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

### Multimodal Techniques in Surface and Interface Engineering at the Nanoscale

**Moderators: Aubrey Hanbicki**, Laboratory for Physical Sciences, **Mausumi Mahapatra**, Loyola University Chicago

9:15am **NS2+2D-TuM-6 On-Surface Synthesis on Inert and Reactive Surfaces***, Rafał Zuzak, **Szymon Godlewski**,* Jagiellonian University, Poland

In recent years the on-surface manipulation and chemical reactions created a playground for atomically precise synthesis and development of new atomic and molecular nanostructures. However, the abilities to produce desired systems are limited, among others, by relying on the catalytic role of the substrate in initiating selected reactions. Therefore striving for the generation of desired systems forces the search of new reaction pathways and catalytic transformations.

In this talk I will demonstrate our approach based on the application of inert and reactive surfaces in the on-surface experiments. First, I will discuss the synthesis of the acene series with the first observation of spin excitation recorded for tridecacene [1]. Subsequently the focus will be shifted toward non-metallic substrates and the new pathway for the synthesis of new molecular compounds [2] with prospects for circumventing the need to exploit the catalytic role of metallic substrates [3]. Finally, concepts for on-surface reactions on chemically active lithium substrates will be presented. They will be focused on preventing catastrophic dendrite formation in battery electrodes.

The research was supported by the National Science Center, Poland: 2019/35/B/ST5/02666, 2022/04/Y/ST5/00156.

References

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[2] R. Zuzak et al., *ACS Nano*, **17**, 2580-2587 (2023)

[3] R. Zuzak et al., *Nat. Commun.* **16**, 691 (2025)

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 crystal[1]. 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 crystal[2]. 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.

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(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/$Fe_3O_4$(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/$Fe_3O_4$(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 $Fe_3O_4$(001). Using X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM), we investigated the activity of such model systems towards $H_2$ and their stability in reducing environments. Our results show that the atomically dispersed $Rh_{ad}$ and $Rh_{oct}$ species do not activate $H_2$, which would result in the formation of surface hydroxyls on $Fe_3O_4$(001). In contrast, the presence of $Rh_{met}$ in $H_2$ results in the formation of hydroxyls and subsequent etching of the $Fe_3O_4$(001) at higher temperatures (≥ 500 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/$Fe_3O_4$ 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 $H_2$ atmosphere.

11:30am **NS2+2D-TuM-15 Hybrid ALD-MLD HfOx 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 $TiO_2$ 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-$sp^2$ 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.

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

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

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11:45am **NS2+2D-TuM-16 Quantitative Comparative Force Spectroscopy on Molecules***, Xinzhe 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 ($(NH_2)_4$CoPc) adsorbed on Ag(111), both of which are of interest in $CO_2$ 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 $NH_2$ 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 $MoS_2$ during CVD Growth***, **Seonha Park,** Sieun Jang, Songkil Kim,* School of Mechanical Engineering, Pusan National University, Republic of Korea

Molybdenum disulfide ($MoS_2$) is a promising semiconducting material due to its atomic flatness and high carrier mobility. In particular, chemical vapor deposition (CVD)-grown $MoS_2$ has been widely explored for electronic applications owing to its high quality and scalability. However, the mismatch in thermal expansion coefficients between $MoS_2$ and the growth substrate induces strain in $MoS_2$ 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 $MoS_2$. To investigate the role of $MoS_2$–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 $sp^2$-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 $sp^2$-hybridized O dopant hosts a characteristic$\pi$-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 dibromo-p-pentaphenyl (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 ($C_6H_6$) 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 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 Wagner***[1], *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 Armillotta***, 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.

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[1] **SSD Morton S. Traum Award Finalist**

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

11:00am **SS+2D-TuM-13 Strongly Correlated Molecules on Surfaces: SPM Study***, **Pavel Jelinek**,* Institute of Physics CAS, Prague, Czechia **INVITED**

Recent progress in on-surface synthesis enabled the preparation of polyradical strongly correlated molecules [1], which are not available by traditional synthetic approaches in solution. However, the characterization of the electronic structure of such molecules with non-trivial electronic structure using scanning tunneling microscopy (STM) provides new challenges. First, interpreting scanning tunneling spectroscopy (STS) maps of the polyradical molecules based on standard one-electron STM theory [2] often fails. Thus, for a precise interpretation of STS maps and their connection to the electronic structure of molecules, a theoretical description, including non-equilibrium tunneling processes going beyond one-electron molecular orbitals, is required. We will show that for an accurate interpretation of strongly correlated molecules; it is necessary to describe the process of removing/adding an electron within the formalism of many-particle wave functions for the neutral and charged states. This can be accomplished by the concept of so-called Dyson orbitals [3]. We will discuss the examples where the concept of Dyson orbitals is mandatory to reproduce experimental STS data.

Secondly, one challenge is to determinethe magnetic ground state unambiguously or visualize the anisotropic exchange interaction at the level of a single molecular magnet. We demonstrate that STS combined with nickelocene-functionalized scanning probe microscopy can determine the magnetic ground state of single, strongly correlated polyradical molecules with nearly degenerated electronic states. Moreover, this technique enables mapping the anisotropic exchange interaction of individual molecules with submolecular resolution.

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11:30am **SS+2D-TuM-15 Vibrational Spectroscopic Identification of Carbon Absorbed Beneath the Metal Surface***, **Santosh K. Singh**, 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 Determining How Ion Clustering Impacts Interfacial Properties and Electrocatalytic Activity***, **Samuel Johnstone**, Matthew Gebbie,* University of Wisconsin - Madison

Electric double layers (EDLs) form at the interface of charged solid electrodes and liquid electrolytes, where intermolecular forces cause electrolyte ions to rearrange within the interfacial environment. The properties of this region, including the chemical species present and the magnitude of local electric fields, determine the environment for electrochemical reactions. Controlling EDL properties can enhance electrocatalytic activity, but a general understanding of EDL structure remains limited in reactive systems, especially those utilizing large polarizations and high ion concentrations. Under these conditions, multi-ion clusters and correlated ion networks dominate the interface and make interfacial properties difficult to predict using classical models, as they assume noninteracting ions. Here, we use electrochemical impedance spectroscopy to explore how the interfacial behavior of ionic liquids dissolved in various organic solvents changes with surface charge and bulk ion concentration. We study solutions of acetonitrile, dimethyl sulfoxide, and propylene carbonate and use complementary molecular dynamics simulations to gain an understanding into how clustering alters the EDL structure. We then connect these results to electrocatalytic activity by studying the electrochemical $CO_2$ reduction reaction in each organic solvent. We find peak $CO_2$ electroreduction rates correspond to the conditions where the number of mobile charge carriers, or the sum of isolated ions and charged ion clusters in solution, are also maximized in all solvents tested. Overall, we highlight the critical impact of ion correlations in electrochemical systems and show that modulating interfacial ion clustering can be an effective method to accelerate electrochemical reactions.

12:00pm **SS+2D-TuM-17 Bimodal Sputter Depletion of Adsorbed Na from Granular, Regolith-Like, Olivine Targets***, **Adam Woodson**, Cassandre Morel, Noah Jäggi, 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 208 W - Session 2D+EM+NS+QS+SS+TF-WeA

### 2D Materials: Synthesis and Processing

**Moderators: Peter Sutter**, University of Nebraska, **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 constraint 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 howdirect 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**, 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 Al2O3 (0001) and Si (111) substrates using an atomic layer deposition SiO2 mask. Etching of the SiO2 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 variously 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**, Sumner B. Harris,* Oak Ridge National Laboratory, USA*; Austin Houston,* University of Tennessee Knoxville*; Ivan Vlassiouk,* Oak Ridge National Laboratory, USA*; Alexander Puretzky,* Oak Ridge Natinal 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,*** 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 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 SnSe[1] 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 thecarrier 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 uncleaved 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-$MoO_3$ Nanosheets on Sapphire***, **Ryan Spangler**,* Pennsylvania State University*; Thiago Arnaud, Joshua Caldwell,* Vanderbilt University*; Jon-Paul Maria,* Pennsylvania State University

α-$MoO_3$ 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-$MoO_3$ exhibits extreme anisotropy of the dielectric function, enabling in-plane and out-of-plane elliptic or even hyperbolic behavior at various wavelengths. Therefore, α-$MoO_3$ 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-$MoO_3$. In this work, we describe a process for the growth of ultra-large, thin, and atomically smooth single crystals of α-$MoO_3$ 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-$MoO_3$ 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-$MoO_3$ 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-$MoO_3$ 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 $ReS_2$ Grown by CVD**, ***Elycia Wright****, Kedar Johnson, Amari Gayle, Robin Rouseau, M.K. Indika Senevirathna, Michael D. Williams,* Clark Atlanta University

Rhenium disulfide ($ReS_2$) 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 $ReS_2$ holds remarkable properties, including anisotropic electronic, optical, and mechanical characteristics. Unlike other TMDs such as $MoS_2$, $MoSe_2$, $WS_2$, and $WSe_2$, $ReS_2$ 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 $ReS_2$ particularly promising for applications in highly responsive photodetectors. To maximize the potential of $ReS_2$ 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 $ReS_2$ can lead to variations in growth rates in different directions, resulting in multidomain structures that complicate the production of single-crystal $ReS_2$ on a large scale.

In this study, we will synthesize $ReS_2$ 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 $ReS_2$.

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 $cm^2/Vs$, 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,*** One Bethel Valley Rd*; Joy Chao, Haoyang Ni,* One Bethel Valley Road **INVITED**

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

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

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

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

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

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

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

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

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

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

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

4:45pm **MI+2D-WeA-11 Surface Electronic Structure Comparison of Fe-Intercalated and 2h-$TaS_2$***, **Dejia Kong**, Sree Sourav Das, Jacob St. Martin,* University of Virginia, USA*; Peter Siegfried,* George Mason University*; Zhiqiang Mao, Seng Huat Lee,* The Pennsylvania State University*; Ian Harrison,* University of Virginia*; Nirmal Ghimire,* University of Notre Dame*; Mona Zebarjadi,* University of Virginia, USA*; Zheng Gai,* Oak Ridge National Laboratory, USA*; Petra Reinke,* University of Virginia, USA

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

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

5:00pm **MI+2D-WeA-12 Strain Induced Magnetism and Interfacial Effects in Pd/$Mos_2$(0001) Heterostructures***, **Bushra Ashraf**,* University of Central Florida

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

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

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

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

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

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

5:30pm **MI+2D-WeA-14 Emergence of local magnetic moment in ternary $TaWSe_2$ single crystal via atomic clustering**, ***Jewook Park,*** One Bethel Valley Rd. Bldg. 8610, MS-6487

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

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

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

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

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

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

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

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

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[1] **Falicov Student Award Finalist**

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

### 2D Materials: Optoelectronics and Moire Excitons

**Moderators: Shengxi Huang**, Rice University, **Daniel Yimam**, Oak Ridge Natinal 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.

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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 Puretzky,* 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 Geohegan,* 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 MoS2 / WS2 @ 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 $WSe_{2,}MoSe_{2,}$ 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**, Nirosha 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 $MoTe_2$ 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 $MoTe_2$ with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

9:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-8 Quantum Confining Excitons with Electrostatic Moiré Superlattice***, **Liuxin Gu**, Lifu Zhang, Sam Felsenfeld,* University of Maryland, College Park*; Rundong Ma,* University of Maryland College Park*; Suji Park, Houk Jang,* Brookhaven National Laboratory*; Takashi Taniguchi, Kenji Watanabe,* National Institute for Materials Science, Japan*; You Zhou,* University of Maryland, College Park

Quantum confining excitons has been a persistent challenge in the pursuit of strong exciton interactions and quantum light generation. Unlike electrons, which can be readily controlled via electric fields, imposing strong nanoscale potentials on excitons to enable quantum confinement has proven challenging. In this study, we utilize piezoelectric force microscopy to image the domain structures of twisted hexagonal boron nitride (hBN), revealing evidence of strong in-plane electric fields at the domain boundaries. By placing a monolayer $MoSe_2$ only one to two nanometers away from the twisted hBN interface, we observe energy splitting of neutral excitons and Fermi polarons by several millielectronvolts at the moiré domain boundaries. By directly correlating local structural and optical properties, we attribute such observations to excitons confined in a nanoscale one-dimensional electrostatic potential created by the strong in-plane electric fields at the moirédomain boundaries. Intriguingly, this 1D quantum confinement results in pronounced polarization anisotropy in the excitons' reflection and emission, persistent to temperatures as high as ~80 Kelvins. These findings open new avenues for exploring and controlling strongly interacting excitons for classical and quantum optoelectronics.

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.

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11:45am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-16 Electrical Manipulation of Valley Polarized Charged Excitons in 2d Transition Metal Dichalcogenides***, **Kuan Eng Johnson Goh**,* Agency for Science Technology and Research (A*STAR), 2 Fusionopolis Way, Innovis #08-03, Singapore 138634, Singapore

The control of excitons in 2-dimensional (2D) Transition Metal Dichalcogenide (TMD) semiconductors is a key enabler for their use in optoelectronic, valleytronic and quantum applications. Reproducible electrical control of excitons remains elusive as excitons are intrinsically charge neutral quasiparticles. Here, we demonstrate that charge defects present in 2D TMDs like single-layer H-phase $WS_2$ [1,2], could be advantageous for electrical control through the coherent coupling of the exciton or biexciton with intrinsic charges in the single-layer $WS_2$, thus enabling a simple and robust method for electrical manipulation of the degree of valley polarization from <10% to >60% [3]. Such robust electrical tunability of the spectral resonance of the charged states indicates resonant control of valley polarization by exploiting the intricate interplay between the charged and neutral exciton/biexciton states, representing a key advance towards using the valley degree of freedom as an alternate information carrier.[4].

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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 revealshow 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 showsdifferent 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 relevant2D materials for scalability.

## 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 FeTe0.55Se0.45. 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 $MoTe_2$***, **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 $MoTe_2$-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 $Bi_2$-$Bi_2Se_3$***, 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'-$WTe_2$***, **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'-$WTe_2$, 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'-$WTe_2$ 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'-$WTe_2$ films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-$WTe_2$ 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.

4:15pm **2D+AQS+MI+NS+QS+TF-ThA-9 High-Efficiency Optoelectronic Training of Two-Dimensional Magnets***, **Ti Xie**, Jierui Liang,* University of Maryland College Park*; Dhritiman Bhattacharya,* Georgetown University*; Hasitha Suriya Arachchige,* University of Tennessee, Knoxville*; Victor Yakovenko,* University of Maryland College Park*; David Mandrus,* University of Tennessee, Knoxville*; Zi Qiang Qiu,* University of California at Berkeley*; Kai Liu,* Georgetown University*; Cheng Gong,* University of Maryland College Park

A magnetic material, while dressed with different spin configurations, can host a variety of emergent phenomena such as chiral domain walls, skyrmions, and Majorana fermions. Traditional preparation of various spin textures in magnetic films by transforming an already established spin pattern demands intensive energy to cause spin flipping or domain wall motion. In contrast, engineering the phase transition kinetics potentially opens up new avenues to achieve desired spin configurations. The two-dimensional (2D) layered magnets, owing to the ultra-thinness, allow the magnetism control by various external stimuli, among which optical approaches promise non-destructive manipulation, both locally and globally. In this talk, I will introduce how we demonstrated a low-power optical control of 2D magnets. By perturbing the phase transition kinetics, we found that optically excited electrons are multiple orders of magnitudes more effective than electrostatically doped electrons in influencing magnetic domains. Our low-power optical operation paves the new avenue to efficiently engineer 2D spin textures for a plethora of emergent quantum phenomena.

## 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) semiconductor[1] with a large room-temperature electron mobility of approximately $10^3$ cm$^2$ V$^{-1}$ s$^{-1}$, is a promising material for high-sensitivity Hall sensors[2], ballistic transistors,[3] and non-volatile memory applications.[4]The In-Se system contains many different stable phases[5] 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.

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**2D-ThP-2 Ultra-sensitive Nitrogen Dioxide Detection Based on MoS2/Porous Silicon***, **Prachi Gurawal**,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA*; Mohit Madaan,* DEPARTMENT OF PHYSICS, IIT ROORKEE, INDIA*; SOMDATTA SINGH,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA*; GAURAV MALIK,* Semiconductor Physics Research Center, JBNU, Republic of Korea*; VIVEK KUMAR MALIK,* DEPARTMENT OF PHYSICS, IIT ROORKEE, INDIA*; RAMESH CHANDRA,* INSTITUTE INSTRUMENTATION CENTRE, IIT ROORKEE, INDIA

The development of high-performance gas sensing devices based on transition metal dichalcogenides (TMDs) has generated considerable research interest in the efficient detection of hazardous gases. The sensing performance of TMDs material-based sensors can be effectively enhanced by increasing the substrate's surface area, i.e., creating the porosity in the substrate to increase the number of sites available for interaction with the target gas molecules. Here, we have grown the porosity on the n-type (100) silicon substrate surface to increase the deposition area of molybdenum disulfide ($MoS_2$). The DC magnetron sputtering is used to synthesize the $MoS_2$ on a porous silicon (PSi) substrate for $NO_2$ gas detection. The fabricated sensor $MoS_2$@PSi exhibited the maximum response at an operating temperature of 120 ℃ at 100 ppm concentration of $NO_2$ gas. The sensor is able to detect the significant low gas concentration of 50 ppb $NO_2$ gas at the operating temperature. Also, the selectivity measurements showed the sensor possessed the best sensitivity for $NO_2$ among $H_2$, CO, and $NH_3$ gases, making it a potential sensor for $NO_2$ gas sensing.

**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+$C_{60}$ to endohedral fullerene Fe@$C_{60}$ through scattering of Fe+$C_{60}$ 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 $C_{60}$ exofullerenes heated to 900 K, i.e. Fe+$C_{60}$ 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.

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**2D-ThP-7 Monolayer H-BN Excitonic Emission Energy Determined by Low Electron Energy Cathodoluminescence***, **Victor Feitosa Marques de Oliveira,** Fábio Costa, Catalina Ruano,* "Gleb Wataghin" Institute of Physics, Brazil*; Guillaume Cassabois,* Laboratoire Charles Coulomb UMR 5221 CNRS-Université de Montpellier, France*; Jonathan Bradford, Peter Beton, Sergei Novikov,* School of Physics and Astronomy, University of Nottingham, UK*; Bernard Gil,* Laboratoire Charles Coulomb UMR 5221 CNRS-Université de Montpellier, France*; Luiz Fernando Zagonel,* "Gleb Wataghin" Institute of Physics, Brazil

Hexagonal boron nitride (h-BN) is a 2D material with a wide electronic band gap. It exhibits bright light emissions in the deep ultraviolet (DUV) spectral range, despite its indirect bandgap in bulk or few-layer forms [1]. Experimental evidence of the indirect-to-direct bandgap crossover in h-BN monolayers (ML) was first reported in 2019 by combining photoluminescence (PL) and reflectance spectroscopies [2]. A peak around 6.1 eV, attributed to the direct excitonic emission from ML h-BN, was observed in PL measurements. However, the presence of complex Raman signals near this peak posed challenges for spectral analysis. In this study, to accurately determine the excitonic emission energy, we performed cathodoluminescence (CL) spectroscopy in a Low Temperature Scanning Tunneling Microscope (STM) operating under ultra-high vacuum conditions [3]. We characterized h-BN samples grown on Highly Oriented Pyrolytic Graphite (HOPG) by high-temperature molecular beam epitaxy and used STM imaging and spectroscopy to select monolayer regions. By exciting the sample luminescence with low-energy electrons (100 to 300 eV), we were able to avoid Raman signals and have sufficient excitation cross-section to reach a good signal to noise ratio even in an atomically thin material.

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**2D-ThP-8 Graphene oxide and Pd nanozyme- Based Carriers Enhance Neurotrophic Peptide Activity***, **Diego La Mendola,*** University of Pisa, Italy*; Cassandra Pichry,* University of Mons, Belgium*; Stefania Sciacca, Carmela Bonaccorso,* University of Catania, Italy*; Lorenzo Chiaverini, Tiziano Marzo,* University of Pisa, Italy*; Crsitina Satriano,* University of Catania, Italy

Graphene oxide (GO) and palladium (Pd) nanozymes, especially in the form of nanocomposites, are being explored for applications in neural engineering, particularly in GP8 cell-based systems. GO's unique properties and the catalytic activity of Pd nanozymes offer potential for stimulating neural cell growth, differentiation, and regeneration.

Neurotrophins (NTs) are secreted proteins crucial for the development and survival of the nervous system. NTs also promote axon regeneration, guide stem cell differentiation into neuronal lineages, modulate synaptic plasticity, and stimulate angiogenesis. The main NTs include nerve growth factor (NGF), brain-derived neurotrophic factor (BDNF), neurotrophin-3 (NT-3), and neurotrophin-4 (NT-4).Due to their biological properties, NTs are considered promising therapeutic agents for treating neurodegenerative diseases, spinal cord injuries, and peripheral nerve damage. However, their clinical application is limited by poor plasma stability and side effects, such as pain.To address these challenges, we synthesized peptides corresponding to the N-terminal domains of NGF, BDNF, and NT-3, named NGF(1–14), BDNF(1–12), and NT-3(1–13), respectively. These peptides mimic the biological activity of their full-length neurotrophins.

We then used GOto develop a delivery platform capable of carrying and enhancing the activity of these peptides.The spontaneous physisorption of neurotrophic peptides onto GO surfaces occurs via supramolecular interactions, allowing the formation of a stable hybrid platform. These biointerfaces were characterized using vUV-VIS spectroscopy, fluorescence spectroscopy, confocal microscopy, and atomic force microscopy (AFM). Molecular dynamics simulations were also conducted to gain deeper insight into the interactions at the atomic level and to visualize the behavior of the platform in aqueous saline solution.

The biological activity of these systems was evaluated through in vitro experiments on the GP8 cell line. Overall, this hybrid platform shows promise for applications in neural tissue engineering due to its ability to support neurite outgrowth, synapse formation, cell migration, and blood vessel formation.

Acknowledgments

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under the program PRIN 2022 - Progetti di Rilevante Interesse Nazionale,project code: 2022ALJRPL "Biocompatible nanostructures for the chemotherapy treatment of prostate cancer"CS and CB acknowledge the financial support by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

**2D-ThP-9 Discretized Atomic Layer Deposition Recipe for Wafer-scale Synthesis of $MoS_2$***, Sachin Shendokar,* ***Shyam Aravamudhan,*** North Carolina A&T State University

Monolayer $MoS_2$, 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 Messecar,*** Western Michigan University*; Chen Chen, Isaiah Moses, Wesley Reinhart, Joan Redwing,* The Pennsylvania State University*; Steven Durbin,* University of Hawaiʻi 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 $MoS_2$, 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 $MoS_2$ 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 Koneru,*** 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 moire superlattices. The findings offer new opportunities for creating quantum emitter arrays for integrated quantum photonics.

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

## 2D Materials: Devices and Applications

**Moderators: Kuan Eng Johson Goh**, National University of Singapore, **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]

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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 $WSe_2$ 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 $MX_2$ (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.

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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 ($NbS_xSe_{2-x}$) 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 $NbS_2$ 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, $WS_2$ 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 $WS_2$ 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 $WS_2$ 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-gown monolayer $WS_2$ 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 Atomic Precision Manufacturing for Carbon Nanotube Field Effect Transistors (CNTFETs) for 10X Microelectronics Energy Efficiency***, **Dawei Wang**, Steffen McKearnan,* Carbon Technology Inc.

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to solve for rapidly growing U.S. computing energy use with its initiative in energy efficiency scaling for two decades (EES2) for microelectronics. Under this initiative, DOE/AMMTO has funded a portfolio of EES2 device technology R&D projects that promise a first >10X energy efficiency increase by 2030. This paper will highlight the most recent of these projects—the use of atomically precise manufacturing techniques to solve carbon nanotube (CNT) device fabrication challenges. Carbon nanotube conduction exceeds that of the best metals by many orders of magnitude. Conduction from Teflon to CNTS varies across 33 orders of magnitude. The size of a human to the universe is only 27 orders. Current semiconductors, even doped, are orders of magnitude worse conductors than CNTs. Because metals are orders of magnitudes better than silicon or GaAs, we metallize them to create circuits. However, copper is close to a million times lower conductivity per atom than a CNT. Even with a double damascene processes, Cu fails due to electromigration at ~1000x the atomic cross-section of a CNT. DOE industry partner Carbon Technology, Inc has pioneered the engineering of atomically precise catalyst particles as small as 10 atoms across. These are used to control CNT diameter in standard chemical vapor deposition CNT synthesis. With diameter control, chiral (semi vs metallic) control becomes a matter of "rusting" the metallic CNTs into $CO_2$. High quality CNTs on silicon using standard metal contacts and interconnects will provide at least a 10x boost in the efficiency speed trade-off by 2030. In the full EES2 time scale of 20 years, All Carbon Electronics (ACE), semiconducting CNTs interconnected with metallic CNTs (or graphene) on diamond substrates, will deliver the full 1000x performance increase over silicon CMOS and the EES2 vision. With smart investments in carbon, we will stop pounding sand and deliver the diamond age. This talk will present transmission and scanning electron, Raman and Atomic Force microscopy as well as electrical data showing the CNT control needed to deliver on EES2. Simple graphics showing improvement over silicon will also be presented.

9:45am **2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of $HfSe_3$***, **Gauthami Viswan**[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 Universite 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.

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10:00am **2D+AQS+EM+NS+QS+TF-FrM-8 Green Synthesis of Pd-Doped 2D Materials for Energy Applications***, Stefania Sciacca,* University of Catania, Catania, Italy*; Cassandra Pichry,* University of Mons, Belgium*; Roberto Fiorenza, Salvatore Scirè, Luisa D'Urso, Carmela Bonaccorso, Giuseppe Forte,* University of Catania, Catania, Italy*; **Cristina Satriano**,* University of Catania, Italy

In this work, we present the preparation and comprehensive physicochemical characterisation of bioinspired nanostructured 2D hybrids based on graphene oxide analogues functionalised with palladium (Pd) nanoparticles, synthesised via a green wet-chemical route. Using glucose as a sustainable reducing agent and polyvinylpyrrolidone (PVP) as a stabilising agent, we achieved controlled deposition of Pd nanoparticles on the 2D surface, ensuring structural integrity and improved dispersion.

The physicochemical properties of the resulting hybrids were thoroughly investigated using X-ray photoelectron spectroscopy (XPS), confocal Raman microscopy, UV-visible absorption and fluorescence spectroscopy analyses to elucidate the chemical and electronic structure. In particular, the ratio of ordered to disordered carbon domains was exploited to gain insight into the structural evolution of the GO-derived materials. This ratio was correlated with the presence of oxygen- and/or sulfur-containing moieties, providing valuable information on the degree of functionalisation and the influence of heteroatom doping on the hybrid structure. Through quantum mechanical calculations, the interaction energy between graphene oxide and the adsorbed palladium nanoparticles was determined, along with the simulation of absorption and Raman spectra generated by this system. Morphological and topographical features were analysed by atomic force microscopy (AFM) and transmission electron microscopy (TEM), revealing uniform nanoparticle distribution and nanoscale hybrid architecture. These Pd-doped 2D hybrids beyond graphene exhibited promising photocatalytic activity, especially in hydrogen ($H_2$) generation under simulated solar illumination, highlighting their potential in sustainable energy conversion applications.

**Acknowledgements**: CS and CB acknowledge the financial support by MUR in the framework of PRIN2022-PNRR call under project CoMu4CaT.

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 $Ti_3C_2T_x$ 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]. Laslty, this talk will highlight recent insights into $WS_2$ nucleation and film growth on sapphire using tungsten hexacarbonyl and

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[1] **SSD Morton S. Traum Award Finalist**

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.

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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 $CO_2$ reduction reaction ($CO_2RR$). 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 $CO_2RR$ 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 Barelli**, 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 $MoS_2$ and $WS_2$ on large area nanostructured samples fabricated by laser interference lithography (either $MoS_2$ nanostripes arrays or conformal $MoS_2$ 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 $MoS_2$ 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 $MoS_2$ 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 ($cm^2$-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked $WS_2$-$MoS_2$ 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 founding by the NEST - Network 4 Energy Sustainable Transition - PNRR partnership.

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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.

11:45am **2D+AQS+EM+NS+QS+TF-FrM-15 Nitrogen Doped Graphene Materials for Solid-State Hydrogen Storage**, ***Peter Rice**, Buddhika Alupothe Gedara, Mi Yeon Byun,* Pacific Northwest National Laboratory; *Sam Johnson,* Colorado School of Mines, USA; *Maria Sushko, Elizabeth Denis, Zbynek Novotny, Zdenek Dohnalek, Bojana Ginovska, Tom Autrey,* Pacific Northwest National Laboratory

In this work we report our recent experimental and computational findings on controlling the interaction of liquid-organic hydrogen carriers (LOHC's) and hydrogen (H) with nitrogen (N)-doped graphene materials for solid-state H-storage. Specifically, density functional theory (DFT) calculations, inverse gas chromatography (iGC), X-ray photoelectron spectroscopy (XPS)and nuclear magnetic resonance (NMR) are used to quantify both the LOHC (benzene and pyridine) and H adsorption thermodynamics, on materials with varying concentrations of pyridinic and graphitic N. We find that N-doping with basal plane graphitic N has the greatest impact on the LOHC adsorption energetics, compared with basal plane pyridinic and edge site N, due to an enhancement of the π-π stacking configuration. Interestingly, the opposite trend is observed for H adsorption, whereby the calculated adsorption energies and XPS binding energy shifts suggest that pyridinic sites are key sites for binding H, compared with basal plane graphitic N. Our findings provide some guiding principles for developing novel N-doped graphene materials for $H_2$ storage.

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