

12-Apr-15
2015 Condensed Matter Physics Group Research Retreat Schedule
Room 1400 BPS

| | Time | Presenter | Group | Title |
|--------------|-------------|---|--------------|--|
| 8:00 | 8:00-8:25 | Serve light breakfast | | |
| | 8:25 | Opening | | |
| | | Mesoscopic physics and transport | | |
| 8:30 | 8:30-8:45 | Yaxing Zhang | Dykman | Spectra of mesoscopic oscillators with dispersive mode-mode coupling |
| | 8:50-9:05 | William Martinez | Birge | Control of spin-triplet supercurrent in ferromagnetic Josephson junctions |
| | 9:10-9:25 | Ian Dayton | Tessmer | Probing topological insulator interfaces |
| | 9:30-10:00 | Discussion | | |
| 10:00 | 10:00-10:45 | Coffee Break and poster session | | |
| | | Quantum materials and dynamics | | |
| 10:45 | 10:45-11:00 | Jenni Portmann | Duxbury | Evidence of stacking disorder induced gap opening in the ground state of 1T-TaS ₂ |
| | 11:05-11:20 | Faran Zhou | Ruan | Nonequilibrium quantum dynamics probed by ultrafast electron diffraction |
| | 11:25-11:40 | Connor Glosser | Piermarocchi | Ab initio Maxwell-Bloch energy transfer in quantum dot systems |
| | 11:45-12:00 | Discussion | | |
| 12:00 | | Lunch break | | |
| | | Water and Biosystems | | |
| 1:00 | 1:00-1:15 | Aimee Shore | Lapidus | Using microfluidics to observe protein folding on the submillisecond timescale |
| | 1:20-1:35 | Jess West | Comstock | Electrical current measurement and manipulation of single cells via optical trapping |
| | 1:40-1:55 | Florian Figge | McGuire | Oriental dynamics of water at an extended hydrophobic interface |
| | 2:00-2:30 | Discussion | | |
| 2:30 | 2:30-3:15 | Coffee Break and poster session | | |
| | | Complex materials and interfaces | | |
| 3:15 | 3:15-3:30 | Zhen Zhu | Tomanek | Few-layer phosphorene and arsenene allotropes and their tiling: A computational study. |
| | 3:35-3:50 | Jiagui Feng | Zhang | Interfacial coupling and electronic structure of two-dimensional silicon grown on the Ag(111) surface |
| | 3:55-4:10 | Mengze Zhu | Ke | Evolution of commensurate-incommensurate magnetic structure in Ca ₃ (Ru,Fe) ₂ O ₇ with magnetic field probed via neutron scattering |
| | 4:15-4:45 | Discussion | | |
| 4:45 | 4:45 | Closing | | |

12-Apr-15

2015 Condensed Matter Physics Group Research Retreat Poster Session

BPS atrium

10:00-10:46 am & 2:30-3:15 pm

| Poster number | Presenters | Title |
|---------------|--------------|-------|
| 1 | Birge | TBD |
| 2 | Tessmer | TBD |
| 3 | Duxbury | TBD |
| 4 | Ruan | TBD |
| 5 | Piermarocchi | TBD |
| 6 | Lapidus | TBD |
| 7 | Comstock | TBD |
| 8 | Hartman | TBD |
| 9 | Tomanek | TBD |
| 10 | Zhang | TBD |
| 11 | Ke | TBD |
| 12 | Ghosh | TBD |

Spectra of mesoscopic oscillators with dispersive mode-mode coupling

Yaxing Zhang and Mark Dykman

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Mesoscopic vibrational systems typically have several nonlinearly coupled modes with different frequencies and with long lifetime. Examples are provided by flexural modes of carbon nanotubes, graphene sheets, and nanobeams. We consider the power spectrum of one of these modes, which we call an oscillator. Thermal fluctuations of the amplitudes of the modes coupled to the oscillator lead to fluctuations of its frequency and thus to the broadening of its spectrum. However, the coupling-induced broadening is partly masked by the broadening due to the oscillator decay. We show that the mode coupling can be easily identified from the change of the spectrum due to weak resonant driving. Despite the coupling-induced frequency fluctuations being non-Gaussian, it is possible to average over them in a path-integral formulation and thus to find the power spectrum. The shape of the spectrum depends on the interrelation between the nonlinear coupling strength and the decay rates of the modes. The characteristic features of the spectrum are analyzed in the limiting cases. We also find that the spectral effect of the internal nonlinearity of the oscillator differs substantially from the effect of mode-mode coupling.

Control of spin - triplet supercurrent in ferromagnetic Josephson junctions

William Martinez

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Superconductivity arises due to electrons in a metal forming Cooper pairs, which then form a coherent Bose condensate. In conventional superconductors, the Cooper pairs are spin-singlets, i.e. the spins of the two electrons point in opposite directions. When a superconductor (S) is placed in contact with a ferromagnet (F), there is a competition between the anti-parallel-spin pairing of the superconductor and the parallel-spin alignment of the ferromagnet. As a result of that competition, pair correlations in the ferromagnet are restricted to a very short distance -- on the order of one nanometer -- from the S/F interface. A lot of excitement has been generated in S/F systems since long-range spin-triplet correlations were predicted [1]. While the ability to generate these spin-triplet pairs has been demonstrated previously [2], the ability to control the triplet generation reliably still needs to be realized before these devices can be used in technological applications. One possible direction to control the state in such structures is to manipulate the magnetizations of the various F layers within, specifically to switch relative layer magnetization directions between collinear and non-collinear. In this work, we will discuss our ongoing efforts as well as present recent successes in controlling spin-triplet generation in such a way.

[1] A.F. Volkov, F.S. Bergeret and K.B. Efetov, Phys. Rev. Lett. 90, 117006 (2003)

[2] T.S. Khaire, M.A. Khasawneh, W. P. Pratt, Jr., and N.O. Birge, Phys. Rev. Lett. 104,137002 (2010)

Presentation at the CMP Research Retreat at Michigan State University, April 12, 2015.

Probing the Superconducting Proximity Effect in a Topological Insulator Using Scanning Tunneling Microscopy

Ian Dayton, Eric Goodwin, Victor Ramirez, Reza Loloee, Duck-Young Chung, Alex Levchenko, Mercouri Kanatzidis, Alex Levchenko, Stuart Tessmer

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Topological insulators (TI) embody a new state of quantum matter characterized by topological invariants; this contrasts with superconductors (S), as superconductivity arises from a spontaneously broken symmetry of the underlying electron system. When a superconductor is placed on the surface of a topological insulator, the behavior of the superconducting condensate across the S/TI interface offers the opportunity to study the interplay between these two distant quantum states. In this talk, we present cryogenic Scanning Tunneling Microscopy measurements to probe the local density of states in proximity to Pb/Bi₂Se₃ interfaces.

Presentation at the CMP Research Retreat at Michigan State University, April 12, 2015.

Evidence of stacking disorder induced gap opening in the ground state of 1T - TaS₂

Jenni Portmann, Dat Thanh Do, Bhanu Mahanti, Phillip Duxbury

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

1T-TaS₂ is a transition-metal layered compound that shows unique electronic properties, leading to variety of temperature dependent ground state phases. At $T < 190\text{K}$, this material displays a commensurate charge density wave (C-CDW) phase characterized by insulating behavior corresponding to the opening of a gap at the Fermi energy. To better understand the C-CDW phase and explain its quantum mechanical origin, we perform density functional theory calculations of the band structure of 1T-TaS₂ and quantify the effect that spin orbit coupling and Hubbard repulsion have on the ground state. Our results show that neither of these interactions is sufficient to reproduce the insulating gap seen in the experimental results, an observation which is confirmed by our calculation of the phonon band structure and absorption spectrum. Next we consider the effect of different stacking configurations of the TaS₂ layers and find evidence of gap opening for bilayers in the presence of disordered stacking, while monolayer configurations remain metallic regardless of whether stacking disorder is included.

Nonequilibrium quantum dynamics probed by ultrafast electron diffraction

Faran Zhou,¹ Tzong-Ru T. Han,¹ Christos D. Malliakas,^{2,3} Phillip M. Duxbury,¹ Subhendra D.

¹Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824;

²Department of Chemistry, Northwestern University, Evanston, IL 60208;

³Materials Science Division, Argonne National Laboratory, Argonne, IL 60439.

Characterizing and understanding the emergence of multiple macroscopically ordered electronic phases over subtle tuning of temperature, pressure and chemical doping has been a long-standing central issue for complex materials research. Unlike classical systems, phase transition of many-body quantum systems can be driven nonthermally by tuning the electron-phonon and electron-electron interactions without involving excessive lattice entropy, which may be enhanced by low-dimensionality. Identifying the origins for the competitive or cooperative emergence of various interaction-driven functional states and their tuning by doping, temperature, strain, or electrostatic and magnetic fields is of vital importance for elucidating the basic physics and in order to leverage their enormous technological potential. We studied a prototypical strongly correlated electron system 1T-TaS₂, exhibiting an assortment of intriguing electronic phases, including various textured charge-density orders, as well as recently reported superconducting phase under chemical doping, and pressure. The electronic phase transitions are triggered by femtosecond infrared pulses and a temperature-optical-density phase diagram is constructed, and substantiated with the dynamics of metastable states highlighting the cooperation and competition through which the macroscopic quantum orders emerge. Our results highlight the previously undisclosed interaction-driven dynamics and hidden states, in contrast to thermally driven phase transformations. The methodology introduced here can be generally applied to survey the complex energy landscape in strongly correlated electron systems, avoiding the difficulty of electrostatic gating or confounding effects due to defects and/or disorder. In particular, the observation of robust non-thermal switching at meso-scales and at ultrafast timescales, provides a platform for designing high-speed low-energy consumption nano-photonics and electronics devices.

***Ab initio* Maxwell - Bloch energy transfer in quantum dot systems**

Connor Glosser^{*1}, Jie Li², Dan Dault², Carlo Piermarocchi¹, and
B. Shanker²

¹Michigan State University, Department of Physics/Astronomy

²Michigan State University, Department of Electrical & Computer
Engineering

In recent years, semiconductor quantum dots have shown promise in a wide array of consumer applications, particularly in areas that require a high degree of control in their optical properties. Modeling the collective response of many-dot systems due to external electromagnetic pulses necessarily requires methodologies that accurately capture both electromagnetic interactions between dots as well as their effects on the time-evolution of the system at large.

Conceptually, the simplest approximation of an exciton in a quantum dot consists of a two-level system interacting with a time-dependent electric field in the optical spectrum. In the presence of such a field, the semi-classical Maxwell-Bloch equations govern the time-evolution of an effective dipole moment in the dot. The driven oscillation of this dipole necessarily gives rise to an emitted field, allowing for energy transfer in ensembles of dots. Moreover, the large difference in timescales describing the incident field and exciton lifetime present novel computational challenges.

In addition to the large disparity in time scales, the loss of accuracy in the field in the vicinity of the dot remains one of the principal challenges when using discrete methods.[1] The equivalence principle provides a viable approach to overcoming this bottleneck by enclosing the dot with a spherical surface and then employing quasi-analytic field computations.[2] Our algorithm makes use of an efficient time-domain integral equation method to solve for representations of incident and radiated electromagnetic fields on arbitrary arrangements of such spheres. By employing a mesh-free representation of surface fields in terms of spherical harmonics, we eliminate singular integrals and dramatically reduce computational complexity over more conventional volume-based approaches. A numerical solution of the optical Bloch equations subsequently couples to the fields described by incident and radiated pulses to govern the evolution of the dot inside each sphere. Consequently, the resulting method accurately captures excitonic dynamics in moderate collections of dots in a self-consistent manner.

[1] A. Baczewski, "Integral equation and discontinuous Galerkin methods for the analysis of light-matter interaction" MSU PhD Thesis 2013

[2] J. Li and B. Shanker, arXiv:1412.8171

Presentation at the CMP Research Retreat at Michigan State University, April 12, 2015.

Using microfluidics to observe protein folding on the submillisecond timescale

Aimee Shore and Lisa J. Lapidus

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Observation of protein folding dynamics is difficult due to the expansive timescales and parameter space over which folding occurs. We use continuous flow microfluidic mixers coupled with various spectroscopic probes including tryptophan fluorescence, spectral shift, and circular dichroism to address these challenges. Experiments on Protein G and ACBP using our multi probe methodology reveal folding kinetics beyond a simple unfolded-to-folded transition indicating that folding is more complex than previously assumed. We also examine how intramolecular diffusion in an unfolded protein changes in response to environmental conditions and its implication in diseases.

Electrical current measurement and manipulation of single cells via optical trapping

Jess L West¹, Adam J Gros¹, Becky J Steidl², Gemma Reguera², Matthew J Comstock¹

¹Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan, USA

²Department of Microbiology and Molecular Genetics, Michigan State University, East Lansing, Michigan, USA

The ability of *Geobacter* bacteria to respire to extracellular electron acceptors such as uranium and electrodes shows promise for applications in bioremediation and bioenergy. Key to these technologies is a better understanding of how individual cells transfer electrons outside the cell to extracellular electron acceptors. We have constructed an experimental setup integrating optical tweezers and sample chambers equipped with micron-scale gold electrodes that allow in situ current measurements down to 50 fA. By performing bulk cyclic voltammetry experiments in these sample chambers, we have found that bias voltages of 200 mV to 500 mV are ideal in our system, producing current of about 100 pA. We have trapped individual *Geobacter sulfurreducens* cells and we can precisely manipulate them onto a gold electrode while simultaneously measuring current. With this technique, we are interrogating the cellular components responsible for current production in *Geobacter*.

Orientational dynamics of water at an extended hydrophobic interface

Florian Figge, Shunhao Xiao, John A. McGuire
Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

We report on the orientational dynamics of water at a model extended hydrophobic interface consisting of a self-assembled monolayer of octadecylsilane on fused silica. At such an interface, a fraction of water molecules has a dangling OH group in which the hydrogen points away from the bulk water and so does not participate in hydrogen bonding. We measure the dynamics of water molecules at the interface by exciting the dangling OH stretch mode with a resonant infrared pump pulse and following the excited vibration in time with a surface-specific sum-frequency probe generated by mixing a second vibrationally resonant infrared pulse and a visible pulse at the interface. As a water molecule with a dangling OH undergoes out-of-plane reorientation such that the dangling OH forms a hydrogen-bond, the vibration shifts to lower frequency, and the vibrational excitation undergoes rapid, irreversible decay. In this way, decay of the dangling OH stretch excitation is correlated with reorientational dynamics. We find that the out-of-plane reorientation of the dangling OH is characterized by a time constant of 1.46 ± 0.08 ps, only half the jump time from one hydrogen-bonded configuration to another in bulk H_2O but about 30% longer than the out-of-plane reorientation at the air-water interface. The acceleration relative to bulk can be understood as a consequence of the dangling OH not needing to break a hydrogen bond to reorient. The deceleration relative to the air-water interface is conjectured to be a consequence of suppression of the shortest wavelength capillary waves at the water surface in contact with the hydrocarbon interface.

Few-Layer Phosphorene and Arsenene Allotropes and their Tiling: A Computational Study

Zhen Zhu, Jie Guan and David Tománek

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA • zhuzhen@msu.edu

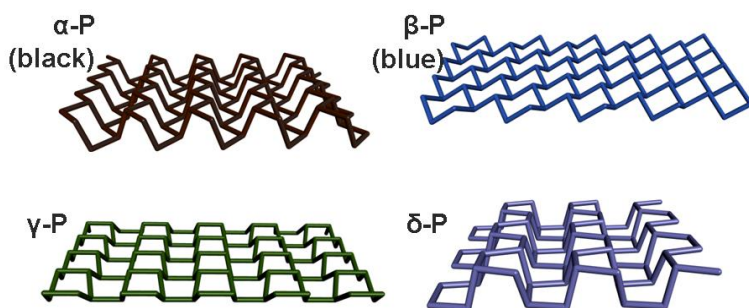


Figure 1. Different structural phases of phosphorene (Ref. [3])

Graphene monolayers, have sparked off unprecedented interest due to their unique electronic structure, but will unlikely replace silicon electronics due to a vanishing fundamental band gap. To still realize the promise of 2D semiconductor electronics, scientists are turning to other layered materials with a nonzero band gap. In this respect,

layered structures of group V elements are rapidly attracting interest. Few-layer phosphorus dubbed phosphorene combines high carrier mobility with an unprecedented tunability of the band gap [1-3]. Multiple allotropes of phosphorene, illustrated in Figure 1, may be synthesized by CVD and coexist within a monolayer with virtually no energy penalty to form grain boundaries [3]. There are countless possibilities to tile a phosphorene monolayer with different allotropes, providing the possibility of complex electronic structure patterning [4]. Similar intriguing electronic properties as found in phosphorene are postulated also for arsenene[5], a monolayer of gray arsenic. Computer simulations are a welcome means to gain microscopic insight into the physical properties and possible ways to synthesize these structures, as a guide to experimental efforts.

This research was supported by the National Science Foundation Cooperative Agreement #EEC-0832785, titled "NSEC: Center for High-rate Nanomanufacturing".

[1] David Tománek, 2014 symposium on phosphorene: An emerging 2D semiconductor, *Mater. Express* **4**, 545 (2014).

[2] Han Liu, Adam T. Neal, Zhen Zhu, Zhe Luo, Xianfan Xu, David Tománek, and Peide D. Ye, *ACS Nano* **8**, 4033 (2014).

[2] Zhen Zhu and David Tománek, *Phys. Rev. Lett.* **112**, 176802 (2014).

[3] Jie Guan, Zhen Zhu, and David Tománek, *Phys. Rev. Lett.* **113**, 046804 (2014).

[4] Jie Guan, Zhen Zhu, and David Tománek, *Phys. Rev. Lett.* **113**, 226801 (2014).

[4] Jie Guan, Zhen Zhu, and David Tománek, *ACS Nano* **8**, 12763 (2014).

[5] Zhen Zhu, Jie Guan, and David Tománek, *Phys. Rev. B (RC)* (2015).

Interfacial Coupling and Electronic Structure of Two - Dimensional Silicon Grown on the Ag(111) Surface

Jiagui Feng

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Freestanding silicene, a monolayer of Si arranged in a honeycomb structure, has been predicted to give rise to mass-less Dirac fermions, akin to graphene. However, Si structures grown on a supporting substrate can show properties that strongly deviate from the freestanding case. Here, combining scanning tunneling microscopy/spectroscopy and differential conductance mapping, we show that the electrical properties of the ($\sqrt{3} \times \sqrt{3}$) phase of few-layer Si grown on Ag(111) strongly depend on film thickness, where the electron phase coherence length decreases and the free-electron-like surface state gradually diminishes when approaching the interface. These features are presumably attributable to the inelastic inter-band electron-electron scattering originating from the overlap between the surface state, interface state and the bulk state of the substrate. We further demonstrate that the intrinsic electronic structure of the as grown ($\sqrt{3} \times \sqrt{3}$) phase is identical to that of the Si(111)-Ag($\sqrt{3} \times \sqrt{3}$)R30° reconstructed Ag on Si(111), both of which exhibit the parabolic energy-momentum dispersion relation with comparable electron effective masses. These findings highlight the essential role of interfacial coupling on the properties of two-dimensional Si structures grown on supporting substrates, which should be thoroughly scrutinized in pursuit of silicene.

Evolution of commensurate-incommensurate magnetic structures in $\text{Ca}_3(\text{Ru,Fe})_2\text{O}_7$ with magnetic field probed via neutron scattering

Mengze Zhu

Physics and Astronomy Department, Michigan State University,
East Lansing, MI 48824, USA

Neutron diffraction studies have revealed an uncommon commensurate-incommensurate magnetic phase transition with decreasing temperature in the 5% Fe-doped bilayer ruthenate $\text{Ca}_3(\text{Ru,Fe})_2\text{O}_7$. An incommensurate phase formed of a cycloidal spiral spin structure coexists with a commensurate one below the phase transition at 42 K and persists down to the lowest temperature, accompanied by higher-order magnetic satellite peaks which indicate the formation of a magnetic soliton lattice. Magnetic field applied along the b axis induces an incommensurate-to-commensurate magnetic phase transition. However, the nucleation of the magnetic soliton lattice with decreasing magnetic field is prohibited by the suppression of the effect of thermal fluctuations on the first-order transitions, which explains the highly history-dependent behavior in the out-of-plane transport measurement. We ascribe these findings to the competing magnetic interactions in $\text{Ca}_3\text{Ru}_2\text{O}_7$. This study demonstrates an effective approach to tune novel magnetic and electronic properties of this complex system via 3d magnetic transition-metal substitution.