomalous coarsening with faster kinetics for growth at higher flux rates [2]. This unusual motion is also directly seen by LEEM with the refilling of an initial vacant circular region generated by a laser pulse, evolving at constant speed x/t instead of the normal $x/t^{1/2}$ diffusive motion (with x the profile edge). An outgoing expanding front is observed whose boundary is the source of material that refills the vacant hole. The combined effect is to observe mass transport over macroscopic distances with unusual long range correlation between the outwards expanding "source" and the inward moving "sink" (the refilling edge), separated by more than 0.200mm. In collaboration with M. Hupalo, P.Miceli, E. Conrad and M. S. Altman.

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[3] K. L. Man, et al. Phys. Rev. Lett., 11036104–5, 2013.

11:06AM I1.00002 Minimum stable height of Ag nano-islands on Si(111)7x7 , YIYAO CHEN, MICHAEL GRAMLICH, SHAWN HAYDEN, PAUL MICELI, University of Missouri-Columbia — The origin of a minimum stable Ag nano-island height of one bi-layer on top of the wetting layer has remained a long-standing mystery in the effort to understand mechanisms that control the growth of supported nanoscale metals. We present the results of synchrotron x-ray scattering studies which demonstrate that the interfacial energy, rather than previously suspected electron confinement effects, is responsible for the minimum island height. In situ measurements of x-ray reflectivity and crystal truncation rods reveal that the Ag nano-islands consume the wetting layer and are, therefore, tri-layers – an effect that cannot be detected by scanning probe measurements. These experiments lead to an energy "phase diagram" that we propose to explain the existence of a minimum island height for supported nanoscale metals. Support from the National Science Foundation under grants DMR-0706278 and DGE-1069091 is gratefully acknowledged. The Advanced Photon Source Sector 6 beam-line at Argonne National Laboratory is supported by the US-DOE under Contract No. W-31-109-Eng-38.

11:18AM I1.00003 Temperature Dependent Electrical Characterization of Graphene Flakes Synthesized Using Liquid Phase Exfoliation , BALEESWARAIAH MUCHHARLA, MITCHELL CONNOLLY, ANDREW WINCHESTER, SUJOY GHOSH, Southern Illinois University Carbondale, SWASTIK KAR, Northeastern University, SAIKAT TALAPATRA, Southern Illinois University Carbondale, SOUTHERN ILLINOIS UNIVERSITY CARBONDALE TEAM, NORTHEASTERN UNIVERSITY COLLABORATION — We will report the synthesis and electrical transport properties of graphene flakes synthesized by exfoliating the bulk graphite in isopropyl alcohol. Temperature dependence of the electrical resistivity of thin films made from exfoliated graphene flakes has been studied over a wide range (10K $<$T $<$300K) of temperature. Temperature dependence of resistance shows a slow linear increase in resistance with decrease in temperature. Electric field effects on charge transport properties e.g. temperature (220K $<$T $<$275K) dependence of carrier mobilities etc. of exfoliated graphene thin film devices under electrochemically gated environment will also be presented and discussed.

11:30AM I1.00004 Interplay between restricted transport and catalytic reaction in nanoporous materials: KMC simulation and analytic theory , ANDRES GARCIA, JING WANG, DAVID ACKERMAN, JAMES EVANS, Iowa State Univ — Behavior of catalytic reactions in narrow pores is controlled by a delicate interplay between fluctuations in adsorption-desorption at pore openings, highly restricted diffusion, and reaction. The resulting concentration profiles determined by KMC simulation, showing reactants mainly near pore openings, are not described by standard mean-field reaction-diffusion equations. For simple A$\rightarrow$B unimolecular reaction kinetics, the challenge in developing a correct theory is to suitably describe chemical diffusion in mixed-component quasi-single-file systems. This is achieved based on a refined picture of tracer diffusion for finite-length pores. For A+B$\rightarrow$C+D bimolecular and other reactions, there are additional complications in describing spatial correlations in reactant locations which can strongly impact the reaction kinetics.

11:42AM I1.00005 Effect of metal and semiconducting nanoparticles on the fluorescence of Dy^{3+} doped lead and bismuth borate glasses , SAISUDHA MALLUR, STEWART FERRELL, P.K. BABU, Western Illinois University — The rapid development of laser research has led to increased theoretical and experimental investigations of fluorescence of rare-earth ions in heavy metal oxide glasses. These glasses containing metallic and semiconducting nanoparticles are very promising systems because the nanoparticles may induce favorable changes in the rare earth ion's fluorescence properties. We prepared Dy^{3+} doped lead and bismuth borate glasses containing Ag, CdSe and ZnSe nanoparticles. Glasses are made through the normal melt quench method. $AgNO_3$ or powders of the semiconducting compounds are added as precursor materials. Glasses obtained through this process contain Ag atoms or molecules of the semiconducting compounds uniformly distributed within the glass system. These are then subjected to a controlled annealing near the glass transition temperature. During this annealing process, Ag atoms or CdSe/ZnSe molecules thermally diffuse and coalesce to form nanoparticles. The sizes of these nanoparticles can be varied by varying the annealing times as confirmed by the TEM. Fluorescence spectra of Dy^{3+} show noticeable changes as a function of annealing times. Variations in the fluorescence spectra are believed to arise from the strong interaction between Dy^{3+} ions and the nanoparticles.

11:54AM I1.00006 Supported shock waves in hydroxyl-terminated polybutadiene melts: A large-scale molecular dynamics study , MARKUS FROEHLICH, THOMAS SEWELL, DONALD THOMPSON, University of Missouri-Columbia — Hydroxyl-terminated polybutadiene (HTPB) melts subjected to supported shock loading were studied by non-reactive all-atom molecular dynamics (MD) simulations to investigate their responses to shock wave passage. An efficient Monte Carlo/MD technique was developed to generate multi-million-atom systems of well-equilibrated linear polymers with chain lengths $n = 64$, 128, or 256 backbone carbons. Explicit shock wave simulations, performed using a reverse-ballistic method, were carried out for all three chain lengths with a shock strength of 8.6 GPa, and for the $n = 128$ system with four different shock strengths ranging from 2.8 to 12.5 GPa. All MD simulations were done using LAMMPS and the OPLS-AA force field with the Lennard-Jones potential replaced by the Buckingham exp-6 potential. Spatial and temporal resolution of the shock response was obtained by analyzing the simulation data in a reference frame centered on the shock front, which traverses the sample with constant speed. Structural properties, global scaling behaviors, and vibrational spectra of the unshocked polymers are in good agreement with literature data. Results for the shocked material indicate a shock-induced transition to a glass-like state based on residual shear stresses and increases of structural relaxation times by several orders of magnitude. Vibrational spectra for the shocked states exhibit considerable broadening and blue shifting.

12:06PM I1.00007 Fluorescence Enhancement and Single Molecule Fluorescence Detection on Nanogap Embedded Plasmonic Gratings fabricated using HD-DVD , AVINASH PATHAK, SAGNIK BASURAY, JOSEPH MATHAI, DREW MENKE, KESHAB GANGOPADHYAY, PETER CORNISH, SHUBHRA GANGOPADHYAY, Univ of Missouri - Columbia — A novel method for producing silver plasmonic gratings for surface plasmon resonance (SPR) based coupling of light has been developed which utilizes soft lithography technique using PDMS stamping of grating from HDDVDs. Further, 20nm wide nano-gaps are formed on the stamp wherein an extreme field concentration occurs leading to enhancements of 118 times with respect to glass. The gratings with nanogaps were used for single molecule studies, with an immobilized layer of tagged DNA molecule. Enhancement with epifluorescence on gratings when compared to total internal reflection microscopy (TIRF) on quartz slides is up to 40 times on nanogaps. Further, single molecule Forster resonance energy transfer imaging used to study the dynamics of DNA performed on the gratings shows intensity enhancement by 10 times on nanogaps in comparison to TIRF on quartz. Finally, in order to improve the reproducibility of the nanogaps, a glancing angle deposition method (GLAD) is coupled with the existing technique in order to form nanogaps. We are thus also able to produce extremely sharp tip regions on these grating structures which further enhance the coupling efficiencies due to a field concentration within these hotspot regions. The layered structure is able to produce height dependent enhancement giving a 3-dimentional view of micromolar concentration of dye on the surface. In conclusion, a method of fabricating plasmonic substrates has been developed which can be utilized for sensing or observation of single molecule interactions using epifluorescence.