Magnetic Interfaces and Nanostructures
Room 209 F W - Session MI+2D-WeA

Magnetic Interfaces and Nanostructures Oral Session

Moderators: Valeria Lauter, Oak Ridge National Laboratory, **Hendrik Ohldag**, Lawrence Berkeley National Laboratory

2:15pm **MI+2D-WeA-1 Probing Heterogeneity in 2D van der Waals Materials via Cryogenic STEM***, **Miaofang Chi**,* One Bethel Valley Rd*; Joy Chao, Haoyang Ni,* One Bethel Valley Road **INVITED**

Quantum materials exhibit unique phenomena and functionalities that extend beyond classical physics. The use of 2D sheets and the construction of hetero- and moiré structures have emerged as promising approaches to inducing exotic quantum effects. However, studying these materials via cryogenic scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) has traditionally been limited by stage instability. Recent advancements in stage design by manufacturers now provide new opportunities for this research. In this talk, I will present our ongoing studies using atomic-scale cryogenic STEM and monochromated EELS to investigate the coupling between lattice and electronic structures in several representative 2D van der Waals materials relevant to magnetic storage and spintronic applications. One key example is the discovery of layer-number-dependent phase transitions in $CrCl_3$ during cooling. Another is the impact of defects and secondary phases on the magnetic structure evolution of $Fe_{5-x}GeTe_2$ (FGT-512). Additionally, we have mapped local excitons in moiré-structured $MoTe_2$. These studies demonstrate that the electronic and magnetic properties of 2D materials can be tuned by controlling the layer number or engineering moiré structures. They also highlight the power of combining high-resolution cryogenic STEM imaging and spectroscopy to advance the understanding of quantum materials.[1]

[1] This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences, and Engineering Division and was performed at the Center for Nanophase Materials Sciences at ORNL.

2:45pm **MI+2D-WeA-3 Examining the influence of magnetic and electron beam probes on the topologically-protected edge states of 2D Bi2Te3 Nanoplates***, **Timothy Carlson**, Swathi Kadaba,* Wake Forest University*; Gabriel Marcus,* Quoherent*; Motahhare Mirhosseini, David Carroll,* Wake Forest University

In this work well defined, stoichiometric two-dimensional (2D) nanoplates of the topological insulator, Bi2Te3, were imaged using magnetic force microscopy (MFM), atomic force microscopy (AFM), and high resolution transmission electron microscopy (HRTEM) including techniques such as electron energy loss spectroscopy (EELS) and cross sectional TEM. Nanoplates with a diameter range of 0.5 to 1.5um and ~6-15nm thick were supported on highly order pyrolytic graphite (HOPG) for the scanning probes and ultra thin, lacy TEM grids for the electron probes imaging and spectroscopy. In the case for the MFM experiments, the relative strength of the edge-fields were characterized by adjusting the lift heights resulting in a unique relationship between the magnetic probe and the nanoplates under observation. For the EELS experiments, the data was collected on the edges of the nanoplates and signatures indicative of edge channels was observed. We suggest in both cases time-reversal symmetry breaking in the Bi2Te3 nanoplate from the field of the magnetic cantilever and the high electron flux from the electron beam. These symmetry breaking interactions are believed to produce induced, topologically protected currents. The addition of an applied DC bias to the tip enabled the controlled filling of Landau levels by lowering or raising the fermi level. Previous studies suggest Bi2Te3 nanoplates of similar proportions to lie within the 3D topological insulator family and therefore harbor 2D surface states, however, based on the nature of the contrast seen in the MFM, electron energy loss spectroscopy (EELS), and our synthesis method we argue these nanoplates fall within the 2D topological insulator family. These studies reveal the existence of persistent currents in our 2D Bi2Te3 system at room temperature and point to MFM and EELS as powerful tools for probing such topologically protected quantum spin hall states.

3:00pm **MI+2D-WeA-4 Surface of Topological Weyl Semimetal PtBi1.6***, **Zheng Gai**,* Oak Ridge National Laboratory*; Dejia Kong,* Department of Chemistry, University of Virginia, Charlottesville, VA 22903*; Rongying Jin,* University of South Carolina, Columbia, SC 29208

$PtBi_{2-x}$ (specifically $PtBi_{1.6}$) is a noncentrosymmetric Weyl semimetal that hosts topologically protected surface states, making it a fascinating platform for exploring exotic surface and bulk phenomena. The material naturally cleaves to reveal two distinct surface terminations: a buckled Bi1 surface with *3m* symmetry, and a flat Bi2 surface with *m* symmetry. $PtBi_{1.6}$ also exhibits giant magnetoresistance, surface superconductivity, and evidence of robust quasiparticle interference patterns, making it a compelling candidate for applications in spintronics, quantum sensing, and topological quantum computing. However, several key questions remain open. One major challenge is understanding the role of surface states in transport phenomena—particularly whether they contribute to the large magnetoresistance observed at low temperatures. Our scanning tunneling microscopy (STM) studies reveal the presence of both Bi1 and Bi2 terminations upon cleaving, consistent with prior surface-sensitive spectroscopic studies. Detailed quasiparticle interference (QPI) analyses highlight contrasting behaviors on the two surface types, suggesting that the electronic structure and scattering mechanisms are highly termination-dependent. Additionally, we examine the impact of atomic-scale defects on the surface states, providing insight into their stability and resilience. These findings deepen our understanding of surface-bulk interplay in noncentrosymmetric topological systems and underscore the importance of surface engineering in future device applications.

The STM work of this research was conducted at the Center for Nanophase Materials Sciences, ORNL, which is a DOE Office of Science User Facility.

3:15pm **MI+2D-WeA-5 Visualizing Electronic and Magnetic Structure at Nanoscale for Spintronics***, **Jyoti Katoch**,* Carnegie Mellon University, USA **INVITED**

Topological semimetals, such as WTe_2 and $TaIrTe_4$, have strong spin-orbit coupling, non-trivial band dispersion, and bulk and surface spin polarized states. A combination of intrinsic spin Hall effect and surface state driven efficient and unconventional spin current generation can be obtained in these systems for manipulating the magnetic order. However, the comprehensive understanding of electronic structure, which is directly responsible for charge to spin conversion, of these systems at mesoscopic scale remains critical missing. I will discuss our results on probing spatially resolved electronic structure of atomically thin layers of WTe_2 and $TaIrTe_4$ using nanoARPES. Moreover, recently, we reported the first experimental realization of field-free deterministic magnetic switching of a perpendicularly polarized van der Waals (vdW) magnet employing spin current with out-of-plane spin polarization in layered WTe_2. We will discuss our efforts to utilize the photoemission electron microscopy (PEEM) paired withx-ray magnetic circular dichroism (XMCD) to obtain a spatially resolved view on the underlaying mechanism of this magnetic switching behavior. Finally, I will discuss our experiments aimed at nanoscale imaging of magnetic structure of atomically thin films of a vdW antiferromagnet, i.e., CrSBr. Layered magnetic systems display highly intriguing properties, such as thickness-dependent magnetic ground state, electric field tunability, enhancement of interlayer AFM exchange coupling in the ultra-thin limit, and tunable magnon-magnon coupling, to name a few. We will report on experiments wherein we employ PEE) paired surface-sensitive XMCD/XMLD to perform layer-dependent domain imaging in mesoscopic sized samples of CrSBr. We will discuss detailed thickness, temperature, and externally applied magnetic field-dependent magnetic domain imaging of atomically thin samples of CrSBr.

4:15pm **MI+2D-WeA-9 Layered Systems for Spintronics and Quantum Sensing of Spin Dynamics***, **Simran Singh**,* Carnegie Mellon University **INVITED**

Low-dimensional systems and their atomically precise heterostructures are a modular material platform to study emergent spin and magnetism related phenomena. I will present our work(s) on exploring topological semimetals and layered magnets based low-dimensional heterostructures to realize novel spin-galvanic effects for electric field control of the magnetic order, demonstrate a new type of unidirectional magnetoresistance, and realize an unconventional form of anomalous Hall effect. First, I will discuss our experiments to employ spin-current with an out-of-plane spin polarization generated in a low-symmetry topological semimetal to deterministically switch and read the magnetic state(s) of perpendicularly polarized magnets. Secondly, I will discuss the experimental realization of unconventional form of anomalous Hall effect in a low-dimensional heterostructures, which is proportional to not only out-of-plane magnetization but also to in-plane magnetization component, potentially expanding the parameter space for designing dissipationless edge transport in low-dimensional systems. Furthermore, spin-defects can be engineered in low-dimensional systems – an appealing prospect for quantum sensing technologies. Time permitting, I will present our work aimed at utilizing designer spin defects embedded in a two-dimensional system to probe broadband spin dynamics.

4:45pm **MI+2D-WeA-11 Surface Electronic Structure Comparison of Fe-Intercalated and 2h-TaS₂**, ***Dejia Kong**, Sree Sourav Das, Jacob St. Martin,* University of Virginia, USA*; Peter Siegfried,* George Mason University*; Zhiqiang Mao, Seng Huat Lee,* The Pennsylvania State University*; Ian Harrison,* University of Virginia*; Nirmal Ghimire,* University of Notre Dame*; Mona Zebarjadi,* University of Virginia, USA*; Zheng Gai,* Oak Ridge National Laboratory, USA*; Petra Reinke,* University of Virginia, USA

Anisotropic ferromagnetic phases can be introduced to transitional metal dichalcogenide (TMD) TaS_2 through intercalating Fe in the van der Waals (vdW) gap. By deviating from the commensurate values (x = ¼ or ⅓), the crystalline structure as well as the magnetotransport properties of the TMD system can be tuned. For instance, $Fe_{1/4}TaS_2$ has a centrosymmetric 2 × 2 structure while $Fe_{1/3}TaS_2$ has a non-centrosymmetric r3 × r3 supercell structure. The magnetic Curie temperature of Fe_xTaS_2 also exhibits a strong dependence on Fe concentration. We evaluate $Fe_{0.28}TaS_2$ and 2H-TaS_2 samples using STM/Spectroscopy (STM/S) and density functional theory (DFT) to investigate the real-space intercalant electronic structure comparatively and the potential phase segregation between the two commensurate compounds. $Fe_{0.28}TaS_2$ shows a supercell at 77 K, whereas 2H-TaS_2 displays no apparent supercell at the same temperature. Fe vacancy defects and clusters are discovered in the intercalated surface, and their surrounding local density of states (LDOS) shows non-trivial differences at energies compared to the pristine $Fe_{0.28}TaS_2$ area, which is related to Fe orbitals contributions based on the DFT calculations.

The STM work of this research was conducted at the Center for Nanophase Materials Sciences, ORNL, which is a DOE Office of Science User Facility.

5:00pm **MI+2D-WeA-12 Strain Induced Magnetism and Interfacial Effects in Pd/Mos$_2$(0001) Heterostructures**, ***Bushra Ashraf,*** University of Central Florida

This research utilizes density functional theory (DFT) calculations, including spin-orbit coupling (SOC), to analyze the interaction between palladium ad-layers and the MoS_2(0001) surface. We find that generally, as expected, the increase in the in-plane Pd-Pd bond length to 3.16 Å that results from the epitaxial growth of Pd on MoS2(0001), leads to a ferromagnetic palladium. Our results indicate that, relative to a free standing Pd layer, single Pd layer on MoS_2(0001) experiences a weakening of ferromagnetism. In contrast, the deposition of two Pd layers on MoS_2(0001) partially restores magnetization, resulting in magnetic moments of 0.091 μB and 0.206 μB per Pd atom for the mid (first) and top (second) layers, respectively. A significant spin splitting is identified in bilayer Pd systems, even without the inclusion of SOC, highlighting the influence of charge redistribution in achieving a spin-polarized state. When SOC is accounted for, band splitting occurs at high-symmetry points (such as K) with magnitudes comparable to intrinsic spin splitting, thereby enhancing the electronic structure. These results underscore the ability to tune magnetism in Pd-MoS_2 heterostructures through strain, charge transfer, and SOC, suggesting promising device applications and quantum well structures. Additionally, our findings affirm the potential for manipulating magnetism through electric fields in strained Pd layers, paving the way for innovative engineering of spin-dependent phenomena in transition metal dichalcogenide-based heterostructures.

5:15pm **MI+2D-WeA-13 Impact of Nanoscale Curvature on the Structural and Magnetic Properties of Co/Pd Alloys**, ***Asma Qdemat**, Asma Qdemat,* ORNL

Researchers have studied a lot about the properties of magnetic thin films grown on flat substrates. This is mostly because it's easy to make them and there are well established ways to process them. However, researchers have not studied enough about how nanoscale curvature affects them. This study aims to fill that gap by directly comparing the structure and magnetic behavior of Co/Pd alloy thin films deposited on flat versus curved surfaces.

In this contribution, we will present a detailed investigation of the effects of how nanoscale curvature affects the structural and magnetic properties of Co/Pd alloys deposited on flat silicon substrates and highly ordered monolayers of 50 nm and 200 nm SiO_2 nanospheres, using molecular beam epitaxy (MBE). We used a variety of advanced methods to study our system, including magnetometry, X-ray reflectivity (XRR), polarized neutron reflectometry (PNR), and grazing-incidence small-angle neutron and X-ray scattering (GISANS/GISAXS) was employed to probe both depth-resolved and lateral properties.

Structural analysis via SEM and XRR revealed that films deposited on flat silicon maintained smoother, while those grown on curved nanospheres exhibited increased surface roughness and disrupted periodicity. In films on curved substrates, a parabolic scattering length density (SLD) model was necessary to capture the curvature-induced gradient in density profiles. GISAXS and GISANS confirmed these findings, showing less nanospheres ordering and greater lateral roughness, particularly in thicker films. Furthermore, magnetically, the nanoscale curvature significantly influenced anisotropy. SQUID measurements showed strong perpendicular magnetic anisotropy (PMA) in films on flat substrates, with square hysteresis loops and high remanence. In contrast, films on curved nanospheres had increased coercivity, reduced saturation magnetization, and a tilted magnetization axis, effects that were more pronounced in thinner films. These observations were further confirmed by PNR, which revealed that curvature changes the magnetic SLD profiles and increases the Co magnetic moment. This is likely due to strain and changes in the interfacial coupling.

Our findings show that nanoscale curvature is important in controlling how magnetic alloys behave. Curvature can reduce the uniformity of the structure and the magnetic properties. But it can also open up new ways to control local magnetic interactions by altering strain and anisotropy. These insights are very important for the development of flexible, conformal magnetic devices where precise control over magnetic anisotropy is required.

5:30pm **MI+2D-WeA-14 Emergence of local magnetic moment in ternary TaWSe₂ single crystal via atomic clustering**, ***Jewook Park,*** One Bethel Valley Rd. Bldg. 8610, MS-6487

Ternary transition metal dichalcogenides (TMDs) provide a versatile platform to explore novel electronic and magnetic ground states via compositional substitution and local structural modulations. Using a combination of scanning tunneling microscopy and spectroscopy (STM/S), magnetic property measurements, and density functional theory (DFT) calculations, we analyze the emergence of local magnetic moments driven by the clustering of Ta atoms in ternary $TaWSe_2$ single crystals. STM topography reveals triangular clusters of Ta atoms embedded within W-rich regions of $TaWSe_2$. These clusters exhibit a consistent shape and an orderly arrangement throughout the surfaces. DFT calculations show that these Ta clusters induce local strain, giving rise to localized magnetic moments. The magnetic behavior is further corroborated by temperature-dependent magnetization measurements, which exhibit a magnetic transition near 50 K. This study offers a pathway to engineer magnetism in TMD systems with potential applications in spintronic and quantum materials.

5:45pm **MI+2D-WeA-15 Lattice-Strain and Anisotropy-Driven Phenomena in Epitaxial Rare-Earth Orthoferrite and Orthochromite Thin Films**, ***Mohit Madaan,*** Indian Institute of Technology Roorkee, India*; Prachi Gurawal,* Indian Institute of technology Roorkee, India*; Anil Jain,* Bhabha Atomic Research Centre, India*; V. K. Malik,* Indian Institute of Technology Roorkee, India

Within the class of functional perovskite materials, rare-earth orthoferrites ($RFeO_3$) and orthochromites ($RCrO_3$) are remarkably explored for their wide range of captivating properties as well as broad span of potential applications. Key properties include spin reorientation (SR) transition, magnetization reversal (MR), exchange bias (EB), spin switching, and magneto-optic effects. These features arise from the complex exchange interactions between the rare-earth and Fe^{3+}/Cr^{3+} magnetic sublattices. Studies on thin films of orthoferrite and orthochromites have presented significant tunability of these properties based on various factors, like-lattice-mismatch with substrate, film-thickness, stoichiometry, and chemical valency.

In this work, we investigate single- and multi-layer epitaxial thin films of $SmCrO_3$ orthochromite and $NdFeO_3$ orthoferrite, grown on single-oriented substrates- $SrTiO_3$ (STO), $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT), respectively using pulsed laser deposited (PLD) technique. High-resolution X-ray diffraction (HRXRD), including θ-2θ scans and reciprocal space maps confirms the epitaxial nature of the film and estimate the strain and its nature (tensile & compressive). Temperature-dependent magnetic susceptibility (ac and dc) reveal the anomaly features in the vicinity of characteristic magnetic transition temperatures (Néel Temperature T_N, SR temperature T_{SR}) for both in-plane (IP) and out-of-plane (OOP) configurations. Additionally, magnetic isotherms clearly demonstrate the impact of strained-relaxed film on magnetic phase stability.

Hence, these findings critically highlight the role of lattice-strain, anisotropy within films in tunning the properties to synthesize multifunctional heterostructures. They also open new avenues of exploration of magnetoelectricity, photovoltaics, and optoelectronics in these systems.

Keywords: Lattice-strain, magnetic anisotropy, spin reorientation.

6:00pm **MI+2D-WeA-16 Chirality, Surface Termination and Anti-ferromagnetic Alignment in Fe(III) Spin Crossover Salts***, **Mohammad Zaid Zaz**[1],* University of Nebraska-Lincoln*; Wai Kiat Chin, Arjun Subedi, Gauthami Viswan,* University of Nebraska - Lincoln*; Alpha T.N'Daiye,* Advanced Light Source, Lawrence Berkeley National Laboratory*; Alexander Wysocki,* University of Nebraska-Kearney*; Rebecca Lai, Peter A Dowben,* University of Nebraska - Lincoln

Switchable molecular materials based on 3d transition metal complexes are a rich platform for exploring phenomenon related to symmetry breaking which include chirality and surface termination. In certain di-nuclear species, magnetic ordering between different metal ions is also witnessed. We explore chirality, surface termination and anti-ferromagnetic alignment in an Fe(III) spin crossover complex namely $[Fe(qsal)_2Ni(dmit)_2]$ where, qsal = N(8quinolyl)salicylaldimine, and $dmit^{2-}$ = 1,3-dithiol-2-thione-4,5-dithiolato. We employ spatially resolved Fe-L3,2 edge X-=ray absorption spectroscopy to probe the chiral signature at the Fe metal center. Surface termination is studied by complementary X-ray photoemission spectroscopy and energy dispersive X-ray spectroscopy. These are further complemented by inverse photoemission spectroscopy and Fe, Ni-L3,2 edge X-ray absorption spectroscopy. Finally, we investigate the anti-ferromagnetic alignment in this system by X-ray magnetic circular dichroism measurements at the Fe and Ni core.

[1] **Falicov Student Award Finalist**

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