

Nanoscale Science and Technology Room 206 A W - Session NS2+2D-TuM

Multimodal Techniques in Surface and Interface Engineering at the Nanoscale

Moderator: Mausumi Mahapatra, Loyola University Chicago

9:30am **NS2+2D-TuM-7 Generalized Defect Quantification of 2D Materials with Atomic Force Microscopy**, **Matthew Rosenberger**, University of Notre Dame

INVITED

Routine defect characterization is a critical capability for understanding defect-property correlations and optimizing growth of two-dimensional (2D) materials. High throughput optical methods for defect characterization, such as Raman spectroscopy, are useful for graphene, but are insufficiently sensitive to defects in some other 2D materials, such as transition metal dichalcogenides (TMDs), particularly for defect densities of about 10^{12} cm^{-2} or less. Typical methods for directly detecting defects at the atomic scale, such as scanning transmission electron microscopy (STEM) and scanning tunneling microscopy (STM), are effective, but they are slow and often require arduous sample preparation. There is a need for 2D material defect characterization techniques that are routine, fast, and reliable. Here, we demonstrate two atomic force microscopy (AFM)-based techniques for locating and quantifying atomic-scale defects in 2D materials. First, we show that conductive AFM can locate and differentiate the same defects as STM by comparing conductive AFM and STM on the same region of a TMD crystal¹. Our work establishes conductive AFM as a higher-throughput alternative to STM for defect quantification. Second, we show that lateral force microscopy (LFM) can locate atomic-scale defects through a direct comparison of LFM with conductive AFM on a TMD crystal². Importantly, we show that LFM can locate atomic-scale defects in TMD monolayers on insulating substrates and in insulating 2D materials, such as hexagonal boron nitride, because LFM is a purely mechanical technique. The AFM-based methods presented here enable routine defect characterization, which will facilitate rapid investigations of defect-property relationships and speed up the development of new growth processes.

(1) Xu, K.; Holbrook, M.; Holtzman, L. N.; Pasupathy, A. N.; Barmak, K.; Hone, J. C.; Rosenberger, M. R. Validating the Use of Conductive Atomic Force Microscopy for Defect Quantification in 2D Materials. *ACS Nano* **2023**, *17* (24), 24743–24752. <https://doi.org/10.1021/acsnano.3c05056>.

(2) Yang, Y.; Xu, K.; Holtzman, L. N.; Yang, K.; Watanabe, K.; Taniguchi, T.; Hone, J.; Barmak, K.; Rosenberger, M. R. Atomic Defect Quantification by Lateral Force Microscopy. *ACS Nano* **2024**, *18* (9), 6887–6895. <https://doi.org/10.1021/acsnano.3c07405>.

11:00am **NS2+2D-TuM-13 Excess Barrier Height Unlocks Andreev Reflection in Scanning Tunneling Microscopy**, **Petro Maksymovych**, Clemson University; **Wonhee Ko**, University of Tennessee Knoxville; **Jose Lado**, Aalto University, Finland

Superconductors are currently entering a new golden age, marked by a renewed quest for higher Curie temperature, explosion of new candidate superconducting materials and emerging applications, such as topological quantum computing. However, the foundational questions—whether the material is actually superconducting and what causes superconductivity—remain as pertinent as ever. Indeed, pairing symmetry—a key property of any superconductor—can be a challenging and contested property, even for materials where superconductivity itself is unambiguous.

To this end, we introduced a new approach to detect Andreev reflection (AR) in metal-superconducting contacts of arbitrarily high resistance, most notably in scanning tunneling microscopy (STM). Fundamentally, AR allows the injection of Cooper pairs from a metal to a superconductor, producing excess conductance and a unique sensitivity to the properties of a superconducting state. However, detecting AR in traditional transport measurements requires low (ideally zero) contact resistance—limiting its application to mesoscale and contact geometries. To remove this limitation, we shifted the experimental observable from the excess conductance to the excess height of the tunneling barrier, providing a new approach to detect, probe, and quantify Andreev reflection.

In this talk, I will discuss how tunneling barrier height spectroscopy functions in superconducting junctions and present our recent computational and experimental results on AR-STM with both conventional and unconventional superconductors. The barrier height spectroscopy has a

rich structure with combined sensitivity to the pairing symmetry, number of superconducting gaps and the detailed structure of the Fermi surface. Moreover, excess barrier height detects special, higher order Andreev reflection processes, that occur in proximate tunneling junctions just before the collapse of the tunneling barrier. As a result, STM can now leverage the unique power of Andreev reflection to probe superconductivity, magnetism and even topological properties from a new perspective. Research sponsored by Clemson University and US Department of Energy. SPM experiments were carried at the Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, a US DOE User Facility. Song/PM, arXiv: 2411.11724; Ko/PM. *Nano Letters*, **2023** *23* (17), 8310-8318; Song/PM, *Nano Letters* **2023** *23* (7), 2822-2830; Ko/PM, *Nano Letters* **2022** *22* (10), 4042-4048

11:15am **NS2+2D-TuM-14 Dynamic Evolution of Rh/Fe₃O₄(001) Catalysts Under Hydrogen Conditions**, **Mausumi Mahapatra**, Loyola University Chicago; **Marcus Sharp**, **Zdenek Dohnalek**, **Christopher Lee**, **Yifeng Zhu**, **Oliver Gutiérrez**, **Bruce Kay**, Pacific Northwest National Laboratory

Metal/oxide interfaces are a new emerging class of catalysts owing to their unique electronic and chemical properties. In this study, we have prepared a series of model Rh/Fe₃O₄(001)catalysts that include Rh adatoms (Rh_{ad}), mixed surface layers with octahedrally-coordinated Rh (Rh_{oct}), as well as metallic Rh clusters and nanoparticles (Rh_{met}) on Fe₃O₄(001). Using X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM), we investigated the activity of such model systems towards H₂ and their stability in reducing environments. Our results show that the atomically dispersed Rh_{ad} and Rh_{oct} species do not activate H₂, which would result in the formation of surface hydroxyls on Fe₃O₄(001). In contrast, the presence of Rh_{met} in H₂ results in the formation of hydroxyls and subsequent etching of the Fe₃O₄(001) at higher temperatures ($\geq 500 \text{ K}$) due to water formation via the Mars-van Krevelen mechanism. Additionally, such surface etching leads to the release of the Rh_{oct} from the surface lattice and their sintering to Rh_{met}. To bridge the material gap between the model and high surface area catalysts, we perform parallel studies on powder Rh/Fe₃O₄ catalysts. The XPS characterization shows remarkable similarities between these systems. Further, our model studies provide an atomistic picture of the behavior of high surface area catalysts in the H₂ atmosphere.

11:30am **NS2+2D-TuM-15 Hybrid ALD-MLD HfO_x Thin Films: The Role of Carbon for Memristive Application**, **Soham Shirodkar**, **Dushyant Narayan**, **Minjong Lee**, **Dan Le**, University of Texas at Dallas; **Jacob N. Rohan**, Cerfe Labs, Austin; **Jiyoung Kim**, University of Texas at Dallas

Resistive switching (RS) memories based on transition metal oxides (TMOs) are a promising class of emerging nonvolatile memory devices for next-generation electronics. However, conventional TMO-based RS memories typically require high forming voltages (V_{form}) during initial operation, consuming excessive power. To address this issue, incorporation of metal dopant species into TMOs is proposed to lower the V_{form} [1]. For example, Hf/Zr doping in TiO₂ ReRAM has been demonstrated to increase the formation of oxygen vacancies, leading to lower forming voltages [2]. In our previous work, we have demonstrated that incorporating carbon into HfO_x films via a hybrid Atomic Layer Deposition (ALD)/Molecular Layer Deposition (MLD) process can eliminate the need for a forming process, enabling 'Born-ON' behavior during the first sweep [3,4]. However, control of carbon incorporation is challenging due to its high atmospheric reactivity. Therefore, the choice of organic precursor during the MLD can significantly influence the film's properties and ultimately the device properties.

In this work, we systematically investigate the impact of different organic precursors during ALD/MLD hybrid process using two linear-chain hydrocarbons Ethylene Glycol (EG) and Glycerol (GL) as well as an aromatic hydrocarbon Hydroquinone (HQ). These organic precursors vary in number of carbon atoms and number and position of OH groups. In this regard, we observed significant differences in growth per cycle (GPC) and carbon bonding states: HQ, being the largest molecule, exhibited the highest GPC-3.1 Å/cycle and carbon composition-45% along with higher expected C-sp² content due to its aromaticity. Whereas EG showed a low GPC-0.2 Å/cycle and less carbon incorporation-15% due to its small size and possible poisoning effects. In contrast, GL, with an additional OH group, likely mitigates these poisoning effects common to linear hydrocarbons, resulting in a GPC of 2.1 Å/cycle and 31% carbon content. Metal-Insulator-Metal devices with these films exhibit distinct 'Born-ON' behavior as well as resistive switching without electroforming, though each precursor-based film requires a different thermal budget to activate this response. This

study underscores the crucial role of precursor chemistry in tailoring the properties of carbon-doped TMO memristors and offers potential pathways for improving RS device performance.

This research is supported by Cerfe Labs and Air Force Research Laboratories.

[1] H.-S. Philip Wong et al., *J Electroceram* (2017) 39:21-38

[2] Yoshio Nishi et al., *ICSSDM, Kyoto* (2012)

[3] C. A. Paz de Araujo et al., *APL Mater.* **10**, 040904 (2022)

[4] M. Lee et al., *ALD/ALE* (2024)

11:45am NS2+2D-TuM-16 Quantitative Comparative Force Spectroscopy on Molecules, *Xinzhong Wang*, Yale University; *Percy Zahl*, Brookhaven National Laboratory; *Jara Trujillo Mulero*, Universidad Autonoma de Madrid, Spain; *Hailiang Wang*, Yale University; *Rubén Pérez*, Universidad Autonoma de Madrid, Spain; *Eric Altman*, *Udo Schwarz*, Yale University
Understanding molecular-scale interactions at surfaces is essential for advancing catalyst design and developing efficient energy conversion processes. Here, we report ongoing efforts to improve the spatial accuracy and quantitative reliability of three-dimensional atomic force microscopy (3D-AFM) by refining data correction techniques for CO-functionalized tips. These developments allow us to minimize tip- and substrate-induced artifacts and isolate the intrinsic molecular interaction at atomic resolution.

As a testbed for this approach, we investigate cobalt phthalocyanine (CoPc) and its amino-functionalized counterpart ((NH₂)₄CoPc) adsorbed on Ag(111), both of which are of interest in CO₂ electroreduction catalysis. By identifying and removing asymmetric force contributions caused by the metallic structure of the tip, we obtain corrected force spectroscopy data that reveal equilibrium interaction distances and energies across individual molecules. Our analysis shows that NH₂ substitution alters the spatial distribution of interaction strength, decreasing equilibrium distances near ligand attachment points while broadly reducing interaction energy with the tip.

These experimental observations agree well with DFT-based simulations and suggest that side-group functionalization directly modulates the molecule's chemical landscape. The methodology provides a direct route toward correlating molecular structure with catalytic behavior at the single-molecule level, thereby enabling a deeper understanding of functional molecular systems on surfaces.

12:00pm NS2+2D-TuM-17 Thermal Strain-Induced Nanogap Formation in Monolayer MoS₂ during CVD Growth, *Seonha Park*, *Sieun Jang*, *Songkil Kim*, School of Mechanical Engineering, Pusan National University, Republic of Korea

Molybdenum disulfide (MoS₂) is a promising semiconducting material due to its atomic flatness and high carrier mobility. In particular, chemical vapor deposition (CVD)-grown MoS₂ has been widely explored for electronic applications owing to its high quality and scalability. However, the mismatch in thermal expansion coefficients between MoS₂ and the growth substrate induces strain in MoS₂ flakes, and the nanogap structure can be formed to release such growth-induced strain. Understanding and controlling this unique nanogap structure is of great interest, as it offers opportunities for applications such as nanogap electrodes, biosensors, and gas sensors. In this work, nanogap formation mechanisms and the factors governing gap size and morphology were systematically investigated in monolayer CVD MoS₂. To investigate the role of MoS₂-substrate interfacial bonding strength in nanogap formation, three samples with different adhesion properties with the substrate are prepared. Strain distribution analysis using photoluminescence (PL) mapping and statistical analysis of multiple SEM images revealed that interfacial bonding strength significantly affects strain relaxation behavior, where weaker bonding facilitates strain release, leading to faster crack propagation and more irregular gap paths. The crystallographic configuration also influenced propagation behavior. Asymmetric bi-crystalline flakes with misorientation angles showed a stronger tendency for cracks to follow grain boundaries due to increased mechanical instability. Additionally, the relationship between flake size and nanogap size was also investigated. In samples with moderate interfacial bonding strength, a linear increase in nanogap size was observed with increasing flake size above a critical threshold. In contrast, strongly bonded samples exhibited smaller nanogaps than the moderate bonding sample, with minimal variation in gap size regardless of flake size. These results suggest that nanogap size can be effectively controlled by tuning the interfacial bonding strength and the flake size.

Surface Science

Room 209 CDE W - Session SS+2D-TuM

Complex Phenomena on Surfaces

Moderators: *Te-Yu Chien*, University of Wyoming, *Bo-Hong Liu*, National Synchrotron Radiation Research Center

8:00am SS+2D-TuM-1 Atomically Precise Synthesis and Characterization of Defect Structures in Graphene, *An-Ping Li*, Oak Ridge National Laboratory
INVITED

Atomically precise engineering of defects and interfaces in graphene, along with a detailed understanding of its structure-dependent electronic properties, is essential for the advancement of graphene-based quantum electronic applications. Here we present recent progress in the controlled synthesis and atomic-resolution characterization of defect structures in graphitic nanomaterials. The first approach involves bottom-up synthesis of graphitic nanostructures using on-surface chemical reactions using rationally designed molecular precursors. Particularly, graphene nanoribbons (GNRs) are obtained on a non-metallic substrate, showing entangled magnetic states that are decoupled from the substrate. The multistep thermally triggered transformations rely on highly selective and sequential activations of C-Br, C-F bonds, followed by cyclodehydrogenation. Scanning tunneling microscopy and spectroscopy (STM/S) are used to monitor the formation of intermediates and GNRs, revealing a weak interaction between GNRs and the substrate. The second approach employs a top-down strategy to introduce oxygen (O) substitutions into epitaxial graphene grown on SiC. Techniques including ion implantation and STM tip-assisted manipulation are used to create sp²-hybridized O dopants and control its configuration. A combination of chemical-bond-resolved non-contact atomic force microscopy (ncAFM) and STM is used to investigate the structural and electronic properties of the O-related defects. The STM/S measurements, supported by DFT calculations, indicate that the sp²-hybridized O dopant hosts a characteristic orbital electronic state below the Dirac point. Tuning the Fermi level with electric field may achieve single-electron occupancy of these atomically defined centers. Such control opens the door to the realization of long coherence electron-spin qubits, providing pathway toward graphene-based quantum technologies.

The research was conducted at the Center for Nanophase Materials Sciences (CNMS), a US Department of Energy User Facility.

8:30am SS+2D-TuM-3 Fabrication of Graphene Nanoribbons/Organic Molecules Interface, *A.M. Shashika D. Wijerathna*, *Markus Zirnheld*, Old Dominion University; *He Zhao*, Central South University, China; *Rockwell Li*, Old Dominion University; *Pingshan Wang*, Central South University and Guangzhou University, China; *Yiming Li*, Central South University, China; *Yuan Zhang*, Old Dominion University

Graphene derivative materials are great superlubricant candidates that can be potentially utilized in molecular devices. Therefore, it is essential to understand the mechanical property at the interface that is formed by organic molecules and graphene derivatives materials. In this study, we fabricated an interface formed by organic molecules with armchair graphene nanoribbons and studied its mechanical properties.

15-carbon-wide armchair graphene nanoribbons (15-AGNRs) were synthesized on Au(111) substrate in a bottom-up approach with dibromopentaphenyl (DBPPP) as precursor molecules. Precursor molecules, DBPPP exhibit two different self-assembly patterns on Au(111) substrate, forming rectangular domains and hexagonal domains. Both self-assembly structures can be successfully transformed into 15-AGNRs through polymerization at 370 K and, subsequently, cyclodehydrogenation at 470 K. 30-GNRs were also observed in some cases.

Subsequently, pentacene molecules, a linear polycyclic aromatic hydrocarbon consisting of five linearly-fused benzene (C₆H₆) rings, were deposited onto the AGNRs to form the interface pentacene/AGNRs. Pentacene molecules exhibited a preference for adsorption on the Au(111) substrate than the graphene nanoribbons. Therefore, they first fill in gapping areas formed in between graphene nanoribbons, and once the metallic surface sites are fully occupied, they adsorb onto the ribbons. Pentacene is adsorbed on AGNRs in different orientations, which include nearly transverse, oblique, and nearly axial. Among these, the most energetically favorable and stable orientation is nearly transverse, where the pentacene molecular long axis is approximately 93° clockwise relative to the GNR axis. Notably, external mechanical energy facilitated the movement of pentacene molecules along the GNRs, suggesting low molecular-scale friction. These findings provide critical insights into the

Tuesday Morning, September 23, 2025

adsorption behavior of pentacene on AGNRs and mechanical properties of the interface, which is essential for advancing their applications in organic electronics.

This work is conducted with a low-temperature (~ 77 K), ultra-high vacuum (10^{-10} mbar) scanning tunneling microscopy (LT-UHV-STM).

Keywords: Armchair Graphene Nanoribbons, Pentacene, Friction at Molecular Interface, Adsorption Orientation, Scanning Tunneling Microscope

8:45am SS+2D-TuM-4 Visualizing the Products of Scattering at Surfaces: Hot Transient Motion of N on Ru(0001) and Coverage Dependent Mobility and Placement of O on Moiré Graphene, Joshua Wagner¹², Steven Sibener, University of Chicago

Diffusion of atomic species is a pivotal process in surface chemistry for topics ranging from catalysis to material stability. This presentation focuses on two types of atomic mobility: the nonthermalized “hot” atomic motion of N atoms following dissociative chemisorption of N_2 and the highly correlated coverage-dependent diffusion of oxygen atoms on moiré patterned graphene. Overall, results provide spatially rich and atomically resolved insight to on-surface dynamics and illustrate a new direction in the study of interfacial reaction dynamics where outcomes such as site-specific reactivity and non-thermalized diffusion can be examined using incident kinetic energy and angle of incidence as reaction control parameters.

Ruthenium based materials serve as more energy efficient catalysts for the dissociative chemisorption of N_2 , the rate limiting step of ammonia synthesis *via* the Haber-Bosch process. Despite the global importance of this chemical process, open questions remain concerning the dissipation of energy following dissociation. Answering these questions may inform catalyst design and will enrich our understanding of fundamental surface dynamics.

To probe the energy dissipation pathways of N_2 dissociation on Ru(0001), tight control of the energy and angle of incident N_2 is achieved *via* supersonic molecular beam fluxes of N_2 molecules. An in-line and *in situ* scanning tunneling microscope (STM) provides atomic-scale visualization of surface products. Analysis of the spatial distributions of N adatoms from the same molecule as a function of incident energy and angle provides insight to the energy dissipation pathways such as energy transfer to phonons and electron hole-pair excitations following dissociative chemisorption.

Exchanging a resistively heated pinhole nozzle for an RF plasma source, the molecular beam can also deliver supersonic ground state atomic oxygen. The site-specificity of atomic oxygen binding on the graphene-Ru(0001) moiré lattice is shown here to be coverage dependent. Furthermore, the stability of oxygen species on epitaxial graphene varies with the number of proximal O atoms as shown by STM imaging. Effects of multiparticle interactions appear in pair-distribution functions, oxygen binding distributions on the moiré lattice, and the diffusivity of O atoms. Comparison of monolayer versus bilayer graphene additionally demonstrates the role that spin-flipping dynamics play in the adsorption of $O(^3P)$ on graphitic surfaces. Overall, results provide insight to the stability of moiré-patterned two-dimensional materials which show promise as platforms for next-generation quantum materials and catalysts.

9:00am SS+2D-TuM-5 Oxygen Diffusion Dynamics on a Rh(111)/(322) Multifaceted Surface, Alexis Gonzalez, Elizabeth Serna-Sanchez, Maxwell Gillum, Stephanie Danahey, Dan Killelea, Loyola University Chicago

The diffusion of oxygen on multifaceted Rhodium (Rh) crystals is of significant interest due to the importance of Rh in heterogeneously catalyzed reactions, such as surface-facilitated oxidation reactions. In this study, we investigate the diffusion dynamics and oxygen species on these two surfaces using temperature-programmed desorption (TPD) and low-energy electron diffraction (LEED) techniques. Despite the structural differences between the (111) and (322) facets, our experiments reveal that the oxygen species on both surfaces are similar, with oxygen existing on the surface as atomic oxygen shortly after adsorption. TPD experiments show that oxygen desorption occurs at comparable temperatures on both surfaces, indicating similar binding energies for oxygen species on each facet. However, LEED shows that there may be different structures forming on either side of the crystal and the orientation of oxygen species are dissimilar. These findings suggest that the oxygen species formed on both (111) and (322) surfaces are essentially the same even though the two

surfaces have different atomic arrangements. This observation highlights the importance of other factors, such as surface defects and temperature, in governing the oxygen diffusion process. The study provides information on how surface structure influences the diffusion behavior of oxygen on Rh crystals and emphasizes the need for considering both surface morphology and adsorption characteristics in the design of catalytic materials.

9:15am SS+2D-TuM-6 CO Adsorption on Gr/Ni(111) Single Point Defects, Francesco Armillotta³, EPFL, Switzerland

Single atom catalysis (SAC) has attracted great interest due to its potential high selectivity, reduced material consumption, and activity. However, a detailed atomistic insight into the active sites and reaction details is still limited, which is fundamental for the understanding and engineering of SAC. We show that even simple molecular adsorption and desorption can reveal non-trivial aspects that affect, for example, the overall sticking probability. We study the CO chemisorption on a model single atom catalyst, where single Co and Ni atoms are adsorbed (or stabilized) in graphene (Gr) vacancies during graphene growth by chemical vapor deposition (CVD) on a Ni single crystal.^{1,2} The study is carried out using a custom designed high-resolution Thermal Desorption Spectroscopy (TDS) instrument in combination with a Variable Temperature STM. In particular, the TDS instrument allows for the study of active sites with a very low surface coverage, of the order of 10^{-3} monolayers. We provide a thorough characterization of the active sites for CO adsorption on Gr (Fig. 1a).^{3,5} In particular, the identification of Ni and Co in Gr di- and tri-vacancies, the dependence on the azimuthal Gr orientation, and an unreported CO chemisorbed state on pristine Gr. We show that the nature of the single point defect can have a huge impact on the CO adsorption probability, accounting for differences up to a factor of 10^4 . We explain the existence of very different main adsorption channels, such as a reverse spillover (Fig. 1b) and activated adsorption *via* a precursor state (Fig. 1c), both known for extended surfaces but never reported for single atoms.^{4,5} The well-defined geometries allow for direct and reliable comparison with *ab initio* simulations, revealing important thermodynamic and kinetic aspects.

(1) Chesnyak, V.; Perilli, D.; Panighel, M.; Namar, A.; Markevich, A.; Bui, T. A.; Ugolotti, A.; Farooq, A.; Stredansky, M.; Kofler, C.; et al. *Sci. Adv.* **2024**, *10* (45), eado8956

(2) Carnevali, V.; Patera, L. L.; Prandini, G.; Jugovac, M.; Modesti, S.; Comelli, G.; Peressi, M.; Africh, C. *Nanoscale* **2019**, *11* (21), 10358–10364

(3) Perilli, D.; Chesnyak, V.; Ugolotti, A.; Panighel, M.; Vigneri, S.; Armillotta, F.; Naderasli, P.; Stredansky, M.; Schied, M.; Lacovig, P.; et al. *Angew Chem Int Ed* **2025**, e202421757

(4) Armillotta, F.; Naderasli, P.; Chesnyak, V.; Brune, H., *J. Phys. Chem. C* **2025**, *129* (10), 4915–4922

(5) Armillotta, F.; Naderasli, P.; Chesnyak, V.; Panighel, M.; Carnevali, V.; Africh, C.; Peressi, M.; Brune, H. Carbon monoxide adsorption on intrinsically defected graphene on nickel *in preparation*

9:30am SS+2D-TuM-7 Spin and Transport in Graphene Nanostructures with π -Magnetism, Thomas Frederiksen, Donostia International Physics Center (DIPC), Spain

INVITED

The emergence of π -magnetism in open-shell graphene nanostructures—long anticipated from theoretical models—has seen remarkable experimental breakthroughs in recent years, driven by advances in on-surface synthesis and scanning probe techniques. These developments have enabled the realization and manipulation of localized spin states with atomic precision, opening new opportunities in spin-dependent phenomena at the nanoscale. In this talk, I will highlight recent progress in understanding and engineering π -magnetism in graphene nanostructures through three complementary theoretical perspectives. First, I will discuss theoretical efforts to interpret scanning tunneling microscopy (STM) experiments that probe spin-resolved phenomena in atomically precise nanographenes. Second, I will present theoretical results on hyperfine interactions in π -magnetic nanographenes, where significant and anisotropic couplings suggest promising avenues for detection via techniques such as ESR-STM and for studying coherent nuclear dynamics. Finally, I will introduce a proposal for a spin-polarizing electron beam splitter based on crossed graphene nanoribbons, showing how such structures could serve as building blocks for spintronics and quantum interference devices. Together, these directions underscore the potential of

¹ AVS Dorothy M. and Earl S. Hoffman Awardee

² SSD Morton S. Traum Award Finalist

Tuesday Morning, September 23, 2025

³ JVST Highlighted Talk

Tuesday Morning, September 23, 2025

graphene nanostructures for both fundamental quantum science and future quantum technologies.

11:00am SS+2D-TuM-13 Simultaneous Electron Spectroscopy and X-Ray Scattering on Model Ceria Catalysts, Baran Eren, Weizmann Institute of Science, Israel

INVITED

Heterogeneous catalysis is a timely and critical research field in basic and applied energy sciences, due to its potential to provide solutions to global environmental issues. However, there is still a lack of a profound understanding of the molecular and structural processes at the interfaces between solids and reactant gases. A detailed understanding of the correlation between the chemistry, structure, and function in these materials requires a multimodal investigation. Over the past few years, scientists at the Advanced Light Source, the Berkeley synchrotron facility, have developed a unique setup attached to an X-ray beamline where chemically-sensitive ambient pressure X-ray photoelectron spectroscopy (APXPS) and structure-sensitive grazing incidence X-ray scattering (GIXS) experiments can be performed simultaneously. Here, we showcase that this tool can provide mechanistic insights that are unparalleled in the literature.

This novel approach allows us to probe the changing surface and bulk chemistry, and surface and bulk structure of the model ceria catalysts in the presence of H₂ and CO₂ gases. In addition to the method itself, the electron density, surface chemistry, and roughness trends observed in ceria during the reaction will be discussed in this talk. Access to such a variety of data from working catalysts in a single experiment can have far-reaching implications, because changes in surface roughness, ability to store hydrogen in the bulk in various forms, and the chemical state of the surface, which all depend on the reactive environment, can directly affect the catalyst performance.

11:30am SS+2D-TuM-15 Vibrational Spectroscopic Identification of Carbon Adsorbed Beneath the Metal Surface, Santosh K. Singh¹, Volkan Cinar, Sylvia T. Ceyer, Massachusetts Institute of Technology

Carbon dissolved in transition metals, also known as subsurface or bulk carbon, plays a critically important role in many technological processes. Subsurface carbon atoms have been recognized as essential for the catalytic growth of carbon nanotubes, graphene synthesis, and operation of direct carbon fuel cells. Despite the recognition of carbon bound beneath the surface of a metal as a crucial species in many chemical and catalytic processes, it has not been identified spectroscopically using methods that do not destroy the sample. We report the first vibrational spectroscopic identification of bulk carbon in a Au-Ni(111) surface alloy by high-resolution electron energy loss spectroscopy (HREELS) and its unambiguous synthesis via collision-induced absorption (CIA). The vibrational modes of carbon embedded beneath the surface alloy are shown to be distinguishable from surface-bound carbon based on their intensity dependence on the incident electron energy. Three distinct peak features, centered around 690, 500, and 380 cm⁻¹, are assigned to modes of subsurface carbon atoms that are located at octahedral sites and triangular misfit dislocation loops of the second layer of Au/Ni surface alloy. Additional confirmation of these assignments come from their appearance after CIA experiments, in which surface bound carbon atoms are hammered into the bulk by collisions with energetic gas phase Xe atoms, accompanied by a decreased intensity of the surface carbon mode at 540 cm⁻¹. This work reports for the first time a new method to spectroscopically identify interstitial carbon below the surface of a solid metal and a non-thermal method to synthesize it.

11:45am SS+2D-TuM-16 Pt-Sn Catalysts for Selective Hydrogenation of Furfural, Donna Chen, Sharfa Farzandh, University of South Carolina; Wenrui Chai, Katherine Mader, Graeme Henkelman, University of Texas at Austin; Mengxiong Qiao, University of South Carolina

The production of high value chemicals from biomass is an attractive option for reducing economic dependence on fossil fuels, and the development of new catalysts for selective transformation of highly functionalized biomass derivatives has become an important area of research. For example, furfural is a platform chemical derived from biomass reforming, and catalysts are needed for the desired selective hydrogenation of furfural to furfuryl alcohol, which is a high-value chemical used in adhesives, resins, and coatings. In this work, model Pt-Sn surface alloy catalysts were prepared in ultrahigh vacuum (UHV) by vapor-depositing Sn on Pt(111) and annealing to various temperatures. Specifically, a $\sqrt{3}\times\sqrt{3}$ -R30 low energy electron diffraction pattern was observed after annealing one monolayer of Sn on Pt(111) to 800 K, while a p(2x2) pattern was observed after annealing

to 1000 K. Low energy ion scattering studies confirmed that these two ordered overlayers have compositions roughly corresponding to Pt₂Sn and Pt₃Sn, respectively. Furfural hydrogenation was studied in a microreactor coupled directly to the UHV chamber under reaction conditions of 0.1% furfural/balance H₂ at 160 °C. On Pt(111), conversion was low (~5%), with THF and furan as the main products and no furfuryl alcohol produced. However, on the p(2x2) surface, the desired furfuryl alcohol product was formed with ~70% selectivity, and conversion was ten times higher than on Pt(111). Furfuryl alcohol was also observed on the $\sqrt{3}\times\sqrt{3}$ -R30 alloy surface, but the yield was only 25% of that on the p(2x2) surface. Furthermore, furfuryl alcohol production was even lower on annealed Pt-Sn surfaces with lower Sn coverages or unannealed surfaces with the same coverage. Density functional theory and minimum energy pathway calculations showed that in the first hydrogenation step, hydrogenation at the carbonyl oxygen is both kinetically and thermodynamically favored on the Pt, Pt₃Sn, and Pt₂Sn surfaces. In the second step, hydrogenation at the C-OH carbon has a low energy barrier (0.3 eV) on the Pt₃Sn surface but is not favorable on Pt(111) or Pt₂Sn (>0.8 eV). These differences are explained by a combination of electronic effects that decrease the binding energy of hydrogen on the Pt-Sn alloy surface and adsorption geometries. Furfural hydrogenation was also studied on bimetallic Pt-Sn clusters supported on TiO₂(110), but these surfaces were always rich in Sn and not active for furfuryl alcohol formation.

12:00pm SS+2D-TuM-17 Bimodal Sputter Depletion of Adsorbed Na from Granular, Regolith-Like, Olivine Targets, Adam Woodson, Cassandra Morel, Noah Jäggli, Catherine Dukes, University of Virginia

Regolith roughness is expected to modulate the sputter flux of surface atoms into the exospheres of airless bodies such as Mercury. Studies have shown that roughness—from the nanometer scale upward—promotes redeposition and diminishes total sputtering yields. Experiments involving irradiation of minerals and single-element powders demonstrate yield reductions anywhere from 15% to 70% as compared to smooth targets, but the grain size dependence of this effect has not been adequately parameterized. Understanding this mechanism is therefore of critical importance for quantifying desorption and sputter ejection and for predicting the relative contributions of release processes from planetary surfaces.

We measured the sputter depletion of adsorbed Na from polished natural olivine and from synthetic granular forsterite targets with narrow grain size distributions from 45 µm up to 520 µm. Na vapor was deposited onto each target in an ultrahigh vacuum system and then irradiated at either 15° or 60° incidence (from global surface normal) to prescribed fluence steps using 4 keV He⁺ ions. All experimental steps were carried out at room temperature (~300 K). After each fluence step an XPS spectrum was acquired and used to quantify the remaining Na surface concentration. Depletion cross sections were then extracted from the concentration vs. fluence data for each target, and sputtering simulations were conducted using SDTrimSP to recreate experimental observations and corroborate target surface structure and stoichiometry.

For the polished targets, Na concentrations exhibited single-exponential decay with increasing fluence, and depletion at 60° incidence outpaced that at 15° as expected from theory. Conversely, for all granular samples the Na concentrations exhibited at least double-exponential decay and depletion occurred more quickly at 15°. We propose that this reflects faster removal of Na that is directly exposed to the incident ion flux, convolved with slower removal of shadowed Na by—primarily—reflected incident ions. We found that the shadowed sodium was sputtered away 10–100 times more slowly than the exposed Na, with a transition from single-exponential to double-exponential decay at some threshold between nanoscale roughness (polished targets) and microscale roughness. These results may help to explain, for example, why current models underestimate the persistence of Na density enhancements in Mercury's dayside exosphere, as observed by the MESSENGER spacecraft's UltraViolet and Visible Spectrometer.

2D Materials

Room 205 ABCD W - Session 2D-TuA

2D Materials: Theory and Applications

Moderator: Kai Xiao, Oak Ridge National Laboratory

5:15pm 2D-TuA-13 Theoretical Study of van der Waals epitaxy of Biayer Silicene on III-Sb substrates, *Kumar Vishal, Hong Huang, Yan Zhuang*, wright state university

Research development of integrated silicon photonics in the mid-infrared (MIR) range has gained considerable momentum over the past decades, driven by its vital applications in biochemical sensing, medicine, and even astronomy communications. However, progress has been hampered by the limitation by the energy bandgap and optical transparency in conventional material. Very recently, it has been reported that 2D bilayer silicon (BLSi) demonstrates unique optical properties across the MIR spectrum. By adjusting the strain, the optical absorptions can be tuned in a wide range of wavelength from 1.5 -11.5 μm . However, experimentally the maximum in-plane strain achieved is $\sim 7\%$ in a lattice-matching epitaxial silicon. Remote- and Van der Waals epitaxy methods can break the lattice-mismatch constraint to obtain single crystal 2D materials, but with an insufficient in-plane strain preserved in the 2D films.

In this work, motivated by the recent achievement of dative epitaxy of single crystalline Cr₅Te₈ on WSe₂ enduring a $\sim 16\%$ lattice mismatch, we conducted a theoretical study based on density function theory (DFT). Our aim is to explore the feasibility of growing BLSi on two III-Sb substrates: GaSb and AlSb. These substrates were chosen due to their ability to provide sufficient in-plane strain (11.92% and 12.23% respectively) to assure energy bandgap opening in BLSi. The generalized gradient approximation (GGA) and the strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA) have been employed in the computation to analyze the chemical bond formation and to optimize the energetically favorable atomic structures. Our findings suggest that Van der Waals epitaxy of BLSi on both of the III-Sb substrates is viable when the substrate's surfaces are terminated with the metallic atoms. By forming the dative bonds between the BLSi and the III-Sb substrates, substantial in-plane strain in BLSi can be preserved, leading to a low buckled BLSi with an opened energy bandgaps.

5:30pm 2D-TuA-14 Tuning Bandgap in Nanoporous Graphene through Molecular Design, *Mamun Sarker, Alexander Sinitskii*, University of Nebraska - Lincoln

Molecular design is a powerful tool for growing graphene nanostructures with atomic precision, enabling control over their electronic and physical properties. Precisely tuning these properties is essential for advancing the next generation of graphene-based 2D electronic devices. In this presentation, I will discuss the on-surface synthesis of novel nanoporous graphene (NPG) materials, whose electronic bandgaps can be tuned from semiconducting to nearly metallic through rational molecular design. These NPGs were synthesized using custom-designed polyaromatic precursors deposited on Au(111) and thermally activated under ultra-high vacuum via surface-assisted chemical reactions. Scanning tunneling microscopy (STM) reveals the structural integrity and periodicity of nanoporous networks. Scanning tunneling spectroscopy (STS), in combination with density functional theory (DFT), shows that strategic modifications in the pore size, topology, and connectivity can reduce the bandgap to as low as 0.05 eV, approaching metallic behavior. This work not only demonstrates the feasibility of tailoring graphene's electronic structure with sub-nanometer precision but also establishes a versatile platform for engineering low-bandgap 2D materials.

5:45pm 2D-TuA-15 How Transparent Is Graphene? An Analytical Model for Remote Epitaxy, *Jason Kawasaki*, University of Wisconsin Madison

We propose an analytical model for the remote bonding potential of the substrate ϕ_{remote} that permeates through graphene during remote epitaxy. Our model, based on a Morse interatomic potential, includes the attenuation due to (1) the increased separation between film and substrate and (2) free carrier screening from graphene. Compared with previous slab density functional theory calculations, which use the electrostatic potential as a proxy for bonding, our analytical model provides a more direct description of bonding, explicitly includes screening (which is often ignored), and is based on simple, interpretable, and well benchmarked parameters. We show that the magnitude of $\phi_{\text{remote}}(z)$ for typical semiconductor and oxide substrates is few meV or smaller, similar to the van der Waals potential of graphene. This suggests that the potential of graphene, plus the interference between the

remote substrate and graphene potentials, must be considered when interpreting experiments on remote epitaxy. We use our model to interpret previous experiments from the remote epitaxy and related literature. True remote effects are often obscured by defect-seeded nucleation, e.g. pinhole epitaxy, that mimics the macroscopic behavior of idealized remote epitaxy. Our model also points to tests, based on tunable screening and spatial extent of the substrate potential, that may increase the strength of the remote potential towards the more idealized picture.

2D Materials

Room 208 W - Session 2D+EM+NS+QS+SS+TF-WeA

2D Materials: Synthesis and Processing

Moderator: Tiancong Zhu, Purdue University

2:15pm **2D+EM+NS+QS+SS+TF-WeA-1 Process Discovery for Quantum Materials, *Stephan Hofmann***, University of Cambridge, UK **INVITED**

Effective heterogeneous integration of low-dimensional nanomaterials in applications ranging from quantum electronics to biomedical devices requires a detailed understanding of different formation and interfacing reactions and the ability to synergize these processes. Process development largely still follows an Edisonian trial-and-error approach, blind and constrained by conventional reactors. This is not only wasteful and frustratingly slow, but hinders scientific breakthroughs in crystal growth and innovation in new deposition technology. This talk will focus on our cross-correlative, high-throughput operando approaches and combinatorial close-space sublimation (CSS) based process design to accelerate process discovery. We show operando spectroscopic imaging ellipsometry and scanning electron microscopy with machine-learning assisted analysis and parameter space exploration for salt-assisted WS_2 layer CVD and TMD oxidation phenomena, and how direct kinetic process data can open data driven approaches to advance the required understanding of underpinning mechanisms.[1] We show that CSS is a highly promising alternative to conventional powder-furnace chemical vapour deposition, offering superior efficiency, precise structural control, scalability, and adaptable process designs. As part of processability and stability assessment, we also explore oxidation kinetics of TMD materials, [2] aided by atomistic modelling using machine-learned force fields.[3]

[1] Yang et al., Chem. Mat. 37, 989 (2025)

[2] Sahota et al., ACS Appl. Nano Mat., asap (2025)

[3] Gsanyi et al., arXiv:2401.00096, 2023

2:45pm **2D+EM+NS+QS+SS+TF-WeA-3 Selective Area Epitaxy of van der Waals Materials, *Ryan Trice***¹, *Stephanie Law*, Penn State University

Two-dimensional (2D) van der Waals (vdW) materials are interesting for a variety of applications, ranging from optoelectronics and photocatalysis to energy storage and topological devices. However, vdW materials synthesized using common techniques like chemical or physical vapor deposition often have a high density of growth-related defects, including grain boundaries, twin defects, pyramidal growth, and spiral defects. While pyramidal growth can be minimized through higher growth temperatures, grain boundaries, twin defects, and spiral defects are much harder to overcome. For many applications, especially in electronics and optics, these defects lead to non-radiative recombination, electron scattering, and other undesirable effects. Furthermore, the fabrication of 2D materials into quantum dots (QDs) through bottom-up methods faces problems with precise location placement and polydispersity in the QDs' diameters. This makes the QDs difficult to characterize and is not ideal for most quantum computing and optical setups. Top-down nanofabrication approaches fix this issue but often cause significant damage to the surfaces or edges of the materials. To address these issues, we used molecular beam epitaxy (MBE) combined with selective area epitaxy (SAE) to grow Bi_2Se_3 thin films. SAE is a technique in which thin films nucleate and grow in defined areas on a wafer. This is done using a patterned mask where growth conditions are selected such that the film will only nucleate on the substrate.

In this talk, we will describe SAE growth of Bi_2Se_3 on Al_2O_3 (0001) and Si (111) substrates using an atomic layer deposition SiO_2 mask. Etching of the SiO_2 mask was done with a wet chemical etch, resulting in micron-scale holes of various shapes and sizes. The processed substrates were then loaded into an MBE chamber for the growth of the Bi_2Se_3 film. First, we will discuss the effects of different substrate temperatures on the selective growth of the Bi_2Se_3 thin films. Second, we will discuss the geometric influence of various shaped patterns on the crystal quality of the selectively grown films. Third, we will look at the effect and viability of nano-scale patterns for selective growth of vdW materials. Further studies will focus on using different materials for the substrate and mask. This approach could allow us to grow wafer-scale, defect-free 2D vdW QDs at specified areas on the wafer, thereby increasing the scalability and applicability of these materials to real-world challenges.

3:00pm **2D+EM+NS+QS+SS+TF-WeA-4 Precision Synthesis and Conversion of 2D Materials by Pulsed Laser Deposition with in Situ Diagnostics, *Daniel T. Yimam***², *Sumner B. Harris*, Oak Ridge National Laboratory, USA; *Austin Houston*, University of Tennessee Knoxville; *Ivan Vlassiouk*, Oak Ridge National Laboratory, USA; *Alexander Poretzky*, Oak Ridge National Laboratory; *Gerd Duscher*, University of Tennessee Knoxville; *Kai Xiao*, Oak Ridge National Laboratory, USA; *David B. Geohegan*, University of Tennessee Knoxville

Over the past few decades, 2D monolayers and heterostructures have become central to nanoscience, offering promising applications in electronics, sensing, and future computing. In addition to their exciting functional properties, significant progress has been made in their bottom-up synthesis and subsequent processing. Techniques such as encapsulation, doping, and implantation in atomically thin 2D materials are crucial to transitioning them from fundamental research to scalable, real-world applications, while enabling the emergence of novel properties. However, the ultrathin nature that makes 2D materials attractive also poses substantial challenges for traditional plasma-based processing methods. To fully harness the potential, it is essential to develop reliable processing techniques that offer precise control and reproducibility.

Pulsed laser deposition (PLD) is a promising non-equilibrium method that allows precise control over the kinetic energy (KE) of ablated species. In this work, we investigate plasma plume interactions with 2D materials using *in situ* plasma diagnostics and optical characterization tools. We demonstrate that a deep understanding and control of plasma plume dynamics enables new approaches for 2D material engineering, including the formation of Janus monolayers, metal atom implantation, and encapsulation with minimal damage. Our approach allows for low temperature substitution and implantation of foreign atoms, such as chalcogens and metals, facilitating the selective synthesis of Janus monolayers and alloys. These findings highlight the potential of PLD to drive the practical advancements in 2D materials for microelectronics and quantum information science.

This work was supported by the U.S. DOE, Office of Science, Materials Sciences and Engineering Division and the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

Keywords: Pulsed laser deposition, chalcogenide substitution, 2D materials, implantation, in situ diagnostics.

3:15pm **2D+EM+NS+QS+SS+TF-WeA-5 AVS Peter Mark Memorial Award Talk: Exploiting Thin Film Phase Diagrams for Synthesizing 2D Transition Metal Dichalcogenides, *Nicholas R. Glavin***, Air Force Research Laboratory **INVITED**

Synthesis of 2D transition metal dichalcogenides for specific applications in electronics, optoelectronic, and advanced coatings remains a critical bottleneck for many industrial applications. In this talk, we will highlight leveraging thin film phase diagrams to rapidly explore the vast parameter space in synthesizing these novel materials. This technique uses laser processing to locally modify regions within the film and coupled with high throughput characterization, rapidly assesses material state and quality for next generation sensors, optical coatings, and low power electronics.

4:15pm **2D+EM+NS+QS+SS+TF-WeA-9 Designer van der Waals Materials for Quantum Optical Emission, *Shengxi Huang, Wenjing Wu***, Rice University **INVITED**

Designer van der Waals (vdW) materials offers enormous opportunities to tune material properties for various applications. Isolated, optically-active defects generated in vdW materials could lead to single photon emission. 2D vdW materials as host materials for single photon emission hold various advantages, such as high optical extraction efficiency from the atomically-thin layered materials, and readiness to integrate with on-chip photonic and electronic devices. However, single photon emission from 2D vdW materials typically suffers from low purity and lack of controllability, due to the sensitivity of these atomically-thin materials to external dielectric environments, surface defects and adsorbents, and strains and wrinkles introduced during material processing. This talk introduces our recent efforts to improve the single photon purity and controllability in vdW materials. We developed novel defect structures that can overcome several current issues, and explored their electronic structure and tunability in optical emission. Through a combination of approaches, including strain engineering, heterostacking, employing optical selection rules for excitation and detection, optimization of material synthesis and handling, we were able to achieve high purity (> 98%) for single photons emitted from 2D

¹ JVST Highlighted Talk

² JVST Highlighted Talk

transition metal dichalcogenides (TMDs) at cryogenic temperature and in hBN at room temperature. This work provides deep insights into the electronic, spin, and valley properties of TMDs and hBN. It also paves the way towards the application of 2D vdW materials for quantum optical applications. The materials engineering approaches developed here can be applied to the optimization of other optical and quantum materials.

4:45pm **2D+EM+NS+QS+SS+TF-WeA-11 Macroscopic Tin Monochalcogenide Van Der Waals Ferroics: Growth, Domain Structures, Curie Temperatures and Lateral Heterostructures, Eli Sutter, Peter Sutter, University of Nebraska - Lincoln**

2D and layered van der Waals crystals present opportunities for creating new families of ferroics with switchable electric polarization, elastic strain, or magnetic order at thicknesses down to the single-layer limit. Synthesis, however, typically leads to small crystals with sizes ranging from below 100 nm (e.g., for SnTe ferroelectrics) to a few μm (e.g., for SnSe ferroelectrics). The limited size and proximity to edges affects the ferroelectric and ferroelastic domain patterns, restricts the experimental methods available to probe emerging properties, and severely limits the ability to fabricate complex device architectures required for accessing functionalities in van der Waals ferroelectrics.

Here, we report the realization of in-plane ferroelectric few-layer crystals of the monochalcogenides tin(II) sulfide and selenide (SnS, SnSe) whose linear dimensions exceed the current state of the art by up to one order of magnitude. Such large crystals allow the investigation of ferroic domain patterns that are unaffected by edges and finite size effects. Analysis of the abundant stripe domains by electron microscopy and nanobeam electron diffraction shows two distinct domain types, twin domains separated by positively charged walls with alternating head-to-head and tail-to-tail polarization as well as not previously observed purely rotational domains connected by neutral domain walls with head-to-tail dipoles. Access to large ultrathin crystals allowed determining the Curie temperatures of few-layer SnSe¹ and SnS van der Waals ferroelectrics.

Finally, we demonstrate the integration of the ultrathin ferroelectric SnSe and SnS into lateral heterostructures.² A two-step process produces crystals comprising an SnSe core laterally joined to an SnS edge-band, as confirmed by Raman spectroscopy, electron microscopy imaging, and diffraction. The ability of the lateral interface to direct excited carriers, probed by cathodoluminescence, shows electron transfer over 560 nm diffusion length from the SnS edge-band. The ferroelectric heterostructures adopt two domain configurations, with domains either constrained to the SnSe core or propagating across the entire SnSe-SnS flakes.

The combined results demonstrate industrial scale in-plane ferroelectrics as well as multifunctional van der Waals heterostructures, presenting extraordinary opportunities for manipulating ferroelectric domain patterns and carrier flow.

(1) Sutter, E.; Ghimire, P.; Sutter, P. *J Am Chem Soc* **2024**, *146* (46), 31961-31968. DOI: 10.1021/jacs.4c11558.

(2) Sutter, E.; Ghimire, P.; Sutter, P. *ACS Nano* **2024**, *18* (44), 30829-30837. DOI: 10.1021/acsnano.4c11341.

5:00pm **2D+EM+NS+QS+SS+TF-WeA-12 Machine Learning Analysis of Molecular Beam Epitaxy Growth Conditions, Mingyu Yu, Ryan Trice, Isaiah Moses, Wesley Reinhart, Stephanie Law, Penn State University**

Machine learning models hold the potential to explore parameter space autonomously, quickly establish process-performance relationships, and diagnose material synthesis in real time. This reduces reliance on manual intervention in parameter space exploration, enabling more precise and efficient mechanistic control. For molecular beam epitaxy (MBE), despite its breakthroughs in materials synthesis, its stringent growth conditions and complex epitaxial mechanisms make the process of optimizing growth process time-consuming and expensive. Therefore, leveraging machine learning to develop autonomous MBE growth platforms presents a highly promising prospect. Our study on the multi-modal machine learning-guided MBE synthesis is based on a comprehensive high-quality dataset of GaSe thin films grown on GaAs (111)B substrates. GaSe is an emerging two-dimensional semiconductor material with intriguing properties, including thickness-tunable bandgaps, nonlinear optical behaviors, and intrinsic p-type conductivity. Moreover, as a representative member of the van der Waals (vdW) chalcogenide semiconductor family, insights gained from studying GaSe can be extended to other vdW chalcogenides. In this work, we aim to leverage machine learning to analyze the relationships between

growth conditions (Ga flux, Se:Ga flux ratio, and substrate temperature) and the resulting sample quality, as well as the correlations among various characterization results including in situ RHEED patterns and ex situ x-ray diffraction rocking curve full-width at half maximum (FWHM) and atomic force microscopy (AFM) root mean square (RMS) roughness. Unsupervised learning on RHEED patterns reveals a well-defined boundary between high- and low-quality samples, capturing physically meaningful features. Mutual information analysis shows a strong correlation between RHEED embeddings and rocking curve FWHM, while the correlation with AFM RMS roughness is weak. Among key growth conditions, growth rate most strongly influences FWHM, whereas the Se:Ga flux ratio primarily affects RMS roughness and the RHEED embeddings. Supervised learning models trained to predict FWHM and RMS roughness demonstrate moderate accuracy, with significant improvement achieved by incorporating RHEED embeddings. Furthermore, anomaly detection via residual analysis in supervised learning aligns well with unsupervised classification from RHEED, reinforcing the reliability of the predictive models. This study establishes a data-driven framework for machine learning-assisted MBE, paving the way for real-time process control and accelerated optimization of thin-film synthesis.

5:15pm **2D+EM+NS+QS+SS+TF-WeA-13 Promoting Crystallographic Alignment in SnSe Thin Films using Step Edges on MgO by MBE, Jonathan Chin, Marshall Frye, Joshua Wahl, Kayla Chuong, Georgia Institute of Technology; Mengyi Wang, Derrick Liu, Pennsylvania State University; Mingyu Yu, University of Delaware; Qihua Zhang, Nadire Nayir, Adri van Duin, Maria Hilse, Stephanie Law, Pennsylvania State University; Lauren Garten, Georgia Institute of Technology**

SnSe is a van der Waals material that can be scaled down to two dimensions,¹ making it a promising candidate for nanoelectronics such as field effect transistors (FETs).² SnSe in the orthorhombic *Pnma* structure exhibits significant electrical anisotropy where the carrier mobility is 45% higher along the [010] direction than the [001] direction in plane,³ making it necessary to control the in-plane alignment of 2D films for integration into electronic devices. SnSe has been shown to form planar coverage on (100) MgO,⁴ with which it has a 1.4% and 5.5% lattice mismatch along the [010] and [001] directions, respectively. However, despite the distinct axial lattice matches, in-situ reflective high-energy electron diffraction (RHEED) shows no preferential SnSe film alignment for films deposited on uncleaned MgO. Therefore, to promote orientation control, we cleaved and annealed the MgO substrates to produce step edges along the surface to increase the local surface energy, thereby encouraging atomic adsorption and alignment. SnSe thin films were then deposited from individual Sn and Se effusion cells via molecular beam epitaxy (MBE) onto the prepared MgO substrates heated to 280 °C for 1-5 minutes with a 1.35:1.00 Se:Sn flux ratio at a 0.083 Å/s growth rate to track the nucleation and growth of SnSe grains. The phase of the SnSe films was confirmed by Raman spectroscopy, exhibiting the characteristic A_g^2 , B_{3g} , A_g^3 , and A_g^4 phonon modes.⁵ In-situ RHEED confirmed the in-plane alignment along the [010] and [001] by RHEED relative to the [100] substrate, matching theory projections made using reactive force field (ReaxFF) simulations. Additionally, atomic force microscopy (AFM) shows SnSe grains nucleating at step edges on MgO, while scanning transmission electron microscopy (STEM) reveals how the aligned SnSe grains propagate laterally off step edges, maintaining crystallographic alignment throughout the film layer. Overall, our results demonstrate that SnSe grains preferentially nucleate along the step edges produced parallel to the [100] edge of the MgO substrates. The alignment of a 2D vdW film facilitated by step edge formation demonstrates how to achieve orientated depositions of similar anisotropic vdW films on a substrate of choice, ultimately facilitating the manufacture of 2D nanoscale electronic devices.

1. Zhang, L.-C. *et al. Sci. Rep.* **6**, 19830 (2016).

2. Chhowalla, M. *et al. Nat. Rev. Mater.* **1**, 1–15 (2016).

3. Zhou, M. *et al. J. Mater. Chem.* **5**, 1247–1254 (2017).

4. Chin, J. R. *et al. Nanoscale* **15**, 9973–9984 (2023).

5. Wu, P. *et al. New J. Phys.* **22**, 083083 (2020).

5:30pm **2D+EM+NS+QS+SS+TF-WeA-14 Synthesis of Millimeter-Scale Single-Crystal α -MoO₃ Nanosheets on Sapphire, Ryan Spangler, Pennsylvania State University; Thiago Arnaud, Joshua Caldwell, Vanderbilt University; Jon-Paul Maria, Pennsylvania State University**

α -MoO₃ is a van der Waals layered semiconductor with biaxial anisotropy that has recently gained interest as an emerging 2D material with a wide band gap (~3 eV), large work function, and high permittivity. Additionally, α -

Wednesday Afternoon, September 24, 2025

MoO₃ exhibits extreme anisotropy of the dielectric function, enabling in-plane and out-of-plane elliptic or even hyperbolic behavior at various wavelengths. Therefore, α -MoO₃ also possesses great potential for nanophotonics through the low-loss and directional propagation of hyperbolic phonon polaritons, which result from the interaction of light with lattice vibrations in highly anisotropic polar materials. However, the lack of single-crystal thin film growth techniques limits further advancement of α -MoO₃. In this work, we describe a process for the growth of ultra-large, thin, and atomically smooth single crystals of α -MoO₃ directly on *a*-plane sapphire using an alkali-assisted physical vapor transport method. Important parameters necessary for high-quality growth to be discussed include substrate selection, alkali-to-MoO₃ ratio, and substrate temperature. The growth proceeds through a vapor-liquid-solid (VLS) mechanism enabled by the formation and liquefaction of low-melting point alkali molybdate phases. This growth mode greatly enhances lateral expansion to several millimeters and thicknesses ranging from hundreds of nm down to <5 nm. This is far thinner and more expansive than crystals grown without alkali metal additives, which can exceed several micrometers in thickness while being limited to a few tens of micrometers in lateral dimensions. The thin alkali-assisted sheets exhibit clean step-flow growth without grain boundaries over mm-scale areas as revealed by atomic force microscopy and polarized optical microscopy. Raman spectroscopy and X-ray diffraction indicate the high crystalline quality of the α -MoO₃ films rivaling that of accessible bulk crystals. We will also investigate the propagation of hyperbolic phonon polaritons using scanning near-field optical microscopy (SNOM) to compare hyperbolic phonon polariton lifetimes to values obtained from exfoliated bulk crystals. We find that this growth technique is suitable for exfoliation-free large-scale single-crystal α -MoO₃ for nanophotonics and other applications.

5:45pm **2D+EM+NS+QS+SS+TF-WeA-15 Studying the Impacts of Growth Temperature and Seeding Promoters on the Structural and Optoelectronic Properties of ReS₂ Grown by CVD**, *Elycia Wright, Kedar Johnson, Amari Gayle, Robin Rousseau, M.K. Indika Senevirathna, Michael D. Williams*, Clark Atlanta University

Rhenium disulfide (ReS₂) is a fascinating member of the transition metal dichalcogenide (TMD) family, which has recently gained significant attention due to its distinct distorted octahedral 1T crystal structure characterized by triclinic symmetry. This distinctive structure shows that ReS₂ holds remarkable properties, including anisotropic electronic, optical, and mechanical characteristics. Unlike other TMDs such as MoS₂, MoSe₂, WS₂, and WSe₂, ReS₂ possesses a band structure that remains consistent regardless of the layer thickness. Due to weak interlayer coupling, it maintains a direct band gap in its bulk and monolayer forms. This unique characteristic makes ReS₂ particularly promising for applications in highly responsive photodetectors. To maximize the potential of ReS₂ for optoelectronic applications, it is essential to address the challenges associated with its anisotropic growth, distorted structure, and weak interlayer interactions. The anisotropic nature of ReS₂ can lead to variations in growth rates in different directions, resulting in multidomain structures that complicate the production of single-crystal ReS₂ on a large scale.

In this study, we will synthesize ReS₂ by chemical vapor deposition (CVD) at various temperatures and utilize seeding promoters to facilitate the growth of single crystals with continuous layers. We will employ advanced techniques such as confocal microscopy, Raman spectroscopy, and photoluminescence spectroscopy to systematically investigate how the growth temperature and seeding promoters affect the structural and optoelectronic properties of ReS₂.

6:00pm **2D+EM+NS+QS+SS+TF-WeA-16 Growth and Characterization of InSe Thin Films on GaAs(111)B and Si(111)**, *Maria Hilse*, Penn State University

Urgent societal and environmental needs have sparked searches for high-mobility 2D materials with sizeable bandgap and decent stability under ambient conditions for use in ultra-low power, ultra-high performance field effect transistors. With a carrier mobility exceeding 1000 cm²/Vs, small electron effective mass, flat electronic band dispersions, excellent optoelectronic, possible ferroelectric properties and a close-to-ideal solar spectrum matched bulk bandgap of 1.26 eV, InSe shows high potential for future use in electronics. Due to the layered nature, and the many members of different polytypes in the InSe materials family, intriguing confinement phenomena and exotic electron-hole coupling mechanisms tunable by the number of single layers add to the potential wealth of properties in InSe.

In this study, InSe thin films were grown by MBE on GaAs(111)B and Si(111). The presence of many InSe phases required a systematic mapping of the growth parameters to identify conditions for single-phase, single-polytype, and single-crystal growth. Through structural characterization in- and ex-situ using reflection high-energy electron and X-ray diffraction, growth conditions for solely gamma-phase, crystalline InSe films were found. Although the structural properties of the films presented nearly unchanged over a small window of growth conditions, the film morphology was seen to sensitively depend on the Se:In flux ratio. Raman spectroscopy confirmed the phase and polytype assignment deduced from large-area structural characterization.

Microstructure analysis, however, revealed a high degree of structural defects in the films. Nano-scale domains of varying single layer stacking sequences, high-angle rotational domains as well as single layers of unusual bonding configuration resulting in a novel InSe polymorph were found in the films. The total number of defects and the general locations of the new polymorph varied in films across GaAs and Si. The highest structural homogeneity was found for InSe films grown on Si.

Density functional theory calculations for a representative selection of the experimentally observed defects confirmed that most defects, including the novel polymorph have formation energies at or below the thermal budget of the MBE synthesis process. Although the bandgaps of all InSe polytypes and polymorphs possess comparable values, large differences were found in their relative offsets. Due to the random distribution of polytypes and polymorphs in the film, our study suggests a high degree of electronic disorder in these films. Electrical transport showed a variable-range hopping-like behavior supporting the hypothesis of electronic disorder.

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, Joy Chao, Haoyang Ni*, Oak Ridge National Laboratory **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 CrCl₃ during cooling. Another is the impact of defects and secondary phases on the magnetic structure evolution of Fe_{5-x}GeTe₂ (FGT-512). Additionally, we have mapped local excitons in moiré-structured MoTe₂. 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 Carlson¹, Swathi Kadaba*, Wake Forest University; *Gabriel Marcus*, Quoharent; *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

¹ JVST Highlighted Talk

Wednesday Afternoon, September 24, 2025

electron energy loss spectroscopy (EELS) and cross sectional TEM. Nanoplates with a diameter range of 0.5 to 1.5 μm and $\sim 6\text{-}15\text{ nm}$ thick were supported on highly ordered 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 Bi_2Te_3 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 Bi_2Te_3 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 Bi_2Te_3 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 $\text{PtBi}_{1.6}$, 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 $\text{PtBi}_{1.6}$) 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. $\text{PtBi}_{1.6}$ 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 with x-ray magnetic circular dichroism (XMCD) to obtain a spatially resolved view on the underlying 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 Zabarjadi*, 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 ($x = \frac{1}{4}$ or $\frac{1}{3}$), the crystalline structure as well as the magnetotransport properties of the TMD system can be tuned. For instance, $\text{Fe}_{1/4}\text{TaS}_2$ has a centrosymmetric 2×2 structure while $\text{Fe}_{1/3}\text{TaS}_2$ has a non-centrosymmetric $\sqrt{3} \times \sqrt{3}$ supercell structure. The magnetic Curie temperature of Fe_xTaS_2 also exhibits a strong dependence on Fe concentration. We evaluate $\text{Fe}_{0.28}\text{TaS}_2$ and 2H-TaS₂ 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. $\text{Fe}_{0.28}\text{TaS}_2$ shows a supercell at 77 K, whereas 2H-TaS₂ 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 $\text{Fe}_{0.28}\text{TaS}_2$ 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 Chirality, Surface Termination and Anti-ferromagnetic Alignment in Fe(III) Spin Crossover Salts, Mohammad Zaid Zaz**, 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 $[\text{Fe}(\text{qsal})_2\text{Ni}(\text{dmit})_2]$ where, $\text{qsal} = \text{N}(\text{8quinolyl})\text{salicylaldimine}$, and $\text{dmit}^{2-} = 1,3\text{-dithiol-2-thione-4,5-}$

Wednesday Afternoon, September 24, 2025

dithiolato. We employ spatially resolved Fe-L_{3,2} 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-L_{3,2} edge X-ray absorption spectroscopy. Finally, we investigate the antiferromagnetic alignment in this system by X-ray magnetic circular dichroism measurements at the Fe and Ni core.

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 SiO₂ 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*, Oak Ridge National Laboratory

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 TaWSe₂ single crystals. STM topography reveals triangular clusters of Ta atoms embedded within W-rich regions of TaWSe₂. 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.

2D Materials

Room 208 W - Session
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM

2D Materials: Optoelectronics and Moire Excitons

Moderator: Daniel Yimam, Oak Ridge National Laboratory

8:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1 Probing the Ultrafast Charge Dynamics and Exciton Emission from Single Atomic Defects in 2D Semiconductors by Lightwave-Driven STM**, *Laric Bobzien, Lysander Huberich, Jonas Allerbeck, Eve Ammerman, Nils Krane, Andres Ortega-Guerrero, Carlo Pignedoli, Oliver Gröning*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland; *Joshua A. Robinson*, The Pennsylvania State University; *Bruno Schuler*, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland **INVITED** Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. This talk explores the intriguing physics of single point defects in transition metal dichalcogenide (TMD) monolayers, investigated through atomically resolved scanning probe microscopy.

We have determined the layer-dependent charge transfer lifetimes of selenium vacancies in WSe_2 on graphene substrates, spanning picosecond to nanosecond timescales [1]. By leveraging our recently developed lightwave-driven scanning tunneling microscope (THz-STM) [2,3], we could probe the ultrafast charge dynamics on the atomic scale. Time-domain sampling with a THz pump-THz probe scheme enabled capturing atomic-scale snapshots of transient Coulomb blockade, a hallmark of charge transport mediated by quantized defect states [4].

Moreover, the extended charge state lifetimes provided by hBN decoupling layers facilitated the local, electrical stimulation of excitonic emission from pristine MoS_2 and individual charged defects via STM luminescence (STML).

By combining the structural and electronic properties accessible by conventional scanning probe microscopy with the optical fingerprint from STML and the excited-state dynamics revealed through pump-probe THz-STM, we gain a comprehensive microscopic understanding of localized quantum states in low-dimensional materials.

References:

- [1] L. Bobzien et al. Phys. Rev. Lett. (accepted, arxiv: 2407.04508)
- [2] J. Allerbeck et al. ACS Photonics 10, 3888 (2023)
- [3] L. Bobzien et al. APL Mater. 12, 051110 (2024)
- [4] J. Allerbeck et al. arXiv:2412.13718 (2024)
- [5] L. Huberich et al. (in preparation)

8:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3 Many-Body Effects on Excitons, Trions, and Defect-Bound States in 2D Materials**, *Kai Xiao, Taegwan Park, Alexander Poretzky*, Oak Ridge National Laboratory, USA; *Xufan Li*, Honda Research Institute; *Kyungnam Kang*, Oak Ridge National Laboratory, USA; *Austin Houston*, University of Tennessee, Knoxville; *Christopher Rouleau, David Geohagan*, Oak Ridge National Laboratory, USA Two-dimensional (2D) materials, particularly transition metal dichalcogenides (TMDs) exhibit strong many-body interactions due to reduced dielectric screening and spatial confinement. These interactions, involving electrons, holes, excitons, phonons, and plasmons, give rise to emergent phenomena distinct from their bulk counterparts. In this talk, I will present our recent investigations into the many-body effects on the optical properties and ultrafast excitonic dynamics of monolayer and bilayer TMDs. Specifically, we synthesized isotopically pure monolayer MoS_2 and highly defective WS_2 via nonequilibrium chemical vapor deposition, enabling a controlled study of isotope effects, defects, and background doping on excitonic behavior. Using ultrafast laser spectroscopy and temperature-dependent optical spectroscopy, we observed pronounced many-body interactions, including exciton-phonon and exciton-electron coupling, which significantly influence exciton energy, dynamics, and light-matter interactions in both monolayer and bilayer TMDs. These strong interactions give rise to novel quantum states and make 2D materials promising platforms for next-generation optoelectronics, quantum information technologies, and fundamental condensed matter physics.

Synthesis science was supported by the U.S. Dept. of Energy, Office of Science, Materials Science and Engineering Division. This work was performed at the Center for Nanophase Materials Sciences, which is a DOE Office of Science User Facility.

8:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4 Proximity-Induced "Magic" Raman Bands in TERS Spectra of MoS_2 / WS_2 @ 1L h-BN-Capped Gold**, *Andrey Krayev*, HORIBA Scientific; *Pavel Valencia Acuna*, PNNL; *Ju-Hyun Jung*, Pohang University of Science and Technology (POSTECH), Republic of Korea; *Cheol-Joo Kim*, POSTECH, Republic of Korea; *Andrew Mannix*, Stanford University; *Eleonora Isotta*, Max Planck Institute for Sustainable Materials, Germany; *Chih-Feng Wang*, PNNL

Recently it was proposed to use the monolayer h-BN – capped gold substrates as an ideal platform for the gap mode TERS and TEPL imaging, that on the one hand, should preserve strong gap mode enhancement of Raman signal due to small thickness (0.3 nm) of the dielectric h-BN layer, and on the other hand preserve strong TEPL response due to de-coupling of 2D semiconductors from the metallic substrate. TERS data collected on mono- and a few-layer-thick crystals of MoS_2 and WS_2 on 1L-h-BN-capped gold show both the TERS and TEPL response, confirming the validity of the proposed approach.

In addition to the enhancement of both the PL and Raman signal, in the course of assessment of TERS/TEPL response of mono- and a few-layer-thick crystals of MoS_2 and WS_2 deposited on 1L h-BN-capped gold we observed in TERS spectra, completely unexpectedly, appearance of Raman bands at about 796 cm^{-1} and 76 cm^{-1} which are not normally observed in regular Raman spectra of h-BN or WS_2/MoS_2 . We can safely state that these "magic" bands belong to h-BN as they appear at the same spectral position in TERS spectra of both the monolayer MoS_2 and WS_2 deposited on the monolayer h-BN capped gold, moreover, the 796 cm^{-1} band often was the strongest band observed in TERS spectra, even stronger than A' mode from WS_2 or MoS_2 . Presence of the transition metal dichalcogenide (TMD) monolayer is mandatory for the appearance of these "magic" bands as they are absent outside of the monolayer TMDs in these samples. Literature search showed that similar (but not identical) phenomenon was observed earlier in h-BN encapsulated $\text{WSe}_2/\text{MoSe}_2$ and WS_2 . There have been several significant differences between our data and the earlier reported one: in our case we have not been able to observe the "magic bands" in MoSe_2 and WSe_2 @ 1L h-BN@Au, while WS_2 monolayers deposited on the same substrate as WSe_2 , showed expected response. More importantly, the excitation laser wavelength dependence in our case was completely different from what was reported earlier: in WS_2 -based samples we observed strong "magic" bands with excitation at 830 nm, 785nm, 594nm, but not 633nm, the wavelength closest to the A exciton in this material. This excitation profile is remarkably reminiscent of the excitation profile of the monolayer WS_2 in intimate contact with silver where we observed strong dip of the intensity of main A' mode in TERS spectra at 633nm excitation wavelength.

We will argue that intricate interaction between the tip-substrate gap plasmon, TMD excitons and most probably, normally mid-IR-active phonons in h-BN is responsible for the appearance of observed "magic" bands.

9:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-5 Correlated Excitons in TMDC Moiré Superlattice**, *Sufei Shi*, Carnegie Mellon University **INVITED**

In a strongly correlated electronic system, Coulomb interactions among electrons dominate over kinetic energy. Recently, two-dimensional (2D) moiré superlattices of van der Waals materials have emerged as a promising platform to study correlated physics and exotic quantum phases in 2D. In transition metal dichalcogenides (TMDCs) based moiré superlattices, the combination of large effective mass and strong moiré coupling renders the easier formation of flat bands and stronger electronic correlation, compared with graphene moiré superlattices. Meanwhile, the strong Coulomb interaction in 2D also leads to tightly bound excitons with large binding energy in TMDCs. In this talk, we will discuss how to use optical spectroscopy to investigate excitonic physics and strongly correlated phenomena in TMDC moiré superlattice, along with correlated exciton states arising from strong interactions.

9:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7 Sub-Stoichiometric Phases in 2D MoTe_2** , *Onyedikachi Alanwoko, Nirasha Rajapakse, Matthias Batzill*, University of South Florida

Atom vacancy formation in crystalline materials is energetically expensive. To lower the energy cost for non-stoichiometry, point defects can condense into energetically more favorable extended defects. Studies on Mo-dichalcogenides have shown that excess Mo is condensed into closed, triangular Mirror Twin Boundary (MTB) loops. These MTBs can form in high densities where the triangular loops connect and form a cross-hatched network of MTBs. Here we show through Scanning Tunneling Microscopy (STM) that periodically ordered MTB networks can obtain a homologous series of sub-stoichiometric MoTe_{2-x} phases. We systematically investigate

the preparation conditions (which include a variation of the growth temperature, Te-desorption by post-growth annealing, and vapor-deposited Mo), enabling the controlled synthesis of these new phases. The different phases require different synthesis procedures, and once formed, these phases appear thermally stable in vacuum. The ability to control and create these different phases of MoTe₂ and other two-dimensional (2D) materials is a promising way of realizing new electronic and chemical properties of 2D materials. Particularly promising is the observation that we can react MoTe₂ with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

11:00am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-13 Microwave Imaging of Excitonic States and Fractional Chern Insulators in 2D Transition Metal Dichalcogenides, Zhurun Ji, SLAC National Accelerator Laboratory/ MIT INVITED

Nanoscale electrodynamics offers a unique perspective on states with bulk-edge correspondence or spatially dependent excitations. I will introduce our latest advancements in optically coupled microwave impedance microscopy, a technique that enhances our capability to explore electrodynamics at the nanometer scale. I will discuss our recent studies utilizing this technology to extract spectroscopic information on exciton excitations within transition metal dichalcogenide systems. Additionally, I will share our recent findings on probing topological and correlated electronic states, specifically the fractional Chern insulator states in twisted TMD bilayers.

11:30am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-15 Control and Properties of Single Dislocations in Van Der Waals Nanowires, Peter Sutter, Eli Sutter, University of Nebraska - Lincoln

Line defects (dislocations) not only govern the mechanical properties of crystalline solids but they can also produce distinct electronic, thermal, and topological effects. Identifying and accessing this functionality requires control over the placement and geometry of single dislocations embedded in a small host volume to maximize emerging effects. We have identified a synthetic route that enables the rational placement and tuning of dislocation in van der Waals nanowires, where the 2D/layered crystal structure limits the possible defect configurations and the nanowire architecture puts single dislocations in close proximity to the entire host volume.¹ While homogeneous layered nanowires carry individual screw dislocations, the synthesis of radial (core-shell) nanowire heterostructures transforms the defect into a mixed (helical) dislocation whose edge-to-screw ratio is continuously tunable via the core-shell lattice mismatch.

Such deterministic control over defects now enables the probing of functionality arising with single dislocations. For example, germanium sulfide van der Waals nanowires carrying single screw dislocations incorporate Eshelby twist and thus adopt a chiral twisted structure,² which for the first time allowed the identification of chirality effects in the photonic properties of a single nanostructure.³ Using cathodoluminescence spectroscopy, whispering gallery modes could be excited and probed to directly compare the photonics of chiral and achiral segments in single nanowires. The data show systematic shifts in energy, which with the help of simulations are assigned to chiral whispering gallery modes in wires hosting a single dislocation.

The ability to design nanomaterials containing individual dislocations with controlled geometry paves the way for identifying a broad range of functional properties of dislocations, with the potential to herald a paradigm shift from the traditional strategy of suppressing dislocations to embracing and harnessing them as core elements of new technologies.

1. P. Sutter, R.R. Unocic, and E. Sutter, *Journal of the American Chemical Society* 145, 20503 (2023); DOI: 10.1021/jacs.3c06469
2. P. Sutter, S. Wimer, and E. Sutter, *Nature* 570, 354 (2019); DOI: 10.1038/s41586-019-1147-x
3. P. Sutter, L. Khosravi-Khorashad, C.V. Ciobanu, and E. Sutter, *Materials Horizons* 10, 3830 (2023); DOI: 10.1039/D3MH00693J

11:45am 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-16 Two-Dimensional Keldysh Theory for Non-Resonant Strong-Field Ionization of Monolayer 2D Materials, Tsing-Hua Her, UNC Charlotte; Che-Hao Chang, NTHU, Taiwan; Kenan Darden, UNC Charlotte; Tsun-Hsu Chang, NTHU, Taiwan; Hsin-Yu Yao, NCCU, Taiwan

Over the past decade, a diverse array of intense light interactions with monolayer two-dimensional (2D) materials have been reported, including low- and high-order harmonic generation (HHG), multiphoton absorption, optical injection of spin and charge currents, terahertz generation, and

laser-induced dielectric breakdown. These processes are all initiated by interband transition of electrons induced by light with photon energy smaller than the bandgap energy. Some modeling efforts based on perturbation theory were attempted but their discrepancies with experiments are at least one order of magnitude, highlighting the lack of theoretical understanding of strong-field ionization in monolayer 2D materials. In this work, we report a new formalism of strong-field ionization for monolayer two-dimensional semiconductors based on 2D Keldysh (KLD) theory [T. -H. Her et al., *Optica* 12, 538-545 (2025)]. We take this approach because the original Keldysh theory [L. V. Keldysh, *Soviet Physics JETP* 20, 8 (1965)] is the only theory that yields, for simplified band dispersion, analytical formulas for the cycle-averaged non-resonant ionization rate in bulk solids induced by a monochromatic electric field of arbitrary strength. It provides a smooth transition between multiphoton and tunneling ionization as what we now call the ‘Keldysh parameter’, γ , varies from $\gamma \gg 1$ to $\gamma \ll 1$. Due to their analyticity, Keldysh’s formulas are widely employed for qualitative modeling of strong-field ionization in bulk solids. In this presentation, we generalize Keldysh’s formulas to monolayer two-dimensional semiconductors. We derive closed-form formulas and their asymptotic forms for a two-band model with a Kane dispersion. We also derive selection rules related to the parity of multiphoton orders near the band edge. We validate our theory by comparing it to recent experiments and modeling of strong-field ionization in monolayer transition metal dichalcogenides (TMDs) with very good agreement (Figs. 1-3 of supplemental document) Specifically, our theory predicts a higher interband electron tunneling rate for 2D compared to 3D in the MIR frequency range, which successfully explains the 10x discrepancy (Fig. 3) between the experiment and modeling for HHG from monolayer TMDs [Liu et al., *Nature Phys* 13, 262–265 (2017)]. Considering the tremendous success of the original Keldysh theory in describing strong-field optical phenomena in atoms and solids, our 2D Keldysh theory is expected to find a wide range of applications in intense light-2D material interaction, such as optical limiting, multi-photon photodetection, THz generation through quantum interference, and photo-carrier doping for HHG.

12:00pm 2D+AQs+EM+MI+MN+NS+QS+SS+TF-ThM-17 Thickness Dependent Band Gap and Electrical Anisotropy of 2DSnSe, Marshall Frye, Jonathan Chin, Joshua Wahl, Jeremy Knight, Georgia Institute of Technology; Walter Smith, Purdue University; Dilara Sen, Samuel Kovach, Kenyon University; Frank Peiris, Kenyon College; Charles Paillard, University of Arkansas; Thomas Beechem, Purdue University; Anna Osterholm, Lauren Garten, Georgia Institute of Technology

2D SnSe presents unique opportunities for optoelectronics, and scalable microelectronics, but it is first critical to understand how the electrical and optical response change upon downscaling. Tailoring the band gap and electrical anisotropy of 2D monochalcogenides, like SnSe, has previously been shown but the mechanisms that drive the changes in band gap are still not understood. This study reveals how changes in bond length and structure drive the thickness dependences of band gap, carrier mobility and lifetime of SnSe thin films. Molecular beam epitaxy is used to deposit (2h00) oriented SnSe thin films with thicknesses ranging from 4 nm to 80 nm. The direct band gap increases from 1.4 eV at 80 nm to 1.9 eV at 4 nm, underscoring the potential of SnSe as a tunable and direct band gap material for thin film optoelectronics. Raman spectroscopy shows different simultaneously changes in the crystal structure and bonding occurring parallel versus perpendicular to the 2D plane with decreasing film thickness. TEM further supports the hypothesis that the increase in the band gap with reduced thickness is due to changes in crystal structure resulting in a contraction of the out-of-plane SnSe covalent bonds, while the in-plane bond length increases. In addition to the reduction in band gap, tracking the time dependent photoluminescence shows an increase in carrier lifetime with decreasing film thickness, while Hall measurements show a change in the carrier mobility with decreasing thickness. Overall, this work provides the critical missing insight needed to design these optically and electronically relevant 2D materials for scalability.

Thursday Afternoon, September 25, 2025

2D Materials

Room 208 W - Session 2D+AQS+MI+NS+QS+TF-ThA

2D Materials: Magnets and Topological Phenomena

Moderators: Rafik Addou, The University of Texas at Dallas, Zhurun Ji, MIT

2:15pm **2D+AQS+MI+NS+QS+TF-ThA-1 Non-Local Transport from Magnetic Topological Superconductivity in 2D Fe-Chalcogenides, Kenneth Burch**, Boston College **INVITED**

Magneto-Chiral topological superconductivity is a rare phase long pursued for error-free quantum computation. Its 1D chiral modes possess topologically protected long-range coherence well beyond that of the Cooper pairs, which could be fruitful for quantum transduction and low-temperature spin transport. While evidence for such modes is mounting, unambiguous signatures, such as non-local transport via co-tunneling, remain elusive. I will describe our realization of 1D chiral hinge modes mediating the direct tunneling of electrons from source to drain in FeTe_{0.55}Se_{0.45}. Specifically, I will discuss our evidence that the non-local tunneling signatures are decoherence-free and emerge from this material's combination of surface magnetism, bulk topology, and superconductivity. Time remaining, I will discuss how these advances can be used for Majorana Circuits and future efforts in cryogenic spintronics

2:45pm **2D+AQS+MI+NS+QS+TF-ThA-3 Integer and Fractional Chern Insulators in moiré MoTe₂, Yihang Zeng**, Purdue University **INVITED**

The fractional Chern insulator (FCI), a lattice analogue of the renowned fractional quantum Hall state, was theorized to exist without external magnetic field. FCI provides a pathway towards novel topologically ordered quantum phases that are useful for decoherence-free quantum computation. Two-dimensional (2D) moiré materials, featuring strong correlation, non-trivial band topology and unparalleled tunability, stands as an ideal platform for realizing FCI. In this talk, I will first present our innovative optoelectronic detection method, which is capable of detecting the chemical potential in arbitrary 2D materials. Employing this new technique, we successfully observed an FCI and integer Chern insulator in the zero magnetic field limit in MoTe₂-based moiré materials. We further study the FCI and ferromagnetism as a function of twist angle.

3:15pm **2D+AQS+MI+NS+QS+TF-ThA-5 Conducting Scanned Probe Investigations of the Bismuthine Termination of Intrinsic Topological Superlattice Bi₂-Bi₂Se₃, Lakshan Don Manuwelge Don, Mysidia Leff, Md. Sakauat Hasan Sakib, Miami University; Seth Shields, The Ohio State University; Joseph Corbett**, Miami University

Topological materials, characterized by symmetry-protected electronic states and robust surface conduction, represent a frontier in quantum materials research. Their non-trivial band topology enables dissipationless edge states, spin-momentum locking, and resilience to disorder, making them strong candidates for spin-orbit torque devices, magnetic field sensors, and polarized light detectors, to name a few. These properties have positioned topological materials as important material of interest as development of scalable quantum technologies grows.

In this study, we explore the atomic and electronic properties of the bismuthine-terminated topological semimetal Bi₂-Bi₂Se₃ using scanning tunneling microscopy (STM) and conductive atomic force microscopy (C-AFM). Bi₂-Bi₂Se₃ is an intrinsic superlattice material s comprised of a Bi₂Se₃ quintuple layer (QL) slab and a 2D Bismuthine (Bi₂) layer separated by a van der Waals gaps. The topological surface state on the 001 orientation depends on the terminating layer, with two distinct possible topologically protected surface states.

The unique step heights between the Bi₂Se₃ QL and Bismuthine layer enable termination characterization through careful step height analysis. Atomically resolved STM measurements on a Bismuthine terminated step reveal a distinct honeycomb lattice, while scanning tunneling spectroscopy (STS) captures a Dirac cone in local density of states centered at the Fermi level, in excellent agreement with angle-resolved photoemission spectroscopy (ARPES).

Using C-AFM under ambient conditions, we investigate force-dependent I-V spectroscopy. Utilizing step height analysis, we find a bismuthine terminated step and perform point spectroscopy. At low applied forces, differential conductance (dI/dV) spectra reveal a Dirac cone, mirroring STM results and confirming the presence of topologically protected surface states even under ambient conditions! As mechanical force increases, we observe a transition in transport behavior, from quantum tunneling to Ohmic conduction. Additionally, a voltage and force-dependent crossover from direct tunneling to Fowler-Nordheim tunneling is identified.

Our findings revealing the atomic structure and Dirac cone of the bismuthine termination in the topological semimetal Bi₂-Bi₂Se₃. Interestingly these feature are observable even under ambient condition. We find no degradation with time, freshly grown sample versus those that have sat for months give the same results.

3:30pm **2D+AQS+MI+NS+QS+TF-ThA-6 Local Spectroscopy Study of Gate-controlled Energy Gap in Monolayer 1T'-WTe₂, Tiancong Zhu**, Purdue University; Zehao He, University of California at Berkeley; Michal Papaj, University of Houston; Samuel Stolz, Department of Physics, University of California, Berkeley; Tianye Wang, Canxun Zhang, Yan-Qi Wang, Joel Moore, Zi Qiang Qiu, Feng Wang, Michael Crommie, University of California at Berkeley

The interplay between strong correlation and topology can lead to intriguing quantum phases of matter. In monolayer 1T'-WTe₂, the non-trivial topology gives rise to the quantum spin Hall insulator (QSHI) phase, characterized by helical 1D edge states surrounding the insulating 2D bulk. While experimental evidences support quantized conductance through the 1D helical edge states, the nature of the insulating bulk, whether attributed to spin-orbit coupling or strong correlation, remains under debate. Here, we employ scanning tunneling microscopy and spectroscopy (STM/S) on gate-tunable 1T'-WTe₂ devices to shed light on this problem. Our samples are fabricated using a combination of molecular beam epitaxy (MBE) and van der Waals (vdW) stacking technique, which allows us to synthesize high-quality monolayer 1T'-WTe₂ films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-WTe₂ at its charge neutrality, which diminishes when the Fermi level is tuned into either the conduction or valence band. STS across the sample edges shows that the edge states persist at all gate voltages, while Fourier transform-STM measurement in the bulk further shows the evolution of the bulk band structure at different carrier densities. We will compare our experimental data with existing theoretical models, such as the SOC-induced gap and the proposed excitonic insulator phase, and suggest future experimental directions to further elucidate the origin of the energy gap.

3:45pm **2D+AQS+MI+NS+QS+TF-ThA-7 Exploring Moiré Magnetism in Twisted Two-Dimensional Magnets, Liuyan Zhao**, University of Michigan **INVITED**

Moiré superlattice emerges from the interference between two mismatched atomic lattices, and it has led to tremendous success in designing and tailoring the electronic states in two-dimensional (2D) homo- and hetero-structures. Yet, the power of moiré superlattice in controlling the spin degree of freedom and thus modifying the magnetic states is much less explored. Only very recently after the development of 2D magnet research, there have been a few experimental attempts in realizing moiré magnetism in twisted 2D magnet homo-structures. In this talk, I will show our recent effort in studying magnetic phases in twisted double bilayer chromium triiodide (CrI₃) and progressive steps towards realizing moiré magnetism. Noting that bilayer CrI₃ is a layered antiferromagnet and that any homogeneous stacking of two bilayers necessarily produces zero magnetization, we have revealed, in twisted double bilayer CrI₃, an unexpected net magnetization showing up at intermediate twist angles and its accompanied noncollinear spin textures. I will show the optical spectroscopy signatures of this twist-induced magnetic phase, then discuss its dependence on twist angle, external magnetic field, and temperature.

2D Materials

Room Ballroom BC - Session 2D-ThP

2D Materials Poster Session

2D-ThP-1 Molecular Beam Epitaxy Synthesis and Characterization of 2D InSe, *Emily Toph, Eric Vogel, Georgia Institute of Technology; Brent Wagner, Georgia Tech Research Institute*

InSe, a monochalcogenide two-dimensional (2D) semiconductor¹ with a large room-temperature electron mobility of approximately $10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$, is a promising material for high-sensitivity Hall sensors², ballistic transistors,³ and non-volatile memory applications.⁴The In-Se system contains many different stable phases⁵ including selenium rich In_2Se_3 and selenium deficient In_4Se_3 phases. The synthesis of InSe is challenging due to the narrow stability range of its stoichiometry on the phase diagram and the need for a surface morphology with large grain lateral growth. Therefore, synthesizing high-quality InSe requires a detailed understanding of how the synthesis parameters affect the structure and stoichiometry of In_xSe_y thin films near and within the narrow range of stability for InSe.

The growth of 2D InSe thin films has been achieved using a novel molecular beam epitaxy (MBE) two-step method involving an indium precursor layer, which effectively suppresses the formation of unwanted phases and allows for high-quality films.⁶ This work builds upon this novel approach by investigating how synthesis parameters, including substrate temperature, precursor flux, and deposition time influence the structural and stoichiometric properties of InSe thin films deposited on sapphire substrates. The chemical bonding, crystalline structure, and morphology of the thin films are characterized by X-ray Photoelectron Spectroscopy, Raman spectroscopy, X-ray diffraction and Atomic Force Microscopy. By understanding how these synthesis parameters impact film quality, the optimal synthesis conditions for InSe thin film deposition can be further refined, enhancing the potential for device applications.

References

1. Camara, M., *et al.*, *Physical Review B* (2002) **65** (12), 125206
2. Bandurin, D. A., *et al.*, *Nature Nanotechnology* (2017) **12** (3), 223
3. Jiang, J., *et al.*, *Nature* (2023) **616** (7957), 470
4. Lu, Y.-Y., *et al.*, *ACS Applied Materials & Interfaces* (2021) **13** (3), 4618
5. Bergeron, H., *et al.*, *Applied Physics Reviews* (2020) **7** (4)
6. Hsiao, S.-W., *et al.*, *Frontiers in Materials* (2022) **9**, 871003

2D-ThP-3 Charge Transfer States at the Monolayer WS_2 /HAT-CN Interface, *Xu He, Antoine Kahn, Princeton University*

Understanding how WS_2 interacts electronically with organic molecules is very important for hybrid optoelectronics and energy harvesting applications, where charge separation at the interface governs device function. In this work, we investigate a heterojunction between monolayer WS_2 and 1,4,5,8,9,11-hexaazatriphenylene hexacarbonitrile (HAT-CN) to study energy level alignment and interfacial charge transfer.

The combined ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy (UPS/IPES) measurements show that the pristine monolayer WS_2 has an ionization energy (IE) of 6.00 eV and an electron affinity (EA) of 3.44 eV with a 2.56 eV electronic gap, while films of pristine HAT-CN show an IE of 9.48 eV and EA of 5.66 eV with a 3.82 eV electronic gap. These values suggest a type-II energy level configuration at the interface, providing an energetic driving force for electrons to transfer from WS_2 into HAT-CN.

Raman and Photoluminescence (PL) spectroscopies, and X-ray photoelectron spectroscopy (XPS) were performed on 1L- WS_2 with 0, 3.75, 7.5, and 15nm HAT-CN thicknesses. The Raman signature of WS_2 remains consistent across different thicknesses of HAT-CN, suggesting that the WS_2 lattice remains intact despite HAT-CN presence. XPS confirms HAT-CN adsorption on WS_2 . PL spectra reveal a >90% quenching of the intrinsic WS_2 emission at around 633nm after HAT-CN deposition without visible PL peak shift. This significant PL quenching indicates the formation of a charge transfer (CT) state at the interface. The large difference in electronic gaps of 1L- WS_2 and HAT-CN suggests that it is not a Frenkel energy transfer. A device with mechanically transferred 1L- WS_2 and HAT-CN is being constructed and tested for photocurrents. We expect to see an external quantum efficiency (EQE) spectra whose absorption in the energy range below the electronic gap of both 1L- WS_2 and HAT-CN will provide direct evidence for the formation of CT states at the interface.

A systematic study on the evolution of the WS_2 VBM and HAT-CN LUMO positions is performed with combined UPS/IPES by evaporating 0, 0.5, 1, 2, 5, and 10nm HAT-CN on 1L- WS_2 on p-Si. This series of energy alignment studies show that the 1L- WS_2 /HAT-CN interface shows a slight relaxation of the CT gap, which aligns well with the loss of electrons from WS_2 into HAT-CN layer.

This work demonstrates how tailoring the energy level alignment in hybrid 2D/organic heterojunctions can enable interfacial charge transfer. Our findings underscore the potential of engineering van der Waals interfaces between TMD monolayers and molecular semiconductors for novel excitonic devices and energy conversion applications.

2D-ThP-4 Enhanced Etching and Surface Cleaning of MoS_2 via Pre-Fluorination and Plasma-Activated Desorption, *Shoaib Khalid, Yuri Barsukov, Stephane Ethier, Igor Kaganovich, Princeton University Plasma Physics Lab*

Transition metal dichalcogenides (TMDs) are a class of layered materials that have garnered significant attention for their unique electronic, optical, and mechanical properties. Their tunable bandgap, high carrier mobility makes them ideal candidates for applications in next-generation electronics, optoelectronics, and energy storage devices. This study, based on ab initio molecular dynamics (AIMD) calculations, suggest that pre-fluorinating the MoS_2 surface before Ar plasma bombardment significantly enhances the etching yield and improves surface smoothness. Additionally, we propose a strategy to remove excess fluorine adsorbed on sulfur using low-energy electrons from the plasma. Our results show that F⁻ ions migrate much faster than neutral F atoms, facilitating their desorption. We also find that when H atoms are adsorbed on the surface, F⁻ ions diffuse until they encounter an H adatom, leading to the desorption of stable HF molecules. This approach of utilizing low-energy reactive species from plasmas offers an effective method for surface transport and cleaning of electronegative adsorbates, such as halogens, from the MoS_2 surface.

This research was supported by the Princeton Plasma Physics Laboratory under U.S. Department of Energy Prime Contract No. DE-AC02-09CH11466.

2D-ThP-5 2d Topological Phases, β -Sn Transformation, and Implications for Topological Superconductivity, *Cheng-Maw Cheng, National Synchrotron Radiation Research Center, Taiwan; Ye-Shun Lan, National Tsing Hua University, Taiwan; Shu-Hua Kuo, National Synchrotron Radiation Research Center, Taiwan; Yen-Hui Lin, National Tsing Hua University, Taiwan; Jing-Yue Huang, National Synchrotron Radiation Research Center, Taiwan; Pin-Jui Hsu, Horng-Tay Jeng, National Tsing Hua University, Taiwan*

Two-dimensional topological materials offer unique electronic properties that are promising for next-generation quantum and spintronic devices. In particular, 2D topological insulators (TIs) host robust spin-polarized edge states protected by a bulk band gap induced by spin-orbit coupling, while topological nodal line semimetals (TNLSMs) feature one-dimensional band degeneracies protected by crystalline symmetries. Despite theoretical predictions, experimental realization of 2D TNLSMs remains scarce. In this work, we report the synthesis and characterization of a monolayer cubic β -Sn phase grown on a Cu(111) substrate via sequential deposition. Starting from low-temperature growth of α -Sn (stanene), we observed a well-defined honeycomb lattice using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), consistent with prior reports. Subsequent Sn deposition led to a structural phase transition into a high-coverage, single-layer β -Sn with a body-centered tetragonal structure. This transition was confirmed by STM and angle-resolved photoemission spectroscopy (ARPES), revealing a dramatic change in the electronic structure. Combined with first-principles density functional theory (DFT) calculations, we demonstrate that monolayer β -Sn hosts two distinct types of nodal lines—coexisting in a single 2D mono-elemental material. This observation marks the first realization of a 2D topological semimetal featuring dual nodal line types. Given β -Sn's known superconductivity in bulk form, our findings establish ultrathin β -Sn as a promising platform for exploring 2D topological superconductivity and potentially hosting Majorana fermions.

2D-ThP-6 Transition of Exohedral Fullerenes Fe+C60 to Endohedral Fullerenes Fe@C60 Upon Its Deposition on the Surface of an Iron Crystal Using Md Simulations, *Danila Alyabev, Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan; Dmitriy Bazarov, Digital Technologies and Artificial Intelligence Research Institute, Tashkent, Uzbekistan*

To date, following the discovery and isolation of fullerenes, there have been a large number of both experimental and theoretical studies on their research. A specific group includes the so-called endofullerenes—

fullerenes with encapsulated atoms or molecules inside their cavities, such structures are of both theoretical and practical interest. In the current study, the possibility of transition of exohedral fullerene Fe+C₆₀ to endohedral fullerene Fe@C₆₀ through scattering of Fe+C₆₀ on the surface of an iron crystal is explored by methods of molecular dynamics.

In this study, we used the LAMMPS software package in combination with a selected Tersoff potential for modeling purposes [1]. To conduct the model experiment, we created two models: a system consisting of Fe and C₆₀ exofullerenes heated to 900 K, i.e. Fe+C₆₀ model (T = 900K), and an iron crystal heated to 300 K (T = 300K). We then isolated a region on the surface of the iron crystal where exofullerenes were deposited normally at a vertical velocity of 4200 m/s (7.15eV, 400 impact points, process time – 5 ps, timestep – 0.0001 ps)

The primary objective of this study was to isolate those fullerenes where the iron atom was encapsulated within the fullerene structure. Dynamic data was acquired and processed as follows: 12 carbon atoms on the lower hemisphere of each fullerene were selected; Vectors were constructed between the iron atom and each of these selected carbon pairs, and the angles formed by these vectors were measured – a total of 66 angle measurements were taken for each of 400 instances. a 400 × 67 data array was generated, where the potential energy value of the iron atom was recorded in a separate column after 5ps model time.

The output data was analyzed using cluster analysis methods, which allowed the classification of fullerenes into groups based on their characteristic geometries. One of the isolated groups included fullerenes with geometries similar to those with endohedral structures, the bond lengths of these fullerenes were compared to those in the study [2]. Based on the simulation results, it is expected that 21-30% of the exofullerenes will transition to endofullerenes under the given initial conditions.

1. K.O.E. Henriksson et al, Journal of Physics: Condensed Matter, 25(44), 445401
2. Cherepanov et al, Crystallogr. Rep. 65, 404–408 (2020)

2D-ThP-9 Discretized Atomic Layer Deposition Recipe for Wafer-scale Synthesis of MoS₂, Sachin Shendekar, Shyam Aravamudhan, North Carolina A&T State University

Monolayer MoS₂, a 2D material, holds enormous promise for transcending the fundamental limits of silicon-based electronics and continuing the downscaling of transistors and logic circuits for energy-efficient computing. However, major research efforts are needed to overcome many fabrication and integration challenges including wafer-scale growth control, doping, contacts, gate stack, and reliability. In this work, we attempt to address one of the challenges, namely wafer-scale synthesis of MoS₂. Atomic Layer Deposition (ALD) is one of the most promising techniques for wafer-scale growth of MoS₂ due to its conformal, self-limiting, and low-temperature characteristics. We present here a novel discretized ALD recipe for wafer-scale deposition of uniformly thick MoO₃, further, to sulfurized to stoichiometric MoS₂. This is an alternative approach for ALD to determine temperature and time based on the Arrhenius equation and first-order reaction kinetics. Wafer-scale uniformity, film morphology, composition and crystallinity were measured using a comprehensive set of characterization techniques including ellipsometry, AFM, XPS, Raman, XRD and Photoluminescence measurements.

2D-ThP-10 Modeling Synthesis Pathways for Transition Metal Dichalcogenide Monolayers with Quantum and Statistical Learning Techniques, Andrew Messecar¹, Western Michigan University; *Chen Chen, Isaiah Moses, Wesley Reinhart, Joan Redwing,* The Pennsylvania State University; *Steven Durbin,* University of Hawai'i at Mānoa; *Robert Makin,* Western Michigan University

The ability for machine learning technologies to estimate patterns from information has made them a top approach for optimizing the growth and characterization of a broad range of material systems, including few and single atomic layer materials such as transition metal dichalcogenides (TMDs). In this work, we have applied both quantum and classical machine learning approaches to investigate and model the metal-organic chemical vapor deposition (MOCVD) of TMD thin films as grown with dihydrogen chalcogenide gas and transition metal hexacarbonyl precursors. Several hundred discrete records of MOCVD-grown TMD samples synthesized in a single laboratory have been organized into material-specific data sets. For each growth trial, Raman spectra characterizing the resulting sample have

been utilized to assess monolayer coverage. The distance between the A_{1g} and E_{2g} Raman mode peaks in each spectrum was measured and associated with the respective growth record as an output variable within the data set. The MOCVD synthesis parameter data was subsequently mapped to the measured A_{1g} and E_{2g} Raman mode peak distance using supervised learning techniques. A combination of p-value calculations, Pearson's correlation coefficients, SHAP values, and regression tree splitting rules were used to analyze the statistical importance of each MOCVD operating parameter for influencing the expected value of the distance between the A_{1g} and E_{2g} Raman mode peaks. Various quantum as well as classical supervised machine learning approaches – including k-nearest neighbors, tree-based models, and quantum support vector machines, were fit to the data and compared for generalization performance. In the case of MoS₂, generalizing beyond the training data indicates that maximizing both the Mo(CO)₆ injector hydrogen gas flow during the growth step and the value of the Mo(CO)₆ flow during the reaction temperature ramp up step is forecasted to result in a minimization of the A_{1g} and E_{2g} Raman mode peak distance. This predicted reduction of the peak distance between the A_{1g} and E_{2g} vibrational modes in Raman spectra acquired of MoS₂ thin films corresponds with improved monolayer coverage. This methodology is applicable to additional TMD materials and characterization features of interest.

*This work was funded by Penn State 2DCC-MIP through the NSF cooperative agreement DMR-1539916 as well as by the National Science Foundation (grant number DMR-2003581).

2D-ThP-11 Investigating Optical Properties of Moiré Excitons in Twisted Transition Metal Dichalcogenide (TMDC) Homobilayers, Dheeraj Koneru², Stevens Institute of Technology

Over the past decade, atomically thin 2D van der Waals (vdW) materials have become powerful systems to study light-matter interaction and electronic confinement. In monolayer transition-metal dichalcogenides (TMDCs), optical absorption is dominated by tightly bound excitons due to reduced screening and enhanced Coulomb interactions. I present the optical study of moiré excitons in twisted WSe₂ homobilayers, where a small interlayer twist generates a periodic potential landscape that traps excitons at specific locations in real space.

To isolate and study these moiré-localized excitons (MXs), I detail the fabrication process of monolayer WSe₂ on SiO₂, followed by tear-and-stack assembly to produce a clean interface between the twisted homobilayers. Through power-dependent, polarization-resolved, and magneto-optical spectroscopy, I demonstrate that the narrow, quantum dot-like spectral lines originate from localized MXs. These results reveal how structural symmetry, twist angle, and magnetic fields impact valley physics in moiré superlattices. The findings offer new opportunities for creating quantum emitter arrays for integrated quantum photonics.

2D-ThP-12 Band Gap Opening in AB-Stacked Bilayer Silicon, Kumar Vishal, Hong Huang, Yan Zhuang, Wright State University

Despite their potential as of being the excellent candidates for advancing CMOS technology to its physical limits, the presence of an opened energy bandgap in either single- or bilayer- silicene poses a significant challenge, hindering its applications in the main stream semiconductor industry. Previous attempts, including applying external electric field, surface decoration, nanopatterning, and applying uniaxial strain along designate directions, have proven insufficient in meeting the stringent demands of CMOS technology concerning operational reliability, processing environment sensitivity, product yield, and achievable processing standards. Recently a number of research reported that applying of the biaxial in-plane strain leads to energy bandgap opening in AA-stacked bilayer silicene, however the maximum energy bandgap opening is limited to 16 meV.

In this work, we present a theoretical study of the opening of energy bandgap in AB-stacked bilayer silicene. Employing the Density Functional Theory (DFT), our investigations have taken into account of the effects of both ferromagnetism and antiferromagnetism, alongside external biaxial in-plane strain/stress and vertical biasing effects. Within a strain range spanning from -5.17% to 10.35%, we observed a strain-tunable energy bandgap opening with a maximum of 380 meV at a strain level of 7.76%. Notably, beyond this strain range, the energy bandgap remains closed. In addition, under compressive strain, the energy band diagram presents spin-

Thursday Evening, September 25, 2025

generated features, with discernible energy band splitting. On the contrary, tensile strain leads to a break of the spin generation, except at specific high symmetry points such as . We further observe a degeneration of the energy band diagram at these high symmetry points upon the application of gate voltage along the vertical direction. The coupling of the ferromagnetism and antiferromagnetism between the two silicene layers results in a transition from metallic material to semiconductor. The potential of the opened bandgap makes the AA-stacked bilayer silicene a very promising candidate material to be applied in the CMOS technology, while the strain-induced tunable bandgap opening offers immediate potential for applications in the infrared (IR) spectrum. In addition, the spin-induced band diagram degeneration may holds promise for integrated spintronics applications.

2D Materials

Room 208 W - Session 2D+AQS+EM+NS+QS+TF-FrM

2D Materials: Devices and Applications

Moderator: Kai Xiao, Oak Ridge National Laboratory

8:15am 2D+AQS+EM+NS+QS+TF-FrM-1 Charge Transport in Printed Films of Two-Dimensional Materials for Printed and Wearable Electronics, *Felice Torrisi*, Imperial College London, UK **INVITED**

Printed electronics has emerged as a pathway for large scale, flexible, and wearable devices[1], Internet-of-Things[2] and smart textiles[3]. Graphene and related two-dimensional (2D) materials offer an ideal platform of novel materials for high performance printed electronics [4,5]. Electronic inks from 2D materials with different electronic properties have been developed to print the different elements of a device: semiconducting or semimetallic inks in the active layer, insulating inks for dielectrics, and conducting inks for electrodes[6].

In this talk I will describe the charge transport mechanisms of surfactant- and solvent-free inkjet-printed thin-film devices of representative few-layer graphene (semi-metal), molybdenum disulphide (MoS₂, semiconductor) and titanium carbide MXene (Ti₃C₂, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS₂ devices is dominated by the intrinsic transport mechanism of the constituent flakes. On the other hand, charge transport in printed few-layer graphene devices is dominated by the transport mechanism between different flakes.[7]

[1] Torrisi, F. & Carey, T. "Graphene, related twodimensional crystals and hybrid systems for printed and wearable electronics" *Nano Today* 23, 73 (2018).

[2] C. Scholten et al. "Advanced Technologies for Industry – Product Watch: Flexible and printed electronics", doi: 10.2826/29513 (2021).

[3] Carey, T. et al. "Fully inkjet-printed two-dimensional material field-effect heterojunctions for wearable and textile Electronics" *Nat. Commun.* 8, 1202 (2017).

[4] Torrisi, F. et al. Inkjet-printed graphene electronics. *ACS Nano* 6, 2992(3006 (2012).

[5] F. Torrisi & T. Carey "Printing 2D Materials" in "Flexible Carbon-based Electronics" Editors P. Samori and V. Palermo, Ed.: Wiley-VCH, Weinheim, Germany, 2018. ISBN: 978-3-527-34191-7.

[6] D. Akinwande "Two-dimensional materials: printing functional atomic layers" *Nat. Nanotechnol.* 12, 287 (2017).

[7] E. Piatti, A. Arbab et al. "Charge transport mechanisms in inkjet-printed thin-film transistors based on two-dimensional materials" *Nature Electronics* 4, 893 – 905 (2021).

8:45am 2D+AQS+EM+NS+QS+TF-FrM-3 Antimony as a Contact Material for Two-Dimensional Semiconductors: Interface Chemistry and Thermal Stability, *Fernando Quintero Borbon, Joy Roy, Robert Wallace, Rafik Addou*, University of Texas at Dallas

Antimony (Sb), a semimetal, has emerged as a promising contact material for two-dimensional (2D) semiconductors. Sb contacts have been shown to achieve ultra-low contact barriers. The formation of a Sb–Se bond has been demonstrated as an effective doping strategy in n- and p-FETs with a single WSe₂ channel through Sb–Pt contact modification. These findings underscore the necessity for further investigation into the interface chemistry and thermal stability of Sb on transition metal dichalcogenides (TMDs), to determine whether the interaction remains van der Waals or becomes chemically reactive upon thermal processing.

The present study offers a comprehensive study of the interface chemistry between Sb and TMDs, in particular MX₂ (M = Mo or W; X = S or Se), using X-ray photoelectron spectroscopy (XPS). Sb was deposited in ultra-high vacuum conditions (UHV) on bulk TMD surfaces, followed by annealing in UHV at 100°C, 200°C, and 300°C. The XPS measurements revealed an absence of chemical or interfacial reactions at room temperature, 100°C, and 200°C. However, upon annealing at 300°C, complete sublimation of the Sb layer was observed. These findings support the van der Waals nature of the interface, confirming that the interaction between Sb and the underlying TMDs remains non-reactive up to 200 °C. This thermal stability and inertness suggest that Sb could be a promising candidate for integration in 2D heterostructures and devices that require clean, weakly interacting interfaces.

[1] Y.-T. Lin et al. *Nano Lett.* (2024) 24, 8880–8886

[2] Z. Wang et al. *Adv. Funct. Mater.* (2023) 33, 230165

[3] T. Su et al. *J. Phys. D: Appl. Phys.* 56 (2023) 234001

[4] Wang et al. *Adv. Funct. Mater.* (2023) 33, 2301651

[5] Chou et al. *IEEE International Electron Devices Meeting (IEDM)*, San Francisco, CA, USA (2021) 7.2.1-7.2.4.

9:00am **2D+AQS+EM+NS+QS+TF-FrM-4 Metal-to-Semiconductor Transition in Niobium Sulfoselenide Alloy and Niobium Sulfide Films by Compositional Control and Post Growth Sulfurization, *Tinsae Alem, Abir Hasan, Kory Burns, Nikhil Shukla, Stephen McDonnell*, University of Virginia**
Transition metal dichalcogenides (TMD) have attracted increasing scientific interest due to their diverse properties including a tunable bandgap, optical anisotropy, low power consumption, and good elasticity. In this study, low-dimensional TMD films were grown with molecular beam epitaxy (MBE) to investigate the effects of varying chalcogen (sulfur and selenium) content in niobium sulfoselenide (NbS₂Se_{2-x}) alloys. Here, we focus on their electrical resistivity and electronic properties, including the transition from metallic to semiconducting behavior to have precise control over the material's electrical conductivity. Additionally, we analyzed the semiconductor-to-metal transition in NbS₂ films following post-growth sulfurization and the corresponding changes in resistivity. These MBE grown films were characterized using in-situ x-ray photoelectron spectroscopy (XPS) to analyze the chemical composition. Next, the electrical resistivity of films was calculated using their sheet resistance measured with a Jandel 4-point probe, and their thickness was estimated using x-ray reflectivity (XRR). We used transmission electron microscopy (TEM) to visualize these MBE-grown films at the atomic scale, enabling the correlation of atomic structure with electronic properties. Lastly, the temperature coefficient of resistance (TCR) measurements was performed to understand the resistivity of the films with temperature dependence and to determine their metallic and semiconducting behavior. Our results demonstrate that the transition from metal to semiconductor occurs with the addition of sulfur into the niobium selenide film. We also observed a trend of increasing resistivity as the sulfur content was increased in niobium selenide film. This work explores the potential of tuning the energy gap of TMD materials, making them ideal candidates for tunable nanoelectronics in various applications.

9:15am 2D+AQS+EM+NS+QS+TF-FrM-5 Evolution of the Electronic Gap of Directly Synthesized Versus Mechanically Transferred WS₂ Monolayer to Multilayer Films, *Xu He, Antoine Kahn*, Princeton University

Transition metal dichalcogenides (TMDs) have emerged as promising electronics and optoelectronics materials for their strong light-matter interaction, large exciton binding energies, and bandgap tunability through the control of composition and the number of layers. Among TMDs, WS₂ stands out for its strong photoluminescence and spin-orbit coupling, making it ideal for exploring charge transfer and interfacial phenomena. However, discrepancies in reported energy levels (electronic gap, ionization energy, electron affinity) remain due to variations in growth and measurement methods, impeding device design.

In this study, we directly compare the band structure of WS₂ films from monolayer to multilayer (up to four layers) prepared by two commonly used methods: direct growth via metal-organic chemical vapor deposition (MOCVD) and mechanical exfoliation with layer-by-layer transfer. We utilize a suite of characterization techniques, including Raman spectroscopy, photoluminescence (PL), UV-vis absorption, and X-ray photoelectron spectroscopy (XPS), to probe vibrational modes and optical transitions. A combination of ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES) allows us to directly study the evolution of ionization energy and electron affinity, hence the electronic gap of the materials.

We find that the electronic gap (E_g) of WS₂ consistently decreases with increasing layer number, reaching bulk-like values by the trilayer for mechanically transferred layers. The exfoliated monolayer is found to have an E_g of 2.43 eV, which reduces to around 1.97 eV at the trilayer and stays at 1.98 eV for the tetralayer. This layer-dependent E_g reduction is driven firstly by an upshift of the valence band maximum (VBM) at the 1L-2L transition and then by a downshift of the conduction band minimum (CBM) at the 2L-3L transition.

Comparing differently processed layers, we find the MOCVD-grown monolayer WS₂ to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E_g in MOCVD-grown monolayers also yields a higher exciton binding energy (~0.55 eV)

than in exfoliated monolayers (~0.43 eV). XPS analysis indicates that MOCVD samples contain more oxygen-related defect species, likely contributing to the subtle band gap differences and a small blue shift of their optical spectra relative to exfoliated layers.

Overall, this comparative study highlights the influence of the fabrication methods on the fundamental electronic structure of WS_2 . These findings provide important guidelines for tailoring band alignments for WS_2 -based heterostructures and optoelectronic devices.

9:30am **2D+AQS+EM+NS+QS+TF-FrM-6 2D Phase Diagram of Iron Sulfides on Au(111): From Hexagonal to Square Atomic Arrangement and Beyond, Andrea Berti**, University of Trieste, Italy; **Marco Bianchi, Paolo Lacovig, Silvano Lizzit**, Elettra-Sincrotrone Trieste, Italy; **Philip Hofmann**, Aarhus University, Denmark; **Alessandro Baraldi**, University of Trieste, Italy

Despite extensive research on two-dimensional (2D) materials, almost all experimentally synthesized 2D systems derive from van der Waals crystals (vdW). While the use of vdW crystals has been remarkably successful, it inherently restricts the 2D materials landscape to compounds that are already layered in their bulk form. Less than 5% of known inorganic materials possess a layered structure suitable for exfoliation, and the vast majority of functional compounds—such as oxides, sulfides, and nitrides—do not belong to this category. In recent years, increasing efforts have focused on the realization of truly two-dimensional monolayers from non-vdW compounds, which could unlock novel properties in fields such as high-temperature magnetism, catalysis, and strongly correlated electron phenomena. Beyond the class of vdW materials, only a limited number of compounds have so far been theoretically predicted to be stable in the 2D limit. In this context, iron-sulfur compounds have recently emerged as promising candidates. Density functional theory predicts that both hexagonal FeS_2 and tetragonal FeS phases can exist as stable monolayers, exhibiting strain-tunable magnetic properties. Although the Mermin-Wagner theorem precludes long-range magnetic order in ideal 2D isotropic systems, magnetic anisotropy can lift this constraint and allow stable ordering, enabling tunable magnetism at the atomic scale, which is essential for spintronics, as well as other emerging phenomena such as topological effects, multiferroicity, and proximity effects in heterostructures. However, compared to their bulk counterparts, Fe-S systems generally display a rich phase diagram, characterized by multiple stoichiometries and atomic arrangements. A similar complexity may also persist in the 2D limit, highlighting the need for a systematic experimental investigation into which 2D FeS_x phases can actually form. For this purpose, we systematically grow and characterize iron sulfide monolayers on Au(111) via in-situ co-deposition of Fe and S. Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and X-ray photoelectron spectroscopy (XPS) reveal two primary phases: one with a hexagonal atomic arrangement consistent with FeS_2 (Fig. 1a), forming a moiré superstructure, and one with a square arrangement (Fig. 1b). By tuning sulfur exposure, we observe additional phases with varying stoichiometry and atomic arrangement, all belonging to the same 5×5 superstructure family (Fig. 1c). These results confirm the existence of a complex 2D phase diagram for FeS_x monolayers, establishing them as a versatile and tunable platform for exploring 2D magnetism in non-vdW systems.

9:45am **2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of HfSe_3 , Gauthami Viswanath**¹, University of Nebraska-Lincoln, USA; **Alexey Lipatov**, South Dakota School of Mines and Technology; **Alexander Sinitskii**, University of Nebraska-Lincoln, USA; **Jose Avila**, Synchrotron SOLEIL and Université Paris-Saclay, France; **Takashi Komesu**, University of Nebraska-Lincoln, USA; **Maria C. Asensio**, Madrid Institute of Materials Science (ICMM), Spain; **Peter A. Dowben**, University of Nebraska-Lincoln, USA

Abstract: The anisotropic structure of Group 4 transition metal trichalcogenides (TMTCs) have gained significant interest due to their possible application in optoelectronics. In this work, the band structure of quasi one-dimensional HfSe_3 was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). HfSe_3 has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is $-0.27 m_e$ which is smaller compared to the effective hole mass along the direction perpendicular to the chains, $-1.17 m_e$. The effective hole mass extracted from the band structure along different high symmetry directions is compared with that of TiS_3 and ZrS_3 from prior studies.¹ X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of HfSe_3 and will be compared to the XAS spectra of HfS_3

² and TiS_3 and ZrS_3 .³ The metal chalcogenide hybridization for Hf differs from the Ti and Zr trichalcogenides. This may be due to the increase in effective atomic number leading to strong spin-orbit interaction of Hf based TMTCs.

References

- (1) Yi, H.; Gilbert, S. J.; Lipatov, A.; Sinitskii, A.; Avila, J.; Abourahma, J.; Komesu, T.; Asensio, M. C.; Dowben, P. A. The Electronic Band Structure of Quasi-One-Dimensional van Der Waals Semiconductors: The Effective Hole Mass of ZrS_3 Compared to TiS_3 . *J. Phys.: Condens. Matter* **2020**, *32* (29), 29LT01.
- (2) Lipatov, A.; Abourahma, J.; Viswan, G.; Acharya, K.; Paudel, T. R.; Loes, M. J.; Bagheri, S.; N'Diaye, A. T.; Mishra, E.; Ekanayaka, T. K.; Zaz, M.; Rodenburg, J.; Dhinra, A.; Streubel, R.; Dowben, P. A.; Sinitskii, A. Electronic Transport and Polarization-Dependent Photoresponse in Few-Layered Hafnium Trisulfide (HfS_3) Nanoribbons. *J. Mater. Chem. C* **2023**, *11* (28), 9425–9437.
- (3) Gilbert, S. J.; Yi, H.; Paudel, T.; Lipatov, A.; Yost, A. J.; Sinitskii, A.; Tsymbal, E. Y.; Avila, J.; Asensio, M. C.; Dowben, P. A. Strong Metal-Sulfur Hybridization in the Conduction Band of the Quasi-One-Dimensional Transition-Metal Trichalcogenides: TiS_3 and ZrS_3 . *J. Phys. Chem. C* **2022**, *126* (41), 17647–17655.

10:30am **2D+AQS+EM+NS+QS+TF-FrM-10 Applications of Two-dimensional Materials in Energy, Water, and Healthcare, David Estrada**, Boise State University

INVITED

The rapidly evolving field of 2-dimensional (2D) materials continues to open new frontiers in fundamental and applied research across water purification, healthcare, and energy applications. This talk will highlight our recent work in the synthesis of 2D and layered-materials-based inks, enabling energy innovations in microsupercapacitors, triboelectric nanogenerators, and electron devices [1-3]. In water applications, we introduce a flowing electrode capacitive deionization (FE-CDI) system utilizing $\text{Ti}_3\text{C}_2\text{T}_x$ MXene electrodes to efficiently remove and recover ammonia from synthetic wastewater and carbonates from simulated ocean water. This FE-CDI system demonstrates promising potential for managing nitrogen and carbon cycles while improving access to clean water [4]. In healthcare, the intersection of graphene and biology offers a powerful avenue for musculoskeletal tissue engineering, where graphene's exceptional physical properties contribute to fundamental biological insights [5-7]. Lastly, this talk will highlight recent insights into WS_2 nucleation and film growth on sapphire using tungsten hexacarbonyl and hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD 3×2 reactor, with in situ photoreflectometry monitoring. Together, these findings highlight the transformative role of 2D materials beyond graphene in addressing critical engineering challenges and advancing sustainable solutions across diverse fields.

This material is based on research sponsored, in part, by Air Force Research Laboratory under agreement number FA8650-20-2-5506, as conducted through the flexible hybrid electronics manufacturing innovation institute, NextFlex. The U.S. Government is authorized to reproduce and distribute reprints for Governmental purposes notwithstanding any copyright notation thereon. The views and conclusions contained herein are those of the authors and should not be interpreted as necessarily representing the official policies or endorsements, either expressed or implied, of Air Force Research Laboratory or the U.S. Government.

References

- [1] F. Rajabi Kouchi, et al., Small Methods, in revision (2025). [2] C. Hollar, et al., Advanced Materials Technologies, 5 (11), 2000600 (2020). [3] T. Pandhi, RSC Advances, 10, 38205-38219 (2020). [4] N. Mansoor, et al., npj Clean Water, 5 (1), 1-11 (2022). [5] M. Sawyer, et al., ACS Applied Materials & Interfaces, in revision (2025). [6] M. Sawyer, et al., ACS Applied Biomaterials, 6 (9), 3717-3725 (2023). [7] S. M. Frahs, et al., ACS Applied Materials & Interfaces, 11, 41906 – 41924 (2019).

11:00am **2D+AQS+EM+NS+QS+TF-FrM-12 Electronic Structure Modulation in 2D Metal-Graphene-Metal Electrocatalysts for CO_2 Reduction and Hydrogen Evolution Reactions, Arturo Medina**, Ines Saih, Vikas Muralidharan, Georgia Institute of Technology; Jinwon Cho, NREL; Faisal Alamgir, Georgia Institute of Technology

Two-dimensional metal-graphene-metal (M/Gr/M) heterostructures provide a versatile platform for tuning electrocatalytic behavior through controlled interfacial strain and charge redistribution. In previous work, orbital-level descriptors were introduced to explain how pseudo-epitaxial strain alters the electronic structure of ultrathin metals, driving changes in

catalytic activity for the CO₂ reduction reaction (CO₂RR). These concepts were grounded in density functional theory and validated experimentally by correlating spectroscopic strain signatures with shifts in catalytic onset potential.

Building on this framework, the present study expands the scope and range of electrocatalytic reactions studied in M/Gr/M systems. We integrate new measurements on the hydrogen evolution reaction (HER), exploring whether the same strain–electronic structure–reactivity relationships observed in CO₂RR extend to HER kinetics. This includes analysis of onset potentials, overpotentials, and durability across a diverse set of M/Gr/M configurations. Various metals from the 3d to 5d series were investigated as candidate electrocatalysts, deposited as atomically thin layers on single-layer graphene. The graphene is supported by both metal and metal oxide substrates, enabling systematic modulation of ligand effects and interfacial bonding.

To probe strain and charge transfer, we employ a suite of synchrotron-based and lab-scale techniques including carbon K-edge near-edge X-ray absorption fine structure (NEXAFS), extended X-ray absorption fine structure (EXAFS), ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), and electron energy loss spectroscopy (EELS). We track strain-induced modifications in electronic structure through synchrotron-based spectroscopy, revealing systematic correlations between interfacial bonding, orbital structure, and catalytic performance. By comparing systems with and without graphene, we isolate the role of interfacial bonding in modulating both electronic structure and catalytic behavior.

This work experimentally explores theoretical predictions for HER in M/Gr/M systems and provides new insight into how strain-induced orbital modulation governs charge transfer and reactivity across multiple electrocatalytic reactions. Together, these results highlight M/Gr/M structures as a model system for disentangling the fundamental interactions between dimensionality, strain, and catalytic function.

11:15am 2D+AQS+EM+NS+QS+TF-FrM-13 Large Area Nanostructuring of Van Der Waals Materials for Photon Harvesting in the Flat Optics Regime, Matteo Borelli¹, Francesco Buatier de Mongeot, Simone Di Marco, University of Genoa, Italy; Rajesh Chennuboina, University of Genoa, India; Giorgio Zambito, Giulio Ferrando, University of Genoa, Italy; Matteo Gardella, CNR-IMM, Italy; Maria Caterina Giordano, University of Genoa, Italy

2D-Transition Metal Dichalcogenides (2D-TMDs) are two-dimensional semiconductors featuring high optical absorption coefficient combined with good transport and mechanical properties. Although mechanically exfoliated TMDs flakes ensure the best optoelectronic properties, homogeneous large-area growth techniques are mandatory for real-world applications [1,2]. At the same time, in view of light conversion applications in the extreme thickness regime of 2D-TMDs, it is essential to develop effective photon harvesting flat optics strategies derived from nanophotonics.

Here we demonstrate that periodic modulation of few MoS₂ and WS₂ on large area nanostructured samples fabricated by laser interference lithography (either MoS₂ nanostripes arrays or conformal MoS₂ layers grown on top of nanogrooved silica templates). These nanopatterned layers can effectively steer light propagation via Rayleigh Anomalies in the flat optics regime, promoting strong in-plane electromagnetic confinement and broadband omnidirectional photon absorption enhancement, with strong impact in photoconversion. [3,4].

As a case study, we investigate the photocatalytic performance of periodically corrugated MoS₂ layers for photodissociation of Methylene Blue (MB), a widely used yet harmful textile dye. Under optimized angles coupling light to photonic anomalies, MB degradation is two times faster compared to planar MoS₂ films [5]. Additionally, periodic TMD nanostripes serve as directional scatterers, expanding possibilities for advanced light manipulation.

Another major challenge is the scalable fabrication of 2D van der Waals (vdW) heterostructures, often limited to micrometric flakes. Here, we demonstrate large-area (cm²-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS₂-MoS₂ heterostructures endowed with type-II band alignment, forming periodic nanogratings [6]. These engineered large-area

vdW heterostructures enable scalable applications in nanophotonics, photoconversion [7], and energy storage.

We recognize funding by the NEST - Network 4 Energy Sustainable Transition - PNRR partnership.

References

1. M.C. Giordano et al. Adv. Mater. Interfaces, 10 (5), 2201408, 2023.
2. C. Mennucci et al. Adv. Opt. Mater. 9 (2), 2001408, 2021.
3. M. Bhatnagar et al., Nanoscale, 12, 24385, 2020.
4. M. Bhatnagar et al. ACS Appl. Mater. Interf., 13, 11, 13508, 2021.
5. G. Ferrando et al. Nanoscale 15,4, 1953, 2023.
6. M. Gardella et al. Small, 2400943, 2025
7. M. Gardella et al. RSC Appl. Interfaces, 1, 1001-1011, 2024

11:30am 2D+AQS+EM+NS+QS+TF-FrM-14 Exploring the Temperature Coefficient of Frequency (TC_f) in Graphene Trampoline Resonators, Yunong Wang, Nawara Tanzee Minim, S M Enamul Hoque Yousuf, Philip Feng, University of Florida

In this work, we report the first experimental investigation of the temperature coefficient of resonance frequency (TC_f) in graphene trampoline nanoelectromechanical system (NEMS) resonators. Trampoline resonators are widely used in photothermal sensing applications thanks to their superior thermal isolation, enabling high sensitivities. Leveraging the exceptional mechanical strength, thermal stability, and ultralow mass of two-dimensional (2D) materials, graphene trampoline resonators offer a compelling platform for ultrafast infrared (IR) detection. Characterizing the TC_f is essential for designing sensors with stable performance across a wide temperature range, enabling high-resolution IR detection, and developing robust NEMS for advanced light sensing applications.

We use focused ion beam (FIB) to make trampoline structure on our graphene drumhead resonator. The resonance characteristics of the device are measured by using a laser interferometry system. An intensity-modulated 405 nm blue laser is employed to drive the device photothermally, and a 633 nm He-Ne laser is used to read out device resonance motions. The reflected light is detected by a photodetector and converted to an electrical signal, which is analyzed by a network analyzer to obtain the resonance response. To measure the resonance frequency at different temperatures, we regulate the temperature of the device with a metal ceramic heater. The temperature of the chip is measured by a platinum resistance temperature sensor.

We measure the resonance response of the device at different temperatures and extract the resonance frequency and quality (Q) factor by fitting the measured spectrum to the damped simple harmonic resonator model. The drumhead resonator with 20 μm diameter shows a resonance frequency $f=3.44$ MHz and $Q=528$, while after FIB, the trampoline structure achieves a significantly higher $f=13.03$ MHz and $Q=5509$. As temperature increases, the negative thermal expansion of graphene causes an upward shift in resonance frequency. We observe a TC_f exceeding 30,100 ppm/°C from the drumhead structure, extracted from frequency shifts between 30 °C and 60 °C. After we FIB the drumhead structure into a trampoline, we found that the TC_f reduced to 588 ppm/°C.

A lower TC_f value from the stage heating-up method is desirable for stable operation across varying thermal conditions. Due to geometric isolation and reduced thermal coupling to the substrate, the trampoline is expected to exhibit a smaller TC_f than its drumhead counterpart. This makes the trampoline resonator a strong candidate for IR sensing applications that require stable performance over a broad range of temperatures.

Bold page numbers indicate presenter

— A —

A. Dowben, Peter: 2D+AQS+EM+NS+QS+TF-FrM-7, **18**
 Addou, Rafik: 2D+AQS+EM+NS+QS+TF-FrM-3, **17**
 Alamgir, Faisal: 2D+AQS+EM+NS+QS+TF-FrM-12, **18**
 Alanwoko, Onyedikachi:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7, **11**
 Alem, Tinsae: 2D+AQS+EM+NS+QS+TF-FrM-4, **17**
 Allerbeck, Jonas:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, **11**
 Altman, Eric: NS2+2D-TuM-16, **2**
 Alyabev, Danila: 2D-ThP-6, **14**
 Ammerman, Eve:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, **11**
 Aravamudhan, Shyam: 2D-ThP-9, **15**
 Armillotta, Francesco: SS+2D-TuM-6, **3**
 Arnaud, Thiago: 2D+EM+NS+QS+SS+TF-WeA-14, **7**
 Avila, Jose: 2D+AQS+EM+NS+QS+TF-FrM-7, **18**

— B —

Baraldi, Alessandro:
 2D+AQS+EM+NS+QS+TF-FrM-6, **18**
 Barelli, Matteo: 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Barsukov, Yuri: 2D-ThP-4, **14**
 Batzill, Matthias:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7, **11**
 Bazarov, Dmitriy: 2D-ThP-6, **14**
 Beechem, Thomas:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**
 Berti, Andrea: 2D+AQS+EM+NS+QS+TF-FrM-6, **18**
 Bianchi, Marco: 2D+AQS+EM+NS+QS+TF-FrM-6, **18**
 Bobzien, Laric:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, **11**
 Buatier de Mongeot, Francesco:
 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Burch, Kenneth: 2D+AQS+MI+NS+QS+TF-ThA-1, **13**
 Burns, Kory: 2D+AQS+EM+NS+QS+TF-FrM-4, **17**

— C —

C. Asensio, Maria: 2D+AQS+EM+NS+QS+TF-FrM-7, **18**
 Caldwell, Joshua: 2D+EM+NS+QS+SS+TF-WeA-14, **7**
 Carlson, Timothy: MI+2D-WeA-3, **8**
 Carroll, David: MI+2D-WeA-3, **8**
 Ceyer, Sylvia T.: SS+2D-TuM-15, **4**
 Chai, Wenrui: SS+2D-TuM-16, **4**
 Chang, Che-Hao:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16, **12**
 Chang, Tsun-Hsu:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16, **12**
 Chao, Joy: MI+2D-WeA-1, **8**
 Chen, Chen: 2D-ThP-10, **15**
 Chen, Donna: SS+2D-TuM-16, **4**
 Cheng, Cheng-Maw: 2D-ThP-5, **14**
 Chennuboina, Rajesh:
 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Chij, Miaofang: MI+2D-WeA-1, **8**

Chin, Jonathan:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**; 2D+EM+NS+QS+SS+TF-WeA-13, **7**
 Chin, Wai Kiat: MI+2D-WeA-12, **9**
 Cho, Jinwon: 2D+AQS+EM+NS+QS+TF-FrM-12, **18**
 Chuong, Kayla: 2D+EM+NS+QS+SS+TF-WeA-13, **7**
 Cinar, Volkan: SS+2D-TuM-15, **4**
 Corbett, Joseph: 2D+AQS+MI+NS+QS+TF-ThA-5, **13**
 Crommie, Michael: 2D+AQS+MI+NS+QS+TF-ThA-6, **13**

— D —

Danahey, Stephanie: SS+2D-TuM-5, **3**
 Darden, Kenan:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16, **12**
 Das, Sree Sourav: MI+2D-WeA-11, **9**
 Di Marco, Simone: 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Dohnalek, Zdenek: NS2+2D-TuM-14, **1**
 Don Manuwelge Don, Lakshan:
 2D+AQS+MI+NS+QS+TF-ThA-5, **13**
 Dowben, Peter A: MI+2D-WeA-12, **9**
 Dukes, Catherine: SS+2D-TuM-17, **4**
 Durbin, Steven: 2D-ThP-10, **15**
 Duschler, Gerd: 2D+EM+NS+QS+SS+TF-WeA-4, **6**

— E —

Eren, Baran: SS+2D-TuM-13, **4**
 Estrada, David: 2D+AQS+EM+NS+QS+TF-FrM-10, **18**
 Ethier, Stephane: 2D-ThP-4, **14**
 — F —
 Farzandh, Sharfa: SS+2D-TuM-16, **4**
 Feng, Philip: 2D+AQS+EM+NS+QS+TF-FrM-14, **19**
 Ferrando, Giulio: 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Frederiksen, Thomas: SS+2D-TuM-7, **3**
 Frye, Marshall:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**; 2D+EM+NS+QS+SS+TF-WeA-13, **7**

— G —

Gai, Zheng: MI+2D-WeA-11, **9**; MI+2D-WeA-4, **9**
 Gardella, Matteo: 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Garten, Lauren:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**; 2D+EM+NS+QS+SS+TF-WeA-13, **7**
 Gayle, Amari: 2D+EM+NS+QS+SS+TF-WeA-15, **8**
 Geohagan, David:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, **11**
 Geohagan, David B.: 2D+EM+NS+QS+SS+TF-WeA-4, **6**
 Ghimire, Nirmal: MI+2D-WeA-11, **9**
 Gillum, Maxwell: SS+2D-TuM-5, **3**
 Giordano, Maria Caterina:
 2D+AQS+EM+NS+QS+TF-FrM-13, **19**
 Glavin, Nicholas R.: 2D+EM+NS+QS+SS+TF-WeA-5, **6**
 Gonzalez, Alexis: SS+2D-TuM-5, **3**
 Gröning, Oliver:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, **11**
 Gutiérrez, Oliver: NS2+2D-TuM-14, **1**
 — H —
 Harris, Sumner B.: 2D+EM+NS+QS+SS+TF-WeA-4, **6**
 Harrison, Ian: MI+2D-WeA-11, **9**

Hasan, Abir: 2D+AQS+EM+NS+QS+TF-FrM-4, **17**
 He, Xu: 2D+AQS+EM+NS+QS+TF-FrM-5, **17**; 2D-ThP-3, **14**
 He, Zehao: 2D+AQS+MI+NS+QS+TF-ThA-6, **13**
 Henkelman, Graeme: SS+2D-TuM-16, **4**
 Her, Tsing-Hua:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16, **12**
 Hilse, Maria: 2D+EM+NS+QS+SS+TF-WeA-13, **7**; 2D+EM+NS+QS+SS+TF-WeA-16, **8**
 Hofmann, Philip: 2D+AQS+EM+NS+QS+TF-FrM-6, **18**
 Hofmann, Stephan: 2D+EM+NS+QS+SS+TF-WeA-1, **6**
 Houston, Austin:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, **11**; 2D+EM+NS+QS+SS+TF-WeA-4, **6**
 Hsu, Pin-Jui: 2D-ThP-5, **14**
 Huang, Hong: 2D-ThP-12, **15**; 2D-TuA-13, **5**
 Huang, Jing-Yue: 2D-ThP-5, **14**
 Huang, Shengxi: 2D+EM+NS+QS+SS+TF-WeA-9, **6**
 Huberich, Lysander:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, **11**

— I —

Isotta, Eleonora:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, **11**

— J —

Jäggi, Noah: SS+2D-TuM-17, **4**
 Jang, Sieun: NS2+2D-TuM-17, **2**
 Jeng, Horng-Tay: 2D-ThP-5, **14**
 Ji, Zhurun:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-13, **12**
 Jin, Rongying: MI+2D-WeA-4, **9**
 Johnson, Kedar: 2D+EM+NS+QS+SS+TF-WeA-15, **8**
 Jung, Ju-Hyun:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, **11**
 — K —
 Kadaba, Swathi: MI+2D-WeA-3, **8**
 Kaganovich, Igor: 2D-ThP-4, **14**
 Kahn, Antoine: 2D+AQS+EM+NS+QS+TF-FrM-5, **17**; 2D-ThP-3, **14**
 Kang, Kyungnam:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, **11**
 Katoch, Jyoti: MI+2D-WeA-5, **9**
 Kawasaki, Jason: 2D-TuA-15, **5**
 Kay, Bruce: NS2+2D-TuM-14, **1**
 Khalid, Shoaib: 2D-ThP-4, **14**
 Killelea, Dan: SS+2D-TuM-5, **3**
 Kim, Cheol-Joo:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, **11**
 Kim, Jiyoung: NS2+2D-TuM-15, **1**
 Kim, Songkil: NS2+2D-TuM-17, **2**
 Knight, Jeremy:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**
 Ko, Wonhee: NS2+2D-TuM-13, **1**
 Komesu, Takashi: 2D+AQS+EM+NS+QS+TF-FrM-7, **18**
 Koneru, Dheeraj: 2D-ThP-11, **15**
 Kong, Dejia: MI+2D-WeA-11, **9**; MI+2D-WeA-4, **9**
 Kovach, Samuel:
 2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, **12**

Author Index

Krane, Nils:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, 11

Krayev, Andrey:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, 11

Kuo, Shu-Hua: 2D-ThP-5, 14

— L —

Lacovig, Paolo: 2D+AQS+EM+NS+QS+TF-FrM-6, 18

Lado, Jose: NS2+2D-TuM-13, 1

Lai, Rebecca: MI+2D-WeA-12, 9

Lan, Ye-Shun: 2D-ThP-5, 14

Law, Stephanie: 2D+EM+NS+QS+SS+TF-WeA-12, 7; 2D+EM+NS+QS+SS+TF-WeA-13, 7; 2D+EM+NS+QS+SS+TF-WeA-3, 6

Le, Dan: NS2+2D-TuM-15, 1

Lee, Christopher: NS2+2D-TuM-14, 1

Lee, Minjong: NS2+2D-TuM-15, 1

Lee, Seng Huat: MI+2D-WeA-11, 9

Leff, Mysidia: 2D+AQS+MI+NS+QS+TF-ThA-5, 13

Li, An-Ping: SS+2D-TuM-1, 2

Li, Rockwell: SS+2D-TuM-3, 2

Li, Xufan:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, 11

Li, Yiming: SS+2D-TuM-3, 2

Lin, Yen-Hui: 2D-ThP-5, 14

Lipatov, Alexey: 2D+AQS+EM+NS+QS+TF-FrM-7, 18

Liu, Derrick: 2D+EM+NS+QS+SS+TF-WeA-13, 7

Lizzit, Silvano: 2D+AQS+EM+NS+QS+TF-FrM-6, 18

— M —

Mader, Katherine: SS+2D-TuM-16, 4

Mahapatra, Mausumi: NS2+2D-TuM-14, 1

Makin, Robert: 2D-ThP-10, 15

Maksymovych, Petro: NS2+2D-TuM-13, 1

Mannix, Andrew:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, 11

Mao, Zhiqiang: MI+2D-WeA-11, 9

Marcus, Gabriel: MI+2D-WeA-3, 8

Maria, Jon-Paul: 2D+EM+NS+QS+SS+TF-WeA-14, 7

McDonnell, Stephen:
2D+AQS+EM+NS+QS+TF-FrM-4, 17

Medina, Arturo: 2D+AQS+EM+NS+QS+TF-FrM-12, 18

Messeccar, Andrew: 2D-ThP-10, 15

Minim, Nawara Tanzee:
2D+AQS+EM+NS+QS+TF-FrM-14, 19

Mirhosseini, Motahhare: MI+2D-WeA-3, 8

Moore, Joel: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Morel, Cassandre: SS+2D-TuM-17, 4

Moses, Isaiah: 2D+EM+NS+QS+SS+TF-WeA-12, 7; 2D-ThP-10, 15

Muralidharan, Vikas:
2D+AQS+EM+NS+QS+TF-FrM-12, 18

— N —

Narayan, Dushyant: NS2+2D-TuM-15, 1

Nayir, Nadire: 2D+EM+NS+QS+SS+TF-WeA-13, 7

Ni, Haoyang: MI+2D-WeA-1, 8

— O —

Ortega-Guerrero, Andres:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, 11

Osterholm, Anna:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12

— P —

Paillard, Charles:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12

Papaj, Michal: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Park, Jewook: MI+2D-WeA-14, 10

Park, Seonha: NS2+2D-TuM-17, 2

Park, Taegwan:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, 11

Peiris, Frank:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12

Pérez, Rubén: NS2+2D-TuM-16, 2

Pignedoli, Carlo:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, 11

Puretsky, Alexander:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, 11; 2D+EM+NS+QS+SS+TF-WeA-4, 6

— Q —

Qdemat, Asma: MI+2D-WeA-13, 10

Qiao, Mengxiong: SS+2D-TuM-16, 4

Qiu, Zi Qiang: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Quintero Borbon, Fernando:
2D+AQS+EM+NS+QS+TF-FrM-3, 17

— R —

Rajapakse, Nirosha:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-7, 11

Redwing, Joan: 2D-ThP-10, 15

Reinhart, Wesley: 2D+EM+NS+QS+SS+TF-WeA-12, 7; 2D-ThP-10, 15

Reinke, Petra: MI+2D-WeA-11, 9

Robinson, Joshua A.:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, 11

Rohan, Jacob N.: NS2+2D-TuM-15, 1

Rosenberger, Matthew: NS2+2D-TuM-7, 1

Rouleau, Christopher:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, 11

Rousseau, Robin: 2D+EM+NS+QS+SS+TF-WeA-15, 8

Roy, Joy: 2D+AQS+EM+NS+QS+TF-FrM-3, 17

— S —

Saih, Ines: 2D+AQS+EM+NS+QS+TF-FrM-12, 18

Sakib, Md. Sakauat Hasan:
2D+AQS+MI+NS+QS+TF-ThA-5, 13

Sarker, Mamun: 2D-TuA-14, 5

Schuler, Bruno:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1, 11

Schwarz, Udo: NS2+2D-TuM-16, 2

Sen, Dilara:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12

Senevirathna, M.K. Indika:
2D+EM+NS+QS+SS+TF-WeA-15, 8

Serna-Sanchez, Elizabeth: SS+2D-TuM-5, 3

Sharp, Marcus: NS2+2D-TuM-14, 1

Shendokar, Sachin: 2D-ThP-9, 15

Shi, Sufei:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-5, 11

Shields, Seth: 2D+AQS+MI+NS+QS+TF-ThA-5, 13

Shirodkar, Soham: NS2+2D-TuM-15, 1

Shukla, Nikhil: 2D+AQS+EM+NS+QS+TF-FrM-4, 17

Sibener, Steven: SS+2D-TuM-4, 3

Siegfried, Peter: MI+2D-WeA-11, 9

Singh, Santosh K.: SS+2D-TuM-15, 4

Singh, Simran: MI+2D-WeA-9, 9

Sinitiskii, Alexander: 2D+AQS+EM+NS+QS+TF-FrM-7, 18; 2D-TuA-14, 5

Smith, Walter:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12

Spangler, Ryan: 2D+EM+NS+QS+SS+TF-WeA-14, 7

St. Martin, Jacob: MI+2D-WeA-11, 9

Stolz, Samuel: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Subedi, Arjun: MI+2D-WeA-12, 9

Sutter, Eli:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-15, 12; 2D+EM+NS+QS+SS+TF-WeA-11, 7

Sutter, Peter:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-15, 12; 2D+EM+NS+QS+SS+TF-WeA-11, 7

— T —

T.N'Daiye, Alpha: MI+2D-WeA-12, 9

Toph, Emily: 2D-ThP-1, 14

Torrisi, Felice: 2D+AQS+EM+NS+QS+TF-FrM-1, 17

Trice, Ryan: 2D+EM+NS+QS+SS+TF-WeA-12, 7; 2D+EM+NS+QS+SS+TF-WeA-3, 6

Trujillo Mulero, Jara: NS2+2D-TuM-16, 2

— V —

Valencia Acuna, Pavel:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, 11

van Duin, Adri: 2D+EM+NS+QS+SS+TF-WeA-13, 7

Vishal, Kumar: 2D-ThP-12, 15; 2D-TuA-13, 5

Viswan, Gauthami: 2D+AQS+EM+NS+QS+TF-FrM-7, 18; MI+2D-WeA-12, 9

Vlassiounk, Ivan: 2D+EM+NS+QS+SS+TF-WeA-4, 6

Vogel, Eric: 2D-ThP-1, 14

— W —

Wagner, Brent: 2D-ThP-1, 14

Wagner, Joshua: SS+2D-TuM-4, 3

Wahl, Joshua:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-17, 12; 2D+EM+NS+QS+SS+TF-WeA-13, 7

Wallace, Robert: 2D+AQS+EM+NS+QS+TF-FrM-3, 17

Wang, Chih-Feng:
2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-4, 11

Wang, Feng: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Wang, Hailiang: NS2+2D-TuM-16, 2

Wang, Mengyi: 2D+EM+NS+QS+SS+TF-WeA-13, 7

Wang, Pingshan: SS+2D-TuM-3, 2

Wang, Tianye: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Wang, Xinzhe: NS2+2D-TuM-16, 2

Wang, Yan-Qi: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Wang, Yunong: 2D+AQS+EM+NS+QS+TF-FrM-14, 19

Wijerathna, A.M. Shashika D.: SS+2D-TuM-3, 2

Williams, Michael D.: 2D+EM+NS+QS+SS+TF-WeA-15, 8

Woodson, Adam: SS+2D-TuM-17, 4

Wright, Elycia: 2D+EM+NS+QS+SS+TF-WeA-15, 8

Wu, Wenjing: 2D+EM+NS+QS+SS+TF-WeA-9, 6

Wysocki, Alexander: MI+2D-WeA-12, 9

Author Index

— X —

Xiao, Kai:

2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3, **11**; 2D+EM+NS+QS+SS+TF-WeA-4, 6

— Y —

Yao, Hsin-Yu:

2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16, 12

Yimam, Daniel T.: 2D+EM+NS+QS+SS+TF-WeA-4, **6**

Yousuf, S M Enamul Hoque:

2D+AQS+EM+NS+QS+TF-FrM-14, 19

Yu, Mingyu: 2D+EM+NS+QS+SS+TF-WeA-12, 7; 2D+EM+NS+QS+SS+TF-WeA-13, 7

— Z —

Zahl, Percy: NS2+2D-TuM-16, 2

Zambito, Giorgio: 2D+AQS+EM+NS+QS+TF-FrM-13, 19

Zaz, Mohammad Zaid: MI+2D-WeA-12, **9**

Zebarjadi, Mona: MI+2D-WeA-11, 9

Zeng, Yihang: 2D+AQS+MI+NS+QS+TF-ThA-3, **13**

Zhang, Canxun: 2D+AQS+MI+NS+QS+TF-ThA-6, 13

Zhang, Qihua: 2D+EM+NS+QS+SS+TF-WeA-13, 7

Zhang, Yuan: SS+2D-TuM-3, 2

Zhao, He: SS+2D-TuM-3, 2

Zhao, Liuyan: 2D+AQS+MI+NS+QS+TF-ThA-7, **13**

Zhu, Tiancong: 2D+AQS+MI+NS+QS+TF-ThA-6, **13**

Zhu, Yifeng: NS2+2D-TuM-14, 1

zhuang, yan: 2D-TuA-13, 5

Zhuang, Yan: 2D-ThP-12, 15

Zirnheld, Markus: SS+2D-TuM-3, 2