

# Sunday Afternoon, September 21, 2025

## AVS Quantum Science Workshop

Room 208 W - Session AQS-SuA

### AVS Quantum Science Workshop Oral Session (ALL-INVITED SESSION)

**Moderators:** Ekta Bhatia, NY CREATES, Charles R. Eddy, Jr., Office of Naval Research Global - London, David Pappas, Rigetti Computing, Andre Schleife, University of Illinois at Urbana-Champaign

3:00pm **AQS-SuA-1 How to Build a Quantum Supercomputer: Scaling from Hundreds to Millions of Qubits**, *John Martinis*, Qolab **INVITED**

In the span of four decades, quantum computation has evolved from an intellectual curiosity to a potentially realizable technology. Today, small-scale demonstrations have become possible on hundreds of physical qubits and proof-of-principle error-correction on a single logical qubit. Nevertheless, the path toward a full-stack scalable technology is largely unknown. There are significant outstanding quantum hardware, fabrication, software architecture, and algorithmic challenges that are either unresolved or overlooked. Here, we show how the road to scaling could be paved by adopting existing semiconductor technology to build much higher-quality qubits and employing system engineering approaches.

3:30pm **AQS-SuA-3 Fault Tolerant Quantum Computation using Majorana-Based Topological Qubits**, *Roman Lutchyn*, Microsoft Quantum **INVITED**

Research in quantum computing has provided numerous new physical insights and the potential to exponentially increase computational power for solving significant problems in science and technology. The primary obstacle to building a scalable quantum computer is errors caused by decoherence. Topological quantum computing addresses this challenge by utilizing topological materials that inherently limit errors.

In this talk, I will discuss the engineering of topological superconductors that support Majorana zero-energy modes at the interface between a conventional superconductor (Aluminum) and a semiconductor with spin-orbit interaction (Indium Arsenide). I will present recent findings from the Microsoft Quantum team that indicate the emergence of topological superconductivity in proximitized semiconductor nanowires. Additionally, I will cover recent measurements of fermion parity, which represent a step towards the fusion of Majorana zero modes. Finally, I will outline a proposal for scalable quantum computing that involves topological qubits composed of superconducting islands in a Coulomb blockade regime, hosting aggregates of four or more Majorana zero modes.

4:00pm **AQS-SuA-5 Enabling the Scaling of Superconducting Quantum Devices in a 300 mm Wafer Fab**, *Ekta Bhatia, Zhihao Xiao, Chung Kow, Stephen Olson, Jakub Nalaskowski, John Mucci, Nicholas Pieniazek, Daniel Romero, Hyuncher Chong, Bryan Egan, Geevanie Telhu, Wenli Collison, Sandra Schujman, Kevin Musick, Thomas Murray, Aleksandra Biedron, Satyavolu Papa Rao*, NY CREATES **INVITED**

Progress in superconducting qubit performance over the past three decades has led researchers to focus on scalable quantum computing. To achieve scalability, the following are among the desiderata: system stability, easy input/output, high component yields, low energy use, and predictable component performance with tight distributions. These demands are even more challenging for quantum computing.

The NY CREATES team, along with our partners, has taken on the scalability challenge by seeking to implement superconducting qubits at 300 mm wafer scale, leveraging state of the art tools and processes to support the development of a Superconducting Quantum Process Design Kit (PDK). A PDK will enable democratization of qubit design and fabrication for start-ups, academia and national labs - but a PDK is only as good as the fidelity with which fabricated devices meet the designer's intent. Hence it is critical to develop fabrication processes that are controlled and repeatable, in tools that are equipped with *in situ* monitors for process control.

This talk will describe our efforts to develop tantalum (Ta)-based qubits at 300 mm scale. We use  $\alpha$ -Ta as the wiring material, and atomic layer deposited tantalum nitride in the tunnel barrier of the Josephson junction. The advantages provided by state-of-the-art 300 mm tools to enable *in situ* process monitoring and control will be described using a few examples from various stages of the process flow. This talk will discuss the impact of two-level systems in material surfaces and interfaces. We have addressed them in many ways - by burying some in a crystalline silicon matrix to eliminate air exposure, and by replacing native oxides with surface treatments providing improved physical characteristics. Implementation of integrated air bridges and lumped element resonators that use high kinetic inductance elements and capacitors that use crystalline silicon as the

dielectric will be discussed. The talk will conclude with a description of the circuit elements that are being developed for the PDK cell library, both as 'fixed geometry' cells, and as parameterized cells.

We thank our many partners, including Brookhaven National Lab, Pacific Northwest National Lab, AFRL-Rome, SEEQC, QCI, Tokyo Electron Ltd, Applied Materials, Cadence, Cornell University, Princeton University, Syracuse University, and Auburn University. The various projects underlying this talk are funded in part by the US Department of Defense (ME Commons), the US Department of Energy (C2QA), and NY CREATES.

4:45pm **AQS-SuA-8 Laboratory-based Experiential Learning for Quantum Information Science**, *Richard S. Ross*, UCLA **INVITED**

UCLA's Master of Quantum Science and Technology program has developed innovative instructional laboratory curricula that provide students with a solid foundation in quantum science. This presentation will showcase several case studies, including "Decohering Michelson" and "Chloroforming Deutsch & Jozsa," which demonstrate how theoretical quantum concepts can be effectively translated into practical laboratory implementations. These laboratory experiences cultivate critical skills—quantum state characterization, gate calibration and compilation, tomography, noise analysis, and signal processing—bridging the gap between abstract quantum theory and technical proficiencies demanded by the quantum workforce. The approach effectively complements traditional educational programs at both advanced undergraduate and early graduate levels, providing students with a unique foundation whether they enter industry or pursue further graduate studies in the field.

5:15pm **AQS-SuA-10 Invited Paper**, *Matthew LaHaye*, Air Force Research Lab **INVITED**

5:45pm **AQS-SuA-12 Invited Paper**, *Athena Sefat*, DOE **INVITED**

# Thursday Morning, September 25, 2025

## 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 National Laboratory

8:00am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-1 Probing the Ultrafast Charge Dynamics and Exciton Emission from Single Atomic Defects in 2D Semiconductors by Lightwave-Driven STM**, Laric Bobzien, Lysander Huberich, Jonas Allerbeck, Eve Ammerman, Nils Krane, Andres Ortega-Guerrero, Carlo Pignedoli, Oliver Gröning, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland; Joshua A. Robinson, The Pennsylvania State University; Bruno Schuler, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland **INVITED**

Two-dimensional (2D) semiconductors provide an exciting platform to engineer atomic quantum systems in a robust, yet tunable solid-state system. This talk explores the intriguing physics of single point defects in transition metal dichalcogenide (TMD) monolayers, investigated through atomically resolved scanning probe microscopy.

We have determined the layer-dependent charge transfer lifetimes of selenium vacancies in  $WS_2$  on graphene substrates, spanning picosecond to nanosecond timescales [1]. By leveraging our recently developed lightwave-driven scanning tunneling microscope (THz-STM) [2,3], we could probe the ultrafast charge dynamics on the atomic scale. Time-domain sampling with a THz pump-THz probe scheme enabled capturing atomic-scale snapshots of transient Coulomb blockade, a hallmark of charge transport mediated by quantized defect states [4].

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

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

#### References:

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

8:30am **2D+AQS+EM+MI+MN+NS+QS+SS+TF-ThM-3 Many-Body Effects on Excitons, Trions, and Defect-Bound States in 2D Materials**, Kai Xiao, Taegwan Park, Alexander Puzetky, Oak Ridge National Laboratory, USA; Xufan Li, Honda Research Institute; Kyungnam Kang, Oak Ridge National Laboratory, USA; Austin Houston, University of Tennessee, Knoxville; Christopher Rauleau, 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  $MoS_2$  /  $WS_2$  @ 1L h-BN-Capped Gold**, Andrey Krayev, HORIBA Scientific; Pavel Valencia Acuna, PNNL; Ju-Hyun Jung, Pohang University of Science and Technology (POSTECH), Republic of Korea; Cheol-Joo Kim, POSTECH, Republic of Korea; Andrew Mannix, Stanford University; Eleonora Isotta, Max Planck Institute for Sustainable Materials, Germany; Chih-Feng Wang, PNNL

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

In addition to the enhancement of both the PL and Raman signal, in the course of assessment of TERS/TEPL response of mono- and a few-layer-thick crystals of  $MoS_2$  and  $WS_2$  deposited on 1L h-BN-capped gold we observed in TERS spectra, completely unexpectedly, appearance of Raman bands at about  $796\text{ cm}^{-1}$  and  $76\text{ cm}^{-1}$  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  $796\text{ cm}^{-1}$  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, Nirasha Rajapakse, Matthias Batzill, University of South Florida

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

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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<sub>2</sub> 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<sub>2</sub> with dissimilar transition metals to create new doped or alloyed 2D materials with potentially desirable properties.

9:45am **2D+AQ5+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<sub>2</sub> 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 moiré domain 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+AQ5+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 electrostatics 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 electrostatics 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+AQ5+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.<sup>1</sup> 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,<sup>2</sup> which for the first time allowed the identification of chirality effects in the photonic properties of a single nanostructure.<sup>3</sup> Using cathodoluminescence spectroscopy, whispering gallery modes could be excited and probed to directly compare the photonics of chiral and achiral segments in single nanowires. The data show systematic shifts in energy, which with the help

of simulations are assigned to chiral whispering gallery modes in wires hosting a single dislocation.

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

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

11:45am **2D+AQ5+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<sub>2</sub> [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<sub>2</sub>, 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].

## References

- [1] Bussolotti, F., et al., *ACS Nano* 15 (2021) 2686
- [2] Bussolotti, F., et al., *ACS Nano* 18 (2024) 8706
- [3] Das, S., et al., *ACS Nano* 18 (2024) 30805
- [4] Goh, K. E. J., et al., *Advanced Quantum Technologies* 3 (2020) 1900123

12:00pm **2D+AQ5+EM+MI+MN+NS+QS+SS+TF-ThM-17 Thickness Dependent Band Gap and Electrical Anisotropy of 2DSnSe**, *Marshall Frye, Jonathan Chin, Joshua Wahl, Jeremy Knight*, Georgia Institute of Technology; *Walter Smith*, Purdue University; *Dilara Sen, Samuel Kovach*, Kenyon University; *Frank Peiris*, Kenyon College; *Charles Paillard*, University of Arkansas; *Thomas Beechem*, Purdue University; *Anna Osterholm, Lauren Garten*, Georgia Institute of Technology

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

# Thursday Afternoon, September 25, 2025

## 2D Materials

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

#### 2D Materials: Magnets and Topological Phenomena

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

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

Magneto-Chiral topological superconductivity is a rare phase long pursued for error-free quantum computation. Its 1D chiral modes possess topologically protected long-range coherence well beyond that of the Cooper pairs, which could be fruitful for quantum transduction and low-temperature spin transport. While evidence for such modes is mounting, unambiguous signatures, such as non-local transport via co-tunneling, remain elusive. I will describe our realization of 1D chiral hinge modes mediating the direct tunneling of electrons from source to drain in FeTe<sub>0.55</sub>Se<sub>0.45</sub>. 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<sub>2</sub>, *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<sub>2</sub>-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<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub>, *Lakshmi 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 Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub> using scanning tunneling microscopy (STM) and conductive atomic force microscopy (C-AFM). Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub> is an intrinsic superlattice material s comprised of a Bi<sub>2</sub>Se<sub>3</sub> quintuple layer (QL) slab and a 2D Bismuthine (Bi<sub>2</sub>) 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 Bi<sub>2</sub>Se<sub>3</sub> 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 Bi<sub>2</sub>-Bi<sub>2</sub>Se<sub>3</sub>. 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<sub>2</sub>, *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<sub>2</sub>, 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<sub>2</sub> 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<sub>2</sub> films on a gate tunable graphene field effective transistor supported by hBN. Gate-dependent STS reveals a substantial energy gap in 1T'-WTe<sub>2</sub> 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 (CrI<sub>3</sub>) and progressive steps towards realizing moiré magnetism. Noting that bilayer CrI<sub>3</sub> is a layered antiferromagnet and that any homogeneous stacking of two bilayers necessarily produces zero magnetization, we have revealed, in twisted double bilayer CrI<sub>3</sub>, 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

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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 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 (MoS<sub>2</sub>, semiconductor) and titanium carbide MXene (Ti<sub>3</sub>C<sub>2</sub>, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> (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<sub>x</sub>Se<sub>2-x</sub>) 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<sub>2</sub> 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 WS<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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.

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Comparing differently processed layers, we find the MOCVD-grown monolayer WS<sub>2</sub> to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E<sub>g</sub> 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<sub>2</sub>. These findings provide important guidelines for tailoring band alignments for WS<sub>2</sub>-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 McKeernan, 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<sub>2</sub>. 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<sub>3</sub>, Gauthami Viswan<sup>1</sup>, 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<sub>3</sub> was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). HfSe<sub>3</sub> has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is -0.27 m<sub>e</sub> which is smaller compared to the effective hole mass along the direction perpendicular to the chains, -1.17 m<sub>e</sub>. The effective hole mass extracted from the band structure along different high symmetry directions is compared with that of TiS<sub>3</sub> and ZrS<sub>3</sub> from prior studies.<sup>1</sup> X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of HfSe<sub>3</sub> and will be compared to the XAS spectra of HfS<sub>3</sub><sup>2</sup> and TiS<sub>3</sub> and ZrS<sub>3</sub>.<sup>3</sup> 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<sub>2</sub>) 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, INVITED, Boise State University

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<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene electrodes to efficiently remove and recover ammonia from synthetic wastewater and carbonates from simulated ocean water. This FE=CDI system demonstrates promising potential for managing nitrogen and carbon cycles while improving access to clean water [4]. In healthcare, the intersection of graphene and biology offers a powerful avenue for musculoskeletal tissue engineering, where graphene's exceptional physical properties contribute to fundamental biological insights [5-7]. Lastly, this talk will highlight recent insights into WS<sub>2</sub> nucleation and film growth on sapphire using tungsten hexacarbonyl and

<sup>1</sup> SSD Morton S. Traum Award Finalist

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hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD  $3 \times 2$  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<sub>2</sub> 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<sub>2</sub> reduction reaction (CO<sub>2</sub>RR). 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<sub>2</sub>RR 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 Borelli*, *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<sub>2</sub> and WS<sub>2</sub> on large area nanostructured samples fabricated by laser interference lithography (either MoS<sub>2</sub> nanostripes arrays or conformal MoS<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub> 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<sup>2</sup>-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS<sub>2</sub>-MoS<sub>2</sub> heterostructures endowed with type-II band alignment, forming periodic nanogratings [6]. These engineered large-area vdW heterostructures enable scalable applications in nanophotonics, photoconversion [7], and energy storage.

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

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11:30am **2D+AQs+EM+NS+QS+TF-FrM-14 Exploring the Temperature Coefficient of Frequency (TC<sub>f</sub>) 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<sub>f</sub>) 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<sub>f</sub> 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

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model. The drumhead resonator with 20  $\mu\text{m}$  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/ $^{\circ}\text{C}$  from the drumhead structure, extracted from frequency shifts between 30  $^{\circ}\text{C}$  and 60  $^{\circ}\text{C}$ . After we FIB the drumhead structure into a trampoline, we found that the  $TC_f$  reduced to 588 ppm/ $^{\circ}\text{C}$ .

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  $\pi$ - $\pi$  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  $\text{H}_2$  storage.

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