Collective Phenomena in Layered and 2D Materials

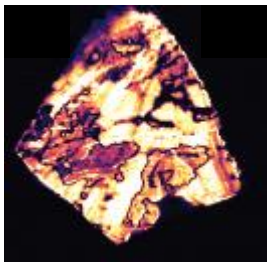
Organizers: Petro Maksymovych, Center for Nanophase Materials Sciences, ORNL
Michael A. McGuire, Materials Science and Technology Division, ORNL

Oak Ridge, TN
August 9-10, 2016

The workshop is dedicated to complex 2D and layered materials that exhibit electronically, structurally and magnetically ordered ground states. We will discuss fundamental properties, prospective new functional properties as well as recent advances enabled by theory, experiments and device integration.

The topics of the workshop include but are not limited to:

- new materials, including transition metal halides, thiophosphates and beyond;
- magnetic, structural and electronic order parameters in layered and 2D materials;
- phase transitions in anisotropic and layered materials;
- advances in synthesis, characterization and theory of complex layered materials and disorder;
- van-der-Waals heterostructures and superlattices.



OAK RIDGE National Laboratory
CENTER FOR NANOPHASE MATERIALS SCIENCES

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Agenda

Tuesday, August 9, 2016

8.30 – 9.00
Petro Maksymovych (ORNL)
A statistical picture of 2D materials research

9.00 – 9.40
Ben Hunt (Carnegie Mellon University)
Quantum Metal and Ising Superconductivity in Two-dimensional $NbSe_2$

9.40 – 10.10
Arnab Banerjee (ORNL)
Prospects and Challenges in the 2D Honeycomb Halide α-$RuCl_3$

10.10-10.30 *Coffee break*

10.30-11.10
Michael Naguib (ORNL)
Two Dimensional Transition Metal Carbides and Carbonitrides "MXenes": Synthesis, Structure, Properties and Applications

11.10-11.50
Mike Susner (ORNL)
Transition Metal Thiophosphate and Selenophosphates as Multi-Functional van-der-Waals Layered Materials

12.00-1.15 *Lunch*

1.15-2.00
Dave Mandrus (University of Tennessee, Knoxville)
Single Layers: An Opportunity to Investigate Crystals of Strongly Correlated and Quantum Materials at the Nanoscale

2.00-2.45
Thomas Maier (ORNL)
Pairing in Dried Out Fermi Seas

2.45-3.00 *Coffee break*

3.00-3.45
David Parker (ORNL)
Gaps, Maps and Traps: The Relationship of Local Structure to Bulk Properties in Iron-Based Superconductors

3.45-4.30
Maxim Ziatdinov (ORNL)
Data Mining and Pattern Recognition in Scanning Probe Microscopy of Layered and 2D Materials

4.30-5.00 *Open discussion*

Wednesday, August 10, 2016

9.00-9.30

Jacilyn Brant (Air Force Research Laboratory, Wright-Patterson, Ohio)

Polycrystalline Powders with Layered Structures: Search for Superconductivity in Oxides and Ion Conductivity in Sulfides

9.30-10.00

Yan Wang (University of Tennessee, Knoxville)

Aspects of Cross Interface Coupling Between FeSe Monolayers and Oxide Substrates

10.00-10.20 *Coffee*

10.20-11.00

Jose Mendoza (Florida State University)

New Computational Methods and Their Applications to Producing and Storing Clean and Sustainable Energy

11.00-11.20

Panchapakesan Ganesh (ORNL)

A High-Throughput Data Based Approach to Materials Discovery

11.20-11.40

David Brown (Georgia Institute of Technology)

Thermal Transport at Interface of Graphene/h-BN

12.00-1.00 *Lunch*

1.00 – 1.30

Kai Xiao (ORNL)

Heterogeneity in 2D systems: From Doped Monolayers to van der Waals Heterostructures

1.30 – 2.00

Di Xiao (Carnegie Mellon University)

Spin Nernst Effect of Magnons in Collinear Antiferromagnets

2.00 – 2.20

Michael McGuire (ORNL)

Magnetism in Layered Transition Metal Halides

2.20 – 2.40

Tom Berlijn (ORNL)

Itinerant Antiferromagnetism in RuO_2

List of abstracts

Quantum Metal and Ising Superconductivity in Two-dimensional $NbSe_2$

Benjamin Hunt

Department of Physics, Carnegie Mellon University

Atomically-thin transition metal dichalcogenides have recently become a very popular subject. $NbSe_2$, a classic layered superconductor, is the first of these that exhibits superconductivity down to one or two atomic layers. I will discuss our recent experiments on bilayer and few-layer $NbSe_2$ and our observation of an anomalous metallic phase in the zero-temperature limit induced by a small perpendicular magnetic field. This quantum metal phase has only been observed in highly-disordered thin film superconductors and its observation in a crystalline superconductor, along with a distinct magnetic field scaling, forces us to reexamine the diagram of possible electronic phases in two dimensions at zero temperature.

The atomic-scale thickness of the $NbSe_2$ crystals also implies that we can explore the regime where quenching of superconductivity is entirely due to paramagnetic effects. We study this regime, where superconductivity can survive up to 30 T in-plane, and find a strong enhancement of the upper critical field relative to the Pauli limit. I discuss the implications of this for spin-orbit coupling effects and possible exotic phases of superconductivity.

Prospects and Challenges in the 2D Honeycomb Halide α-$RuCl_3$

Arnab Banerjee

Quantum Condensed Matter Division, Oak Ridge National Laboratory

As dimensions get reduced, the effects of quantum fluctuations increase. Transition metal halide α-$RuCl_3$ is a 2D layered honeycomb magnet where the layers are bound only with weak Van-der-Waal's interaction, just like graphene. A high spin-orbit coupling in presence of an octahedral crystal field ensures a S=1/2 ground state which further enhances the fluctuations. These conditions make this material one of the most promising candidates for the Kitaev quantum spin liquid (QSL) physics which occurs when the three types of bonds of the honeycomb lattice have mutually incompatible Ising interactions. A Kitaev QSL is particularly interesting since its magnetic excitations are theorized to realize solid-state qubits which are topologically protected from thermal fluctuations.

α-$RuCl_3$ material crystallizes into a long-range zig-zag magnetic order which is one of the classical ground states predicted by the Kitaev-Heisenberg Hamiltonian. In the first part of the talk I show that the long range order in this 2D material is strongly affected by stacking of the 2D layers. Stacking faults are common in 2D layered compounds and can destroy long-range order. Quite non-intuitively however, the introduction of stacking faults increases the transition temperature of long-range order in α-$RuCl_3$. I will discuss how such ground state properties can relate to the strong Kitaev physics. In the second part of the talk, I will discuss the inelastic scattering results in this material in both single-crystal and powder form. We explicitly measure a thermally resilient broad magnetic continuum of scattering which is independent of the long-range zig-zag ordering and cannot be explained by classical spin-wave theories. On the other hand, this mode matched the predictions of the high-energy 2D Majorana Fermions expected from pure Kitaev calculations, placing this material proximate to the pure Kitaev ground state. We measured detailed energy-momentum resolved dispersion of this mode using single-crystal TOF neutron scattering, which would be the first measurement of its kind on a Kitaev continuum. Our measurements yields critical insights into *how* and *by how much* non-Kitaev interactions in a real material modify the ideal Kitaev behavior, and help to pave the path forward towards ideality.

Two Dimensional Transition Metal Carbides and Carbonitrides "MXenes": Synthesis, Structure, Properties and Applications

Michael Naguib

Materials Science and Technology Division, Oak Ridge National Laboratory.

MXenes -a new family of two dimensional (2D) transition metal carbides and carbonitrides- joined the constellations of 2D materials few years ago. With more than 15 different compositions (e.g. Ti_3C_2, Ti_3CN, Mo_2C, V_2C, Nb_2C, $V_{1.5}Cr_{1.5}C_2$) synthesized so far and many more are expected to be stable, MXenes can be considered as the fastest growing family of 2D materials. The surface of the as-synthesized has a mixture of terminations (O, OH, and F) that can be tuned to control MXenes' electronic structure and properties. In addition to their chemical compositions versatility, MXenes offer unique combinations of properties. For example, they have high electrical conductivity and they exhibit hydrophilic behavior, which is a rare combination of properties in layered materials. Since their discovery, MXenes proved themselves to be very promising materials for many applications including electrochemical energy storage (e.g. ion batteries and supercapacitors), robust support for catalysts, conductive additives for polymers, sensors, etc. In this presentation, the recent progress in the synthesis of new MXenes, understanding their structure, and exploring their properties will be summarized. MXenes performance in various applications will be discussed as well.

Transition Metal Thiophosphate and Selenophosphates as Multi-Functional van-der-Waals Layered Materials:

Michael A. Susner[1], Marius Chyasnavichyus[2], Michael A. McGuire[1], Dongwon Shin[1], Panchapakesan Ganesh[2], and Petro Maksymovych[2]

[1]Materials Science and Technology Division, Oak Ridge National Laboratory
[2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Transition metal thiophosphates (TMTPs) are an interesting materials class containing a variety of structures, some of which exhibit ferromagnetic, ferroelectric, or photoluminescent behavior. TMTPs as a general materials class will be discussed, focusing on research into their functional properties and current lines of investigation. In particular, the ferrielectric compound $Cu_{1-x}In_{1+x/3}P_2S_6$ will be discussed in terms of a novel phenomenon, coherent spinodal decomposition, that allows nanoscale engineering of ferroic ordering due to interaction between the ferrielectric $CuInP_2S_6$ and paraelectric $In_{4/3}P_2S_6$ phases within the same single crystal. High energy synchrotron data will be presented that show the structural effects of this mechanism when different kinetics are investigated, i.e the effects of quenching and the formation of nanodomains where the ferroic ordering is suppressed. In addition, a new compound, $CuScP_2S_6$, is investigated and its ordering is probed.

Research was sponsored by the Laboratory Directed Research and Development Program of Oak Ridge National Laboratory, managed by UT-Battelle, LLC, for the U. S. Department of Energy. Microscopy experiments were conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

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Single Layers: An Opportunity to Investigate Crystals of Strongly Correlated and Quantum Materials at the Nanoscale

Dave Mandrus

University of Tennessee, Knoxville

I will discuss some of the opportunities and challenges of studying single layers of correlated and quantum materials. Then I will discuss CrSiTe3 as a specific example of a magnetic semiconductor.

Pairing in Dried out Fermi Seas

Thomas Maier

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The nature of the pairing mechanism in the layered, quasi-2D copper-oxygen and iron-based high-temperature superconductors remains an open problem of great interest in condensed matter physics. The origin and nature of the pseudogap state in the cuprates and its impact on superconductivity as well as the high transition temperatures observed in mono-layer and heavily electron-doped iron-selenides are among the key questions facing modern theory and experiment in this field. This talk will present recent theoretical investigations of these issues and discuss spin-fluctuation pairing in systems where parts of the Fermi surface are missing as a common thread to understand the behavior of these systems.

Gaps, Maps and Traps: The Relationship of Local Structure to Bulk Properties in Iron-Based Superconductors

David S. Parker

Materials Science and Technology Division, Oak Ridge National Laboratory

A topic of intense yet enduring interest in condensed-matter physics is the following: How do *bulk* properties, such as magnetism or superconductivity, arise from *local* chemical and electronic structures? This problem is of particular relevance given the great yet challenging goal of attaining *predictive* capacity for these properties in real materials. In this talk I will describe three recent ORNL findings on superconductivity and magnetism in iron-based materials:

1) The discovery [1] that magnetoelastic coupling in thallium-doped $BaFe_2As_2$ is sufficiently strong as to *reverse* the usual trend of diminished Néel temperature with charge doping;

2) The finding [2] that while the tetragonal phase of FeS can display a novel coexistence of antiferromagnetism and superconductivity depending on iron content, the hexagonal phase has a robust magnetism; and

3) The revelation [3] that while annealing renders the antiferromagnet $BaFe_2As_2$ *more* electronically homogeneous, it makes the superconductor $BaFe_{2-x}Co_xAs_2$ *less* so [4], and it raises transition temperatures in *both* materials.

I close with an outlook for this exciting area of research.

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Data Mining and Pattern Recognition in Scanning Probe Microscopy of Layered and 2D Materials

Maxim Ziatdinov[1,2]

[1]Institute for Functional Imaging of Materials, Oak Ridge National Laboratory

[2]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

We discuss a recent progress in applying data mining and pattern recognition techniques to experimental scanning probe microscopy of 2D and layered materials. To illustrate the developed approaches, we selected three different systems: i) graphene, ii) "parent" state of unconventional iron-based superconductor, and iii) 2D molecular film.

Direct data mining the structure-property relationships in graphene. The link between changes in the material crystal structure and its mechanical, electronic, magnetic, and optical functionalities – known as the structure-property relationship – is the cornerstone of the contemporary materials science research. The recent advances in high-resolution scanning transmission electron and scanning probe microscopies (SPM) have opened an unprecedented path towards examining the materials structure–property relationships on the angstrom-scale level. Hence, it should be in principle possible to "break" the crystal lattice system down to the individual structural fragments and/or distortion modes and identify the geometric features that most influence the physical property of interest. To date, however, there has been no general and statistically-meaningful framework for realizing this vision. To address this problem, we have developed a comprehensive approach for correlative analysis of information obtained in structure and electronic 'channels' of atomically-resolved scanning probe microscopy experiments, and illustrated our approach using data obtained on graphene.

We applied a combination of sliding window fast Fourier transform, Pearson correlation matrix, and linear and kernel canonical correlation, to study a relationship between lattice distortions and electron scattering from SPM data on graphene with defects. Our analysis revealed that the strength of coupling to strain is altered between different paths in a momentum space, which can explain a peculiar coexistence of several quasiparticle interference patterns in nanoscale regions of interest. In addition, the application of kernel functions allowed us to extract a non-linear component of the relationship between the lattice strain and scattering intensity in graphene.

Separation of intertwined electronic responses in a "precursor state" of iron-based superconductor: a statistical learning approach. Electronic interactions present in material compositions close to the superconducting dome play a key role in the manifestation of high-T_c superconductivity. In many correlated electron systems, however, the parent or underdoped states exhibit strongly inhomogeneous electronic landscape at the nanoscale that may be associated with competing, coexisting, or intertwined chemical disorder, strain, magnetic, and structural order parameters. To analyze this spatially inhomogeneous electronic landscape, we have used statistical learning algorithms such as *k*-means clustering, principal component analysis and Bayesian linear unmixing, which allowed us to decorrelate scanning tunneling spectroscopic dataset recorded over the nanoscale surface area of the gold-doped $BaFe_2As_2$ sample. We showed that electronic behaviors uncovered in such statistically meaningful way

have a direct relevance to fundamental physical properties of this material, such as SDW spectral gap, pseudogap-like state, and impurity-induced resonance states.

Machine learning on molecular level. The ability to utilize individual molecules and molecular assemblies as data storage elements has motivated scientist for years, concurrent with the continuous effort to shrink a size of data storage devices in microelectronics industry. One of the critical issues in this effort lies in being able to identify individual molecular assembly units on a large scale in an automated fashion of complete information extraction. Here we present a novel method of applying machine learning techniques for extraction of positional and rotational information from scanning tunneling microscopy (STM) images of π-bowl sumanene molecules on gold.

We use Markov Random Field (MRF) model to classify inversion state of each bowl-shaped molecule based on both the theoretical simulations and experimental data. We further develop an algorithm that uses a convolutional Neural Network (cNN) combined with MRF and input from density functional theory to classify molecules into different rotational classes. Our results have demonstrate that a molecular film is partitioned into distinctive rotational domains consisting typically of 20-30 molecules. Finally, by applying the outlined approach to a sequence of STM images on the sumanene adlayer, we were able to track and "read-out the tip-induced changes in the rotational states of the molecules on a scale of hundreds of molecules.

This work was supported by the U.S. Department of Energy (DOE), Office of Science, Basic Energy Sciences (BES). Research was conducted at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Polycrystalline Powders with Layered Structures: Search for Superconductivity in Oxides and Ion Conductivity in Sulfides

Jacilynn A. Brant,[1] David C. Vier,[2] Thomas J. Bullard,[1] Timothy J. Haugan[1]

[1]The Air Force Research Laboratory, AFRL/RQQM, Wright-Patterson AFB, OH
[2]University of California San Diego, La Jolla, CA

The talk will focus on two points: (1) the search for superconductivity in oxides and (2) lithium ion conductivity in sulfides. The phenomenon of superconductivity in high-temperature superconductors is often ascribed to specific layers within a crystal structure. Here, Magnetic Field-Modulated Microwave Spectroscopy (MFMMS), which can be used to selectively detect superconducting transitions with high sensitivity and selectivity, is used to search for signatures of superconductivity in polycrystalline powders with layered structures. In addition to natural mineral samples, synthetic rare earth (RE) oxides were screened. The structures and phase compositions were analyzed via X-ray powder diffraction (XRPD). In some cases, high resolution synchrotron XRPD data was used to assess low-weight fraction phases in samples that gave rise to peak-like responses in MFMMS data. Zero-field cooled (ZFC) and field-cooled (FC) vibrating sample magnetometry (VSM) was used to evaluate magnetic properties.

Diamond-like thiogermanates with the formula Li_2-II-GeS_4 represent a new class of Li^+ ion conductors, while the rock salt-like Li_2SnS_3 is a fast Li+ ion conductor ($\sigma_{100\ ^\circ C}$ = 1.6x10^{-3} S/cm). In Li_2-II-GeS_4 materials, different lithium diffusion pathways are accessed by varying the divalent metals and the highest conductivity observed is on the order of 10^{-4} S/cm. Li^+ ions conduct between square lattice layers of $[CdGeS_4]^{2-}$, while anionic frameworks with topologies of the zeolite ABW or cubic diamond are accessed in Li_2-II-GeS_4 with II = Mn or II = Fe, respectively. In Li_2SnS_3, the structure can be viewed as $[SnS_3]^{2-}$ layers of honeycomb nets with lithium ions residing between the layers and within the 6-membered rings. The lithium ion mobility likely arises from the ions that reside between tin sulfide layers.

Aspects of Cross Interface Coupling Between FeSe Monolayers and Oxide Substrates

Yan Wang, Steve Johnston

Department of Physics and Astronomy, University of Tennessee, Knoxville

FeSe thin films grown on $SrTiO_3$ and $BiTiO_3$ substrates exhibit a tenfold enhancement in superconducting critical temperature over that found in bulk FeSe at ambient pressure. A number of proposals have been advanced for the mechanism of the enhanced superconductivity. One possibility is the introduction of a cross-interface electron-phonon interaction between the FeSe electrons and oxygen phonons in the substrates that is peaked in the forward scattering (small q) direction due to the two dimensional nature of the interface system. I will first explain the origin and the consequence of such an interaction using a simple and essential microscopic model. I will then discuss ab initio calculations aimed at understanding the nature of this interaction. While we find a strong forward scattering peak at q=0 in the coupling constant of a polar oxygen branch with an energy ~100 meV from the ab initio calculations, the calculated total electron-phonon coupling strength ~0.2--0.3 cannot account for the high Tc~70 K observed in these systems. Our results point towards a cooperative role for the electron-phonon interaction, where the cross-interface interaction acts in conjunction with a purely electronic interaction.

New Computational Methods and Their Applications to Producing and Storing Clean and Sustainable Energy

Jose L. Mendoza-Cortes[1,2,3,4]

[1]Department of Chemical and Biomedical Engineering, Florida State University and Florida A&M, College of Engineering, [2]Scientific Computing Department, Dirac Science, [3]Materials Science and Engineering, High Performance Materials Institute, [4]Condensed Matter Science, National High Magnetic Field Laboratory.

Computational chemistry and materials science algorithms are now powerful enough that they can predict many properties of materials and molecules before they are synthesized. By imple- menting and developing new approaches to calculate materials and chemical properties in super- computers, we have predicted over 100,000 materials for energy storage and catalysis.[1−10] The computations predicted several new materials which were made and tested in the lab, leading to the discovery and development of five new materials that overcome the DOE-targets for methane and molecular hydrogen storage as well as new mechanistic insights allowing to design better catalysis.[7−10] The intend of all this work is towards developing an alternative way to generate and store energy; i.e. conversion of sunlight into chemical fuels.

Our approach is thus inspired in Nature, where sunlight, water, and carbon dioxide is converted to chemical fuels called carbohydrates. However, we intend to convert sunlight and water into another fuel called molecular hydrogen. The advantage of "burning" molecular hydrogen in fuel cell reaction is that it can generate electricity and as only side product is water vapor. Thus we can close the cycle and approach a carbon neutral source of energy and storage that can restored. [11−12] In a recent effort to close the loop towards a possible sustainable and clean energy, we found a new strategy for tuning the band gap of 2D layered materials to capture light which may couple to its intrinsic water-splitting catalytic properties, thus resembling photosynthesis.[13] What this means is that we can capture sunlight effectively with abundant and cheap elements, which is also good at converting water into molecular Hydrogen and Oxygen. This is a promising building block to make the entire process sustainable.

Our ultimate goal is to use sunlight, water and carbon dioxide and generate chemical fuels easier to handle such as methanol or ethanol. We will present our first efforts done in this direction.[14]

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A High-Throughput Data Based Approach to Materials Discovery

Panchapakesan Ganesh

Center for Nanophase Materials Sciences, ORNL

Current outstanding challenges in fundamental understanding of materials, or discovery of new material-solutions for energy and environment challenges, requires a fast-paced discovery route. Current advances in large-scale computers allows us to do just that, but requires a framework that caters to this need while taking advantage of the latest supercomputer architectures. I will talk about our efforts in developing such a scalable high-throughput framework to perform density functional theory (DFT) based *ab initio* calculations and draw examples from ongoing studies using this approach, with experimental validation of novel insights from computations. In addition we are also working on a parallel data analysis suite, that efficiently explores the computed large-datasets to enable data-based discovery.

Thermal Transport at Interface of Graphene/h-BN

David B. Brown, Thomas L. Bougher, Baratunde A. Cola, Satish Kumar

Georgia Institute of Technology

As the power dissipation increases and device dimension scales down in electronic devices, inefficient thermal management can become challenging and cause degradation in performance and reliability. The power consumption and heat removal in these electronic devices is limited by the thermal boundary conductance (TBC) at the interfaces. Graphene, a two-dimensional (2D) material made up of a single layer up to a few layers of sp^2 bonded carbon atoms, has attracted considerable interest because of its electronic (e.g. high carrier mobility) and optical properties (e.g. transparency) [1-3]. Graphene can be stacked with other 2D materials such as h-BN to build layered hetero-structures which introduce compositional and structural diversities to further enrich the properties and applications of 2D materials. For example, h-BN can be used as a promising dielectric for graphene based field effect transistors (FETs) and improve mobility of FET's channel [4] and may open a small bandgap in graphene (~50 meV) [5]. A fundamental understanding of phonon transport and estimation of TBC at the interfaces of 2D materials is of great importance for improved heat dissipation and energy efficiency; however, thermal transport across the interfaces of these hetero-structures is still not well understood. This work fabricates layered hetero-structures of graphene with h-BN by transferring graphene/h-BN to surface of substrate (i.e. SiO_2) to create stacked layers. Raman spectroscopy is used to determine the quality of graphene and h-BN, while atomic force microscopy (AFM) is performed to study the topology of the surface. Time-domain thermoreflectance (TDTR) is used in order to decipher the TBC at the interfaces of graphene and h-BN. TDTR is a pump-probe optical technique which uses a modulated laser beam (pump) to heat the surface of a sample and an unmodulated beam (probe) is used to measure the change in optical reflectivity of the surface. Modulation of the pump beam allows the signal to be measured using lock-in amplification. The experimental data is fit to a thermal model in order to extract the thermal properties of the sample and Monte Carlo simulations are used to determine uncertainties associated with TBC estimation.

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Heterogeneity in 2D systems: From Doped Monolayers to van der Waals Heterostructures

K. Xiao[1], X. Li[1], M. Mahjouri-Samani[1], M-W. Lin[1], K. Wang[1], A. A. Puretzky[1], M. Yoon[1], C. M. Rouleau[1], A-P. Li[1], Wu, Zhou[2], M. Chi[1], B.C. Sumpter[1], J. C. Idrobo[1], D. B. Geohegan[1]

[1]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

[2]Materials Science and Technology Division, Oak Ridge National Laboratory

[3]Dept. of Materials Science and Engineering, University of Tennessee, Knoxville

Two-dimensional (2D) materials have emerged as promising candidates for next-generation atomically-thin electronic and optoelectronic devices due to the pronounced influence of surface states and interactions, as well as quantum confinement. This talk will discuss the fundamental understanding of the roles of heterogeneity in the form of defects, dopants, and atomic interface in 2D materials on their electronic and optoelectronic properties. The isoelectronic doped (W and S) $MoSe_2$ monolayer crystals were synthesized by chemical vapor deposition (CVD) and pulse laser deposition (PLD). We found that isoelectronic substitutions not only tune the carrier type, but also suppress the deep level defects to control the heterogeneity of 2D TMDs. In addition, GaSe/$MoSe_2$ misfit bilayer heterostructures were synthesized by van der Walls epitaxy through a two-step CVD process and characterized by atomic resolution transmission electron microscopy to reveal the atomistic orientation that generates the periodic Moiré superlattices. The *p-n* heterojunctions exhibit a gate-tunable photovoltaic response. Therefore, the understanding of compositional and structural heterogeneities will enable the design of new 2D materials taking advantage of specific functionalities offered by heterogeneities, allowing us to tailor physical properties of 2D materials for optoelectronic devices.

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Spin Nernst Effect of Magnons in Collinear Antiferromagnets.

Di Xiao

Carnegie Mellon University

In a collinear antiferromagnet with easy-axis anisotropy, symmetry guarantees that the spin wave modes are doubly degenerate. The two modes carry opposite spin angular momentum and exhibit opposite chirality. Using a honeycomb antiferromagnet in the presence of the Dzyaloshinskii-Moriya interaction, we show that a longitudinal temperature gradient can drive the two modes to opposite transverse directions, realizing a spin Nernst effect of magnons with vanishing thermal Hall current. We find that magnons around the Γ-point and the K-point contribute oppositely to the transverse spin transport, and their competition leads to a sign change of the spin Nernst coefficient at finite temperature. Possible material candidates are discussed.

Magnetism in Layered Transition Metal Halides

Michael A. McGuire

Materials Science and Technology Division, Oak Ridge National Laboratory

I will give a brief review of layered transition metal halides, mostly binary compounds, with a focus on crystallographic and magnetic properties. This is a reasonably large family of easily cleavable materials, many or all of which are electrically insulating. Specific attention will be given to recent results from chromium trihalides, which undergo structural and magnetic phase transitions with evidence for some magnetoelastic coupling.

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Itinerant Antiferromagnetism in RuO_2

Tom Berlijn

Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

RuO_2 has long been considered a Pauli paramagnet. Based on our combined theoretical and experimental study we conclude that RuO_2 exhibits a hitherto undetected lattice distortion below approximately 900 K. The distortion is accompanied by antiferromagnetic order up to at least 300 K, possibly as high as 900 K, with a small room temperature magnetic moment of approximately 0.05 B. The combination of high Neel temperature and small itinerant moments make RuO_2 unique among ruthenate compounds and among oxide materials in general.