Nanoscale Science and Technology
Room 206 A W - Session NS1-MoM

Frontier in Nanoscale Electron, Ion, and Scanning Probe Imaging

Moderators: Marek Kolmer, Ames National Laboratory, **Robertus Elberse**, NIST

8:15am **NS1-MoM-1 Design, Construction, and Performance of a Dilution Refrigerator-Based Esrspm System with Cryogenic Switches***, **Robertus Elbertse**, Dengyu Yang, Sungmin Kim, Dilek Yildiz, Daniel Walkup, Steven Blankenship, Joseph Stroscio,* NIST **INVITED**

Electron Spin Resonance using a Scanning Tunneling Microscope (ESRSTM) relies on reaching crogenic temperatures to achieve favorable thermal population distributions of quantum states. To date, most ESRSTMs operate between 300 mK and 4 K. Here, we present an ESRSTM that can operate down to 10 mK using a dilution refrigerator (DR). The design of the system is multi-modal, combining STM, AFM, electrical transport and ESR measurement capabilities. To characterize the microwave transmission, we have measured the frequency-dependent radio frequency (RF) transmission using a Josephson tunnel junction, consisting of an Al probe tip and Al (111) sample at 10 mK. Excellent transmission was observed up to 40 GHz in comparison to previous measurements in other laboratories. At the base temperature of the DR (10 mK) scanning tunneling spectroscopy can reach an energy resolution of ≈10 µeV, comparable to the energy broadening expected at base temperature [1]. However, when RF lines are sufficiently transmissive, as we have measured in our DR ESRSPM, the thermal noise introduced by photons originating at room temperature can cause increased broadening effects. This may reach orders of magnitude higher than broadening given by the base temperature of the DR. We will show how adding attenuators and cryogenic switches may help reduce such photonic noise and subsequently show its effect on the decoherence time of single atom qubits.

[1] J. Schwenk *et al.*, "Achieving µeV tunneling resolution in an in-operando scanning tunneling microscopy, atomic force microscopy, and magnetotransport system for quantum materials research," *Rev. Sci. Instrum.*, vol. 91, no. 7, p. 071101, Jul. 2020, doi: 10.1063/5.0005320.

8:45am **NS1-MoM-3 Magnetic Coupling in Graphene Nanoribbon Quantum Dots and Looking Beyond***, **Percy Zahl**,* Brookhaven National Laboratory*; Alexander Sinitskii, Mamun Sarker,* University of Nebraska-Lincoln, USA*; Peter H. Jacobse, Michael F. Crommie,* University of California, Berkeley*; Anshul Saxena,* Walker Department of Mechanical Engineering University of Texas*; Ziyi Wang,* Materials Sciences Division Lawrence Berkeley National Laboratory Berkeley*; Emma Berger,* Department of Physics University of California, Berkeley*; Narayana R. Aluru,* Walker Department of Mechanical Engineering University of Texas

Carbon-based quantum dots (QDs) enable flexible manipulation of electronic behavior at the nanoscale, but controlling their magnetic properties requires atomically precise structural control. While magnetism is observed in organic molecules and graphene nanoribbons (GNRs), GNR precursors enabling bottom-up fabrication of QDs with various spin ground states have not yet been reported. Here the development of a new GNR precursor that results in magnetic QD structures embedded in semiconducting GNRs is reported.

Inserting one such molecule into the GNR backbone and graphitizing it results in a QD region hosting one unpaired electron. QDs composed of two precursor molecules exhibit nonmagnetic, anti ferromagnetic, or anti ferromagnetic ground states, depending on the structural details that determine the coupling behavior of the spins originating from each molecule.

We present on surface precisely synthesized GNR structures imaged using high-resolution atomic force microscopy (HR-AFM) together with high resolution scanning tunneling spectroscopy (STS) to identify local spin properties localized at specific sites within those carbon based structures at the atomic scale.

The synthesis of these QDs and the emergence of localized states are demonstrated through HR-AFM, scanning tunneling microscopy (STM) imaging, and spectroscopy, and the relationship between QD atomic structure and magnetic properties is uncovered. GNR QDs provide a useful platform for controlling the spin-degree of freedom in carbon-based nano structures.

Looking Beyond: Such structures are promising molecular building blocks of carbon based future devices with spin controllable or quantum computing capable elements. Challenges remain to build or move such structures from metal support onto insulating surfaces to decouple spins from the substrate and create a potentially significant long de-coherence time to be practically useful. Furthermore control and readout certainly will be challenging. First steps have been demonstrated using SPM techniques and manipulation on atomic scale. Still, instrumentation has to allow for convenient and efficient future experiments.

Reference to this work:

[1] Small 2024, 20, 2400473; DOI: 10.1002/smll.202400473

9:00am **NS1-MoM-4 Direct Observation of Mg Diffusion Through Screw-type Dislocations in a GaN Device Using Atom Probe Tomography***, **Yimeng Chen**, Michael Salmon, Xiuhong Han,* EAG Laboratories

Large band gap vertical GaN power devices have been developed for high efficiency switch devices [1]. These devices incorporate p-type GaN through Mg doping in selective regions. Precise control of dopant concentration is crucial for semiconductor devices. However, interfacial diffusion or through defect migration of dopants can degrade the performance. Dopant segregation at threading dislocations inducing current leakage was reported [2].

We analyzed a GaN device removed from a USB charger, purchased from the market, that contained the NV6125 microchip for power switching control. The microchip was mechanically de-processed at EAG down to the field-effect-transistor level, exposing the source/drain region for microstructural characterization. A ~0.5 µm thick lamella in cross-section was made along the gate via Focused Ion Beam (FIB) and observed using Scanning Transmission Electron Microscopy (STEM). STEM observation confirmed a layered structure composed of dielectric oxide, metal contact, p-type GaN and AlGaN layers on GaN. The GaN epi exhibits a high threading dislocation density (TDD) that we estimate to be ~1E9/cm^2. Using a simple 2-beam tilting strategy in STEM, we were able to identify each dislocation as either edge, screw, or mixed type.

Precise STEM carbon-deposition was utilized to mark and target defect free regions as well as individual dislocations. Small pillars, ~0.5µmx0.5µmx4µm, containing the marked locations from the existing STEM lamella were extracted and welded to specific grids suitable for both APT and STEM. The samples were then re-imaged and marked again in STEM. Using the STEM marks to guide further FIB machining, the pillars were further processed into needle-shaped samples suitable for atom probe tomography (APT), centered at the precise locations of the threading defects. Composition and elemental distribution, in and around dislocations, were studied using APT. In the presentation, we will compare dopant distribution in dislocation-free regions and at dislocation cores.

APT analysis confirmed approximately 100 ppm Mg dopant in the p-type GaN region. The results clearly indicate Mg diffusion along the dislocation core through the electron blocking layer, resulting in a line concentration of ~80 dopant atom per 100 nm inside the GaN. The study demonstrates the unique capability of site-specific analysis of defects in device structures using correlative STEM and APT analysis, providing detailed insight into the diffusion behavior of dopant in and around threading defects.

[1] T. Oka, T. Ina, Y. Ueno, J. Nishii, Appl. Phys. Express 2015, 8, 6.

[2] H. Sakurai, et. al., Appl. Phys. Express 2020, 13, 086501.

9:15am **NS1-MoM-5 Focused Ion Beam Low Energy Implantation***, **Alex Belianinov**, Michael Titze, Chris Smyth,* Sandia National Laboratories*; Jonathan Poplawsky,* Oak Ridge Natinal Laboratory*; Barney Doyle,* Sandia National Laboratories

Ion implantation is a key capability for the semiconductor industry. As devices shrink, novel materials enter the manufacturing line, and quantum technologies transition to being more mainstream, traditional implantation methods fall short in terms of energy, ion species, and positional precision. However, lowering the implantation energy while maintaining nanometer scale spot size is a technological challenge. This presentation will show an overview of techniques at Sandia National Laboratories Ion Beam Facility that allow focused ion implants 10-200 keV range for quantum relevant applications.

Additionally new developments in sub-1 keV focused ion implants into Si and 2D devices, using a focused ion beam system, validated by atom probe tomography will be shown. We illustrate that identical results for low energy ion implants can be achieved by either lowering the column voltage, or decelerating ions using bias – while maintaining good spatial resolution.

Furthermore, our data reveal that standard implant modeling approaches overestimates experimental depth by a significant margin. Finally, we discuss how our results pave a way to much lower implantation energies, while maintaining high spatial resolution.

9:30am **NS1-MoM-6 Silicon-Containing Poly(Phthalaldehyde) Hard Mask Materials for Simplified High-Resolution and Grayscale Patterning via Thermal Scanning Probe Lithography (t-SPL) - A NanoFrazor Use Case***, **Nicholas Hendricks**, Emine Çağin,* Heidelberg Instruments Nano AG, Switzerland

Enabled by the NanoFrazor technology, thermal scanning probe lithography (t-SPL) has established itself as a mature and reliable direct-write nanolithography technique for generating nanoscale structures [1-4]. The NanoFrazor technology offers an alternative and complementary process to conventional lithography techniques of photolithography and electron-beam lithography (EBL). With an advanced cantilever, t-SPL generates patterns by scanning an ultrasharp tip over a sample surface to induce local changes with a thermal stimulus, which allows for various modifications to the sample via removal, conversion, or addition. Along with an ultrasharp tip, the t-SPL cantilever contains other important functions such as an integrated thermal height sensor and an integrated heating element, both of which are advantageous for fabricating devices for quantum computing, nanoelectronics, and photonics.

The main thermal imaging resists used in t-SPL are poly(phthalaldehyde) (PPA) based materials that are commercially available from Allresist and Polymer Solutions. PPA is an all-organic based resist capable of direct sublimation when exposed to temperatures greater than the decomposition temperature, ~180°C. With such characteristics, PPA has been able to produce sub-10nm lateral dimensions while providing sub-nm vertical resolution but with limited etch selectivity in oxygen-based reactive ion etches. To overcome this, t-SPL utilizes a four-layer film stack, that includes a silicon-containing hard mask, deposited either by spin-coating or evaporation, for high-resolution patterning. To simplify the high-resolution patterning process, a two-layer film stack utilizing a spin-coatable silicon-containing PPA (Si-PPA) material, functioning both as a hard mask material and a thermal imaging resist, is assessed here. One of the advantages of using Si-PPA is that a simplified film stack is used (from four steps to two steps) while maintaining sub-20nm processing capabilities.

Within this presentation, the background of t-SPL will be introduced as well as the experimental results of the two-layer film stack for high-resolution patterning. Sub-40nm patterns transferred into a silicon substrate and sub-20nm features patterned into the Si-PPA film by t-SPL will be further elaborated upon. Initial results from grayscale patterning generated in Si-PPA films and etch amplifications will be discussed.

[1] S. Howell et al., Microsystems & Nanoengineering, 6, 21 (2020)

[2] V. Levati et al., Adv. Mater. Technol. 8, 2300166 (2023)

[3] L. Shani et al., Nanotechnology, 35, 255302 (2024)

[4] Mukherjee et al., ACS Nano, 19, 9327 (2025)

9:45am **NS1-MoM-7 Tunable Electronic Properties Within Highly Unoccupied Electronic Bands of Graphene-SiC Heterostructures Determined by Scanning Tunneling Spectroscopy***, **Marek Kolmer**, Umamahesh Thupakula, Shen Chen,* Ames National Laboratory*; Hoyeon Jeon,* Oak Ridge Natinal Laboratory*; Wonhee Ko,* The University of Tennessee, Knoxville*; An-Ping Li,* Oak Ridge Natinal Laboratory*; Michael C. Tringides,* Iowa State University

Manipulation of the interlayer couplings in vertically stacked two-dimensional (2d) materials results in highly tunable electronic properties, often stemming from emerging novel electronic and topological phases. Here, we will focus on the epitaxially grown graphene (EG) on a silicon carbide (0001) surface, where thermal decomposition of the top silicon carbide layers provides a synthesis of epitaxial graphene layer(s) with exceptional uniformity and control over their structural properties, i.e., number of graphene layers. Subsequent intercalation of heteroatoms under graphene layer(s) becomes a promising strategy for the synthesis of designer 2d quantum materials. In the talk we will discuss how control over these buried graphene interfaces and metal intercalation affects the resulting electronic structure of these model systems. In particular, we will focus on the less understood interface states located within the unoccupied electronic band regime above the vacuum level. Such states, especially for energies larger than ~20 eV, are not easily accessible with most spectroscopies, while here, both the pristine and intercalated systems can be easily measured and compared. The low-temperature scanning tunneling microscope operating in the high-sample bias voltages reaching ~40 V is used to study the interaction between the interface states and high-bias resonances formed within the triangular tip-sample potential. We show the methodology of how to extract the intrinsic electronic density of states of highly unoccupied bands as a function of graphene thickness and intercalated phase from these high-bias scanning tunneling spectroscopy (STS) experiments. Due to the 2d nature of systematically studied graphene heterostructures, their high-bias STS spectra show pronounced features within this energy regime, i.e., in contrast to typical bulk, half-plane metals' spectra, which strongly depend on the interlayer couplings between the heterostructure interfaces.

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Nanoscale Science and Technology
Room 206 A W - Session NS2-MoM

Advanced Nanomaterial for Quantum and Energy Applications

Moderators: Alex Belianinov, Sandia National Laboratory, **Wonhee Ko**, University of Tennessee, Knoxville

10:30am **NS2-MoM-10 Fabricating Color Centers using Liquid Metal Alloy Ion Source Focused Ion Beams***, **Michael Titze**,* Sandia National Laboratories **INVITED**

Color centers are interesting candidates for transmitting quantum information. However, experiments using color centers are hindered by the difficulty of fabricating color centers deterministically. Liquid metal alloy ion source based focused ion beams (FIBs) hold the potential to deterministically fabricate color centers at scale. Often the challenge lies in having a source material that contains the ion of interest to form the color center of relevance. Example challenges include lack of wetting the filament material, evaporation of the element of interest, formation of hard to break oxides, and too little or too high viscosity of the source material, leading to a lack of formation of an emitting Taylor cone. In this talk we will discuss our current efforts in realizing a Na and Pb source. We will discuss the use of a AuSi eutectic where Na is added as an impurity that shows Na is outgassing during source fabrication. We will also present current results using a eutectic NaPb alloy, including the observation of evaporation of the source material when using standard source fabrication recipes, highlighting the need for in-situ thermometry. We will also present our work on fabricating quantum devices utilizing FIB created tin-vacancy centers in diamond and silicon vacancies in SiC showing how FIB enables the required targeting resolution for integration of color centers with quantum devices once a suitable source is fabricated.

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.

11:00am **NS2-MoM-12 Atomic-scale Vibrational Excitations at Amorphous/Crystalline Interfaces***, **Kory Burns**,* University of Virginia, USA*; Nooreen Qureshi,* University of Virginia*; Tymofil Pieshkov, Pulickel Ajayan,* Rice University*; Jordan Hachtel,* Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

Isotopically pure amorphous Boron Nitride has an extremely low nuclear cross-section (inhibiting the absorption of thermal neutrons), high thermal stability, good measurement precision, and robustness to external perturbations; making it an ideal candidate for next-generation quantum sensors. Some of the most prominent issues in understanding thermal transport in candidate materials is the difficulty in fabricating dissimilar interfaces at scale and accurately characterizing their properties. In this presentation, amorphous BN is deposited on 3 different substrates by pulsed laser deposition. Next, an aberration-corrected scanning transmission electron microscope (STEM) with a monochromator on the electron energy loss spectrometer (EELS) is used to measure phonon modes at atomic resolution at the interface between the BN film and the substrate. The epitaxial strain between BN and the substrate is measured using off axis EELS, where the bright field disc is displaced in q-space relative to the EELS aperture to collect electrons that scatter at high angles. This ensure that electrons that scatter off the nucleus are interpreted in the EEL spectrum, and not ones that scatter of the material's electron cloud. This approach ensures that we can measure a localized response from individual atoms by suppressing long-range excitations from the dielectric environment. Accordingly, we reimagine the process used to calculate the localized phonon transport at interfaces and enhance the selection criteria of thin films and substrates for quantum sensing applications. Ultimately, this work reinforces the need to study the structure-property relationship of amorphous solids and discusses their implication in novel applications, including quantum sensors and radiation-hard electronics.

11:15am **NS2-MoM-13 Revealing Quantum Functionality of Topological Thin Films by *in situ* Characterization with Materials Cluster System***,* ***Wonhee Ko,*** University of Tennessee, Knoxville

Achieving unique quantum functionality from the nanostructures is a key to realizing novel electronic and quantum devices. Thin films of quantum materials are a promising candidate, but the quantum states in these films are highly fragile to the ambient condition and require *in situ* growth and characterization techniques. We build materials cluster system that combines *in situ* epitaxial film growth and characterization instruments, such as molecular beam epitaxy (MBE), pulsed laser deposition (PLD), angle-resolved photoemission spectroscopy (ARPES), and scanning tunneling microscopy (STM). With the materials cluster system, we grew thin films of topological insulators and observed lattice and electronic structures in atomic scale. Interestingly, we found that the step edges possess Rashba edge states with unique spin texture, which interacts with topological surface states depending on the film thickness. Moreover, the strength of Rashba interaction was tunable by functionalizing step edges with selenium atoms. The results demonstrate that the unique quantum functionality can be exhibited by materials cluster system, which will become a foundational system to realize quantum devices with these films.

11:30am **NS2-MoM-14 Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor***,* ***Desiree Salazar,*** Energetics Inc.*; Shashank Misra,* Sandia National Laboratories, USA

Atomically Precise vertical Tunnel Field Effect Transistor (vTFET) for 10X Microelectronics Energy Efficiency in a General Purpose Transistor.Desiree Salazar, S. Misra, Emilie Lozier and T. Kaarsberg

The United States Department of Energy (DOE) Advanced Materials and Manufacturing Technology Office (AMMTO) is leading a multi-organization effort to counter alarming trends in U.S. computing energy use (e.g. **LBNL 2024 [https://usdoe-my.sharepoint.com/personal/tina_kaarsberg_ee_doe_gov/Documents/lbnl-2024-united-states-data-center-energy-usage-report.pdf]** forecasts that data centers will account for 26% of US electricity use by 2028 when cryptocoin mining is included) 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 >10X energy efficiency increase by 2030. This paper will highlight the first of these projects with Sandia National Laboratories to build on atomically precise manufacturing techniques to create a vertical tunnel field effect transistor (vTFET). Updates will be provided on the successful integration of front end of line (FEOL), back end of line (BEOL) and mid-! (MEOL) manufacturing processes (especially thermal budget) to fabricate this vTFET in a CMOS compatible process. One important discovery of the research in this area is "ultradoping" which makes the abrupt doping profiles needed for efficient vTFETs far more manufacturable. This talk also will present how these Sandia results integrate with version 1.0b of the EES2 roadmap that will be issued in Summer 2025. Version 1.0a of the Roadmap is available at EES2 Roadmap Version 1.0 [https://eere-exchange.energy.gov/FileContent.aspx?FileID=f4234e29-cc0c-4a56-a510-86b616ab5535] .

11:45am **NS2-MoM-15 Microwave-Assisted Direct Upcycling of Lithium Ion Battery Cathodes***,* ***Clare Davis-Wheeler Chin,*** Sandia National Laboratories*; Kirsten Jones,* University of New Orleans*; Boyoung Song, Bryan Wygant, Anastasia Ilgen,* Sandia National Laboratories*; Candace Chan,* Arizona State University*; C.J. Pearce,* Sandia National Laboratories*; Winson Kuo, John Watt,* Los Alamos National Laboratory*; John B. Wiley,* University of New Orleans*; Kevin Leung,* Sandia National Laboratories

Rapid market growth of lithium ion-batteries (LIB) for electric vehicles has generated critical materials and sustainability challenges. LIB cathodes require cobalt, which is costly and primarily mined in conflict regions. In response, recent efforts focus on developing efficient, scalable methods for recycling spent LIB cathode materials. Here we report a direct-upcycling approach that exploits microwave (MW) heating for exfoliating layered cathode oxides $LiCoO_2$ (LCO) and $LiNi_xMn_yCo_zO_2$ (NMC) into nanosheets (NSs), which facilitates manipulation of Co:Ni:Mn stoichiometry and reassembly into functioning cathode materials. MW irradiation interacts directly with reaction species to promote heterogeneous heat distribution and instantaneous localized superheating, accelerating exfoliation rates and increasing conversion from bulk oxides to NSs. Our "one-pot" MW method decreases exfoliation time from 2 days (leading-edge electrochemical method) to 2 hours and is easily scaled to generate multi-gram yields. High-resolution transmission electron microscopy (HR-TEM) of MW-exfoliated LCO and NMC indicates conversion into mono- and bilayer NSs with yields >99%. LCO NSs also show increased catalytic activity over starting materials, indicating expanded use cases for recycled materials. The results of this work help establish a fundamental science foundation for sustainable scale-up and securing the LIB supply chain, which is a DOE priority.

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Nanoscale Science and Technology
Room 206 A W - Session NS-MoA

Light-Matter Interactions at the Nanoscale

Moderators: Nikolai Klimov, National Institute of Standards and Technology, **Sesha Challa**, NIST-Gaithersburg

1:30pm **NS-MoA-1 Ultrafast and Ultrasmall Characterization of Excitations in Two-Dimensional Heterostructures***, **Archana Raja,*** Lawrence Berkeley National Laboratory (LBNL) **INVITED**

Atomically thin van der Waals crystals allow for the creation of arbitrary, atomically precise interfaces simply by stacking disparate monolayers without the constraints of covalent bonding or epitaxy. By leveraging the environmental sensitivity of interactions at the ultra-thin, two-dimensional (2D) limit, we can "paint" potential energy landscapes to create and control the electronic structure and excitations in these systems. We have characterized and discovered phenomena in such 2D potential landscapes from the atom scale to the application scale using multimodal photon and electron-based spectroscopies.

I will provide an overview of our joint experimental and theoretical work on the prototypical 2D semiconductor interface of monolayer WS_2 and monolayer WSe_2. In part one, we use ultrafast electron diffraction to reveal the role of layer-hybridized electronic states for controlling energy and charge transport across atomically sharp junctions [1]. In part two, we align the registry of the two layers to create a moiré superlattice ~9 nm in size and use electron energy loss spectroscopy to directly visualize the real space localization of excitonic states within a single moiré unit cell [2]. This suggests the possibility of engineering excitonic superlattices with nanometer precision. In the third and final part, I will discuss the transport of energy across the plane of such a superlattice potential using interlayer excitons [3]. We uncover unexpected trends in the temperature dependent exciton diffusivity, which suggests that the moiré potential landscape is dynamic down to very low temperatures

[1] A. Sood*, J. Haber*, A. Rajaet al. "Bidirectional phonon emission in two-dimensional heterostructures triggered by ultrafast charge transfer," *Nature Nanotechnology* 18 (1), 29-35 (2023)

[2] S. Susarla*, M. H. Naik*, A. Rajaet al. "Hyperspectral imaging of excitons within a moiré unit-cell with a sub-nanometer electron probe," *Science* 378 (6625), 1235-1239 (2022)

[3] A. Rossi*, J. Zipfel*, I.Maity*, A. Raja et al. "Anomalous interlayer exciton diffusion in WS_2/WSe_2 moiré heterostructure," *ACS Nano* 18 (28), 18202-18210 (2024)

2:00pm **NS-MoA-3 Towards the Development of Robust Chip-Scale Photonic Thermometers*, Sesha Challa,*** *Michal Chojnacky, Kevin Douglass, Thinh Bui, Daniel Barker, Nikolai Klimov,* NIST-Gaithersburg

Accurate, high-precision temperature metrology is critical for industries, defense, and healthcare. Temperature also is ranked as the second most measured physical property, following time and frequency, underscoring its role in both applied and fundamental sciences. Resistance-based temperature sensors such as standard platinum resistance thermometers (SPRTs), are the benchmark for conventional temperature metrology due to their high accuracy and widespread acceptance. However, their performance is hindered by sensitivity to environmental conditions and mechanical stress. These inherent limitations, coupled with the critical need to reduce dependence on the calibration chain, have spurred significant interest in developing alternative technologies such as photonic thermometry.

At the National Institute of Standards and Technology (NIST), we are developing an integrated photonic-based temperature sensing platform that can bypass the limitations of SPRTs and transform the way temperature is realized and disseminated. Photonic-based sensors also offer the potential to eliminate costly and disruptive recalibration processes. At the core of this sensing platform is an ultra-sensitive photonic thermometer (SPoT). It consists of an on-chip integrated silicon nanophotonic resonator. The device's optical resonance frequency shifts with temperature, enabled by the high thermo-optic coefficient of single-crystal silicon. This allows precise tracking of temperature variations with exceptional sensitivity. The performance of the SPoT device is critically influenced not only by the sensor design but also by key factors in photonic packaging, which together determine its overall sensitivity, stability, and reliability. Reproducibility in sensor performance is often compromised by fabrication variability, especially in shared nanofabrication facilities.

In this work, we address fabrication-induced variability by investigating sensor designs that are inherently tolerant to process deviations. Our study focuses on photonic crystal cavities, ring resonators, and tapered-width resonators, all fabricated under identical conditions. These structures are implemented on a commercially available 220 nm silicon-on-insulator platform to evaluate their robustness and suitability for reliable, reproducible photonic thermometry.

2:15pm **NS-MoA-4 SpoT On: Precision Photonic Thermometry System with Packaged Sensor and Modular Readout Architecture*, Michal Chojnacky,*** National Institute of Standards and Technology (NIST)/ University of Maryland, College Park*; CH. S. S. Pavan Kumar, Kevin Douglass, Thinh Bui, Nikolai Klimov,* National Institute of Standards and Technology (NIST)

Photonic temperature sensors have attracted significant interest as alternatives to resistance thermometers due to their high-temperature sensitivity, robustness to electrical interference and mechanical shock, small form factor, manufacturing scalability, and compatibility with CMOS fabrication processes. Different types of sensing elements, including photonic crystal cavities, fiber Bragg gratings, and microresonators have been demonstrated, along with strategies for device packaging and characterization. Each of these photonic temperature sensors relies on a temperature-dependent shift in the device's optical resonance frequency due to a combination of thermo-optic and thermal expansion effects, which can deliver sensitivities of 10s of pm/K and resolve sub-mK level temperature changes. However, implementing these technologies in a practical thermometry platform capable of providing stable, reliable, and repeatable temperature measurements remains a challenge. In this work, we describe the development of a chip-scale, silicon microresonator-based photonic thermometer, with the goal of delivering a packaged, functional, field-deployable thermometer and the supporting photonic readout to enable its use in both calibration laboratories and demanding field environments.

The Sensitive Photonic Thermometer (SPoT) described in this presentation is based on a silicon microring resonator integrated in a photonic chip. The device is fiber-bonded and packaged in a capsule format suitable for performance testing in International Temperature Scale of 1990-defining fixed point cells and thermometric baths. We present the metrological characterization of SPoT and benchmark its performance against the state-of-the-art Standard Platinum Resistance Thermometer (SPRT). We provide an overview of different device interrogation architectures that can be used for deployable and cost-effective photonic readout of SPoT. We also outline further steps for achieving a metrology-grade SPoT platform with an absolute frequency axis suitable for replacing SPRTs in calibration laboratories.

2:30pm **NS-MoA-5 Development of New Chip-Scale Photonic AC-DC Thermal Transfer Standard***, Sesha Challa, Michal Chojnacky, Kevin O. Douglass, Daniel S. Barker,* NIST*; Stefan Cular,* Howard Community College, Columbia, MD*; **Nikolai Klimov,*** NIST

One of the state-of-the-art ac-dc thermal transfer standards, such as Multijunction Thermal Converter (MJTC), relies on comparing the Joule resistive heating of an unknown ac signal to a known dc signal. The resistive temperature sensor, a thermocouple array, detects the heat generated by an electrical signal applied to the heater. Despite being accurate, MJTC reached its fundamental limitations. MJTC suffers from frequency-dependent heater impedance due to capacitive coupling between the ac current flowing through the resistive heater and the thermocouple array. Furthermore, the precision of ac-dc difference cannot be increased much further by increasing the size of the thermocouple array. To address these limitations and to reduce the ad-dc difference calibration chain, we are developing an alternative, photonics-based technology to perform ac-dc difference measurements. Our new chip-scale Photonic Thermal Transfer Standard (PTTS) device is designed to match or exceed the metrological performance of conventional thermal transfer standards, overcome the current technological barriers, and reduce the ac-dc difference calibration chain. The PTTS device, similar to the MJTC standard, detects local temperature changes from Joule heating induced by ac/dc electrical currents. However, in contrast to MJTC, the temperature sensing element in PTTS is photonics-based. Waveguide-integrated microscale photonic thermometer not only has ultra-high resolution and precision but is also immune to RF interference and does not have a capacitive coupling with the resistive heater. In this work, we demonstrate the first prototype chip-scale photonic device to perform ac-dc difference. The device exhibits a larch ac response above 100 kHz, typical of conventional MJTCs due to fixture constraints (cables, wire bonding, leads). The following generation of PTTS chips will address these limitations. At the end of the presentation, we will outline the future directions toward the development of the new photonics-based thermal transfer standard.

2:45pm **NS-MoA-6 Deterministic Design of Pseudo-Randomly Distributed Nanostructures for Antireflectivity in the MWIR.** *, **Samir Paudel**, Menelaos K. Poutous,* University of North Carolina at Charlotte

Binary-phase subwavelength gratings (SWG) can perform as antireflective structures. Fabricating SWG for applications in the mid-wave infrared (MWIR, 3-5 µm wavelength) can be challenging due to a substrate's optical index and hardness. For high index contrast, antireflective SWG are required to have a depth which can be of the order of a wavelength [1]. The SWG fill-factor can be numerically optimized to improve antireflective efficiency, without any conceptual insight into the SWG profile. Recent experimental results show that pseudo-randomly distributed nanostructures (PRnS) can enhance optical transmission through dielectric windows as well [2,3]. In contrast to optimization by numerical iteration techniques, we have utilized deterministic principles to design PRnS with a-priori minimum-feature dimensions, and specific selection rules for off-axis transmitted intensity scatter profiles. To enhance antireflectivity, we used more than one binary phase transition within the periodic basis cell, to control the effective index value and off -axis scatter profile. We selected linear, low and high scatter PRnS patterns, with a universal critical feature size of 400 nm, to achieve optical surface transmission enhancement above Fresnel limits within the MWIR bandwidth. To ease fabrication requirements, the designs were restricted to a binary phase-depth close to π/2, and unit cell periodic dimensions between 0.8 µm and 4 µm. The PRnS patterns were fabricated using direct two-photon laser-writing in a negative-tone polymer film on a sapphire substrate. To verify fabrication fidelity and tolerance, the PRnS patterns were characterized using a contactless UV-laser confocal microscope. Unpolarized spectral transmission was measured at normal angle of incident using a spectrophotometer in the 2 – 5 µm wavelength band. The measured unpolarized spectral transmission indicates that, with the same critical feature size, wide off axis scatter PRnS patterns exhibit superior antireflectivity performance compared to narrow off-axis scatter PRnS patterns. The experimental results were in good agreement with numerical rigorous coupled-wave analysis simulation predictions.

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3:00pm **NS-MoA-7 Plasmonic Behavior in Boron-Doped Diamond Arising from Low Energy, Intervalence Band Electronic Excitations***, **Souvik Bhattacharya**, R. Mohan Sankaran,* University of Illinois at Urbana Champaign

Diamond is well-known for its extraordinary mechanical, thermal, and optical properties. The introduction of impurity dopants can further tune and transform diamond. For example, boron, a p-type dopant, has been used to enhance electronic conductivity[1] and produce superconductivity[2]. In recent years, a whole host of other impurity atoms in combination with vacancies have been found to create color centers with unique spin properties that have potential for quantum technologies.[3]

In this talk, we will discuss our recent discovery of low energy (<0.5 eV) plasmonic excitations emerging from the valence subbands as a result of boron doping of diamond.[4] Our study was made possible by recent advancements in characterization techniques including scanning transmission electron microscopy-valence electron energy loss spectroscopy (STEM-VEELS) and near-field infrared (IR) spectroscopy. Applying these techniques to boron-doped diamond, we obtain complementary information about the material response in terms of the energy loss and absorption. A theoretical treatment based on first-principles calculations is then carried out to elucidate the fundamental band origin of the response. We show that boron doping leads to emptying of valence subbands, opening up intervalence band (IVB) transitions. Further analysis of the real dielectric component of the calculated response function reveals a resonance and zero-crossing that blue shifts with increasing carrier density, indicating the emergence of metallicity and plasmonic behavior. This mechanism is notably distinct from the collective Drude-like intraband excitations that are reported in traditional metals and other doped semiconductors. The possibility of plasmonic properties in diamond is yet another insight into this remarkable material that could be combined to for example, enhance the fluorescence of color centers for quantum sensing applications.

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3:15pm **NS-MoA-8 Two-Layer Dual-Mode Reflective-Transmissive Polarization Converter by Stereometamaterials***, **Sanchita Sarker**, Mohammad Parvinnezhad Hokmabadi,* University of North Carolina at Charlotte

The ability to control light polarization is vital for applications in imaging, communications, metrology, among others. and. This work reports a systematic approach using supercells of periodic metamaterials to achieve enhanced polarization control. The use of supercells, with identical resonators, provides enhanced parameter flexibility, enabling facile control over the phase and polarization of scattered beams through rotation, flipping, and shifting of the resonators. In particular, we show that by changing the symmetry of the structure from reflection to inversion in a subwavelength two-layer supercell, a transmissive polarization conversion device can be transformed into a reflective counterpart, both with near-unity polarization conversion ratios. This systematic use of supercells highlights their potential for advanced polarization manipulation in electromagnetic and optical devices.

3:30pm **NS-MoA-9 Metamaterial Enabled Semiconductor Lasers***, Sanchita Sarker, **Mohammad Parvinnezhad Hokmabadi**,* University of North Carolina at Charlotte

Over the past two decades, metamaterials—judiciously designed subwavelength structures—have revolutionized optics, enabling breakthroughs in imaging and optical analog computation, among other areas. Recently, interest has expanded to include their use in on-chip beam manipulation and light outcoupling in passive systems. However, their potential within *active* photonic devices—particularly for controlling light inside laser cavities and shaping unconventional cavity geometries—remains largely unexplored. While techniques such as photonic crystals, topological photonics, and optical supersymmetry have been leveraged to enhance laser performance, metamaterials have yet to be fully utilized in this context.

Metamaterials offer distinct advantages that distinguishes them from other structures, particularly their ability to manipulate phase and amplitude at subwavelength scales that are not readily available in other platforms. In this work, we exploit these properties to engineer surface phase profiles that couple into the laser cavity, thereby enhancing the performance of semiconductor lasers. Our devices are based on InGaAsP quantum wells, emitting near 1550 nm. In a standard configuration, the laser cavity supports higher-order lateral modes, which degrade the spatial coherence and brightness of the emitted beam. To address this, we have integrated metamaterial nano-resonators into the cavity of this laser to manipulate light propagation in the lateral direction.

Through careful design of these subwavelength structures, we demonstrate suppression of higher-order lateral modes in favor of the fundamental mode. As a result, the laser emits predominantly in the fundamental lateral mode, significantly enhancing its brightness. To our knowledge, this is among the first demonstrations of incorporating metamaterials directly into the active region of a semiconductor laser cavity, paving the way for novel applications of metamaterials in active photonic devices.

4:00pm **NS-MoA-11 Direct-Write Ion Patterning of Aluminum Nitride Towards Tuning Integrated Photonics*, Bogdan Dryzhakov*,** *Kyle Kelley,* Oak Ridge National Laboratory

Leveraging focused ion beams, this study spatially patterns point defects into wurtzite aluminum nitride (AlN), achieving defect-driven tunability of ferroelectric, optical, and thermal properties. The robust bonding and strong restoring forces of the AlN lattice help preserve long-range polar order even at ion irradiation doses up to 10^{18} ions/cm^2, enabling highly localized defects that act as domain nucleation sites for ferroelectric polarization reversal. Notably, ion irradiation induces stable ferroelectricity in nominally piezoelectric AlN and reduces the ferroelectric switching barrier in boron-substituted aluminum nitride ($Al_{0.94}B_{0.06}N$) by more than 40%. Advanced spectroscopic imaging, including photo- and cathodoluminescence, Raman spectroscopy, and thermal conductance mapping, spatially tracks evolving signatures of defect states and directly correlates them with the emergent ferroelectric functionality and significant (>10×) thermal tunability. Finally, integrating this localized defect engineering of AlN films into quantum photonic integrated circuits enables on-chip tuning of piezoelectric and nonlinear optical coefficients, demonstrating its promise as a practical method for advanced electro-optic and photonic device engineering.

4:15pm **NS-MoA-12 Actively Tunable in-Plane Hyperbolicity in Excitonic Single-Walled Carbon Nanotubes*, Jason Lynch,*** *Deep Jariwala,* University of Pennsylvania

Hyperbolicity allows for the confinement of extremely large electric fields on the nanometer scale and the control of the propagation of electromagnetic energy within it. Hyperbolic metamaterials in the visible and near infrared rely on free-carrier effects since plasmonic media were the only ones with strong enough optical responses to host negative permittivities in this energy range. As a results of using plasmonic media, hyperbolic systems lack tunability and emissivity without the implementation of an adjacent active layer. However, narrow, inorganic excitons have recently been shown to exhibit negative permittivities in several different media just above their resonant energies. Therefore, excitons promise to enable hyperbolic media that is intrinsically emissive and highly tunable. Most of these systems require low temperatures (with the exception of chiral-pure single-walled carbon nanotubes (SWCNTs) and hBN-encapsulated, exfoliated WS_2), and they typically lack in-plane optical anisotropy. Here, we study the electro-optical properties of chiral-pure, aligned SWCNTs, and we observe that SWCNTs have a hyperbolic region that is actively tunable using electrostatic doping. We first use the Lorentz oscillator model to provide insights on the requirements for excitons to exhibit negative permittivity, and what would be needed for a true epsilon-near-zero excitons. Using these insights, we find that excitonic SWCNTs must be chiral-pure and high-density to exhibit negative permittivities. Next, micro-Mueller matrix ellipsometry is used to observe actively-tunable, in-plane hyperbolicity in aligned SWCNT films. The hyperbolic window is tuned by 50 meV by injecting ≈10^{13} carriers/cm^2. For comparison, the Drude model predicts that the plasmon resonance would be tuned by < 1 meV in ITO at the same transition energy. Therefore, SWCNTs have a 60x improvement in hyperbolic tunability than free-carrier systems when normalized for energy. Additionally, the loss in the SWCNTs at the hyperbolic transition is found to be comparable to TiN showing that it could be implemented in similar hyperbolic systems. When combined with the ability for SWCNTs to be globally-aligned on the wafer-scale, our work demonstrates that SWCNTs has great potential as a hyperbolic medium for both emissive and active photonics.

4:30pm **NS-MoA-13 Imaging Photonic Resonances within an All-Dielectric Metasurface via Photoelectron Emission Microscopy*, Andrew Kim,*** Sandia National Laboratories*; Chloe Doiron,* Sandia National Laboratories, USA*; Fernando Vega,* Purdue University, USA*; Jaeyeon Yu, Alex Boehm, Joseph Klesko, Igal Brener, Raktim Sarma, Alexander Cerjan, Taisuke Ohta,* Sandia National Laboratories, USA

Dielectric nanophotonics aims to achieve precise control of light-matter interactions by confining light within subwavelength structures and manipulating the electromagnetic fields therein. Such precise control is utilized towards technological applications that include imaging, holography, and sensing, among others. Here, we use photoelectron emission microscopy (PEEM) to demonstrate near-field imaging of optical resonances within a dielectric metasurface in the ultraviolet to visible wavelength range. This approach involves far-field photonic excitation akin to the illumination conditions of photonic devices and allows for near-field imaging at a sub-optical wavelength spatial resolution. We analyze the local volumetric field variations within the meta-atoms as a function of excitation wavelength and polarization by comparing photoelectron images to finite-difference time-domain simulations. The metasurface supports two distinct resonances that occupy regions of different material thickness within the metasurface, resulting in a contrast in photoemission intensity due to the inelastic mean free path (IMFP) of the photoelectrons. The simulations replicate the intensity distribution in PEEM images by accounting for this IMFP as the two resonances shift their intensity as wavelength is varied. Through our analysis, we determine the IMFP of very low kinetic energy (<1 eV) photoelectrons to be ~35 nm, which is comparable to the meta-atom height and thus highlights the PEEM sensitivity to resonances within the volume. Overall, these results demonstrate that photoelectron imaging with sub-wavelength resolution is suitable for examining light-matter interactions in volume-type (as opposed to surface) photonic modes within dielectric nanophotonic structures.

This work was supported by the US Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574) and by the LDRD program at Sandia National Laboratories. This work was performed in part at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy, Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. The views expressed in the article do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

4:45pm **NS-MoA-14 Investigation the Photocatalytic effect of RuO_2 loading on TiO_2 towards Hydrogen Evolution in Visible Light*, Moses Ashie,*** *Bishnu Bastakoti,* North Carolina A&T State University

The significant role that fossil fuels have played in energy utilization cannot be underestimated. However, owing to the non-renewable and CO_2 emission associated to its usage has paved a way for a search for a more renewable and environmentally unfriendly energy sources of which hydrogen energy identified as a potential target. A highly porous TiO_2-RuO_2 heterogenous solvothermally engineered photocatalyst revealed how varying synthesis conditions can contribute to the modification of TiO_2 towards effective photocatalytic water splitting in the visible region of the electromagnetic spectrum. Characterization techniques such as XRD, SEM, TEM, UV-Vis DRS, and electrochemical analysis revealed that TiO_2-RuO_2-20 exhibited reduced band gap, improved light absorption capability, lower electron-hole recombination rate, lower solution resistance which collectively contributed to effective photocatalytic activity. In addition, a high surface area and mesoporous nature contributed to 1794.8 mmolg^{-1}h^{-1} of hydrogen gas. Compared to the pristine RuO_2 (21.9 mmolg^{-1}h^{-1}) and the commercially available TiO_2 (246.4 mmolg^{-1}h^{-1}), the TiO_2-RuO_2-20 sample produced a yield that is almost 81 times and 7 times respectively. This therefore proves the effectiveness of the solvothermal method and the ruthenium dioxide in modulating the photocatalytic properties of TiO_2 photocatalyst for photocatalytic water splitting in visible light.

Nanoscale Science and Technology
Room 206 A W - Session NS1-TuM

AI for Material Discovery and Characterization

Moderators: Yongtao Liu, ORNL, **Son Le**, University of Maryland

8:00am **NS1-TuM-1 Advancing Scanning Probe Microscopy as a Tool for Nanoscale Scientific Discovery with AI***, **Rama Vasudevan**, Ganesh Narasimha, Jawad Chowdhury,* Oak Ridge National Laboratory*; Soumendu Bagchi,* Oak Ridge Natinal Laboratory*; Yongtao Liu,* Oak Ridge National Laboratory **INVITED**

Scanning probe microscopy (SPM) methods have been a mainstay of nanotechnology since their inception in the 1980s, helping to image and map functional properties of a wide variety of samples, ranging from ceramics to thin films to nanoparticles to biomolecules. More recently, the advent of machine learning and artificial intelligence (AI) has led to an increasing adoption of AI-based methods within core physical sciences.

In this talk, it will be shown how AI can significantly improve SPM in terms of scientific discovery, by adapting AI algorithms and tailoring them for purposes of microscopy characterization and manipulation. Traditional spectroscopic characterization in SPM is carried out in a point by point manner across a grid of points, which is highly redundant. We propose the use of curiosity-based algorithms that can adaptively sample different locations to improve exploration, and boost the robustness of generated structure-function models. The proposed algorithm is trialed on several microscopy platforms and is shown to be superior to random sampling, and is suitable for circumstances when no scalarizer function is available for optimization.

In contrast to materials characterization, where the task is generally purely one of materials prediction, material manipulation requires knowledge of how to act under different environment states, constuting a sequential decision making problem, which is usually formulated as a reinforcement learning problem. This can be solved via traditional policy-based learning methods such as policy-gradient, Q-learning, etc. Here, we show how RL-policies can be learned to manipulate ferroelectric domain structures in thin films, given a surrogate model for domain wall-SPM tip bias interactions, as well as extensions of this RL approach for atomic scale manipulations with other microscopy platforms. This research was supported by the Center for Nanophase Materials Sciences (CNMS), which is a US Department of Energy, Office of Science User Facility at Oak Ridge National Laboratory.

8:30am **NS1-TuM-3 Understanding and Controlling Atomic Transformations in 2D Materials Through in situ STEM***, **Raymond Unocic**, Caitlyn Obrero,* North Carolina State University*; Kevin Roccapriore,* AtomQ*; Ayana Ghosh,* Oak Ridge National Laboratory*; Maxim Ziatdinov,* Pacific Northwest National Laboratory*; Sergei Kalinin,* University of Tennessee Knoxville*; Matthew Boebinger,* Oak Ridge National Laboratory, USA

The discovery and design of next-generation functional 2D materials demand an atomic-level understanding of how structure and chemistry govern performance. At the nanoscale, where materials are often only a few atomic layers thick, minute structural or chemical changes can trigger profound shifts in electronic, magnetic, optical, and catalytic properties. Unlocking control over these properties requires deep insight into the transformation mechanisms that govern atomic-scale behavior. Scanning transmission electron microscopy (STEM) has emerged as a vital tool due to high spatial resolution imaging, diffraction, and spectroscopy. Recent breakthroughs in *in situ* and *operando* STEM now allow us to go beyond static characterization, opening the door to real-time observation of structural evolution and chemical reactions under dynamic conditions. In this work, we leverage *in situ* STEM to investigate the formation pathways, reaction kinetics, and energy landscapes involved in the synthesis of novel 2D materials. Using controlled heating experiments, we directly visualize the transformation of amorphous precursors into crystalline layered structures, capturing how temperature and electron dose influence nucleation and growth mechanisms at the atomic level. Further, we demonstrate atomic engineering of 2D materials through feedback-controlled electron beam techniques to create targeted defects and nanopores with atomic precision. To deepen our mechanistic understanding, we integrate machine learning tools to analyze transformation dynamics and uncover hidden patterns in atomic-scale behavior. These insights pave the way for predictive control over material design. The presentation will conclude with a forward-looking perspective on how advanced microscopy, paired with machine learning, is redefining the limits of materials discovery - transforming our ability to design and engineer 2D functional materials.

8:45am **NS1-TuM-4 Advancing Autonomous Experimentation with Human-AI Synergy and Cross-Platform Integration***, **Yongtao Liu**,* 1 Bethel Valley Road

Advancements in artificial intelligence are rapidly transforming materials research by enabling autonomous experimentation. In this talk, I will present our recent progress in developing automated and autonomous experimentation frameworks that accelerate discovery across diverse materials systems. Our approach integrates computer vision-enabled high-throughput experimentation, AI-powered decision-making, prior knowledge-guided exploration, and cross-platform co-optimization. By leveraging computer vision, we enable rapid, automated exploration of complex experimental parameter spaces. We further incorporate AI algorithms into experimental loops to perform real-time data analysis and decisions making. A key feature of our framework is the incorporation of expert knowledge and human oversight, enabling context-aware experimentation grounded in physical understanding. Beyond single-platform optimization, we also introduce a cross-platform strategy of autonomous experimentation that enables coordinated operation between synthesis and multimodal characterization tools. This distributed yet collaborative strategy requires no physical integration, offering an approach for autonomous research across diverse research platforms.

9:00am **NS1-TuM-5 Nanovision: An Integrated Platform for Two–Dimensional Material Discovery and Device Assembly***, **Son Le**, Jeffrey Schwartz,* Laboratory for Physical Sciences*; Ruihao Ni, You Zhou,* University of Maryland, College Park*; Karen Grutter, Aubrey Hanbicki, Adam Friedman,* Laboratory for Physical Sciences

Two-dimensional (2D) materials are crucial for enabling next-generation computing, electronics, sensing, and communication technologies. Currently, most breakthroughs in 2D material research rely on atomically thin (few-layer), exfoliated crystals. Frustratingly, identifying candidate crystals typically requires tedious, time-consuming, manual processes performed by trained researchers. This bottleneck severely limits device complexity, fabrication throughput, and overall research efficiency. To address this challenge, we created an integrated hardware and software platform that rapidly and automatically images, identifies, and catalogs exfoliated 2D crystals at full-wafer scales. Our platform enables researchers to visualize and to interact with ultra-high-resolution multimodal images of 2D materials using a web-accessible interface that supports remote operations, promotes data sharing, and enhances researcher productivity. By leveraging artificial intelligence and computer vision strategies, our platform eliminates the need for researchers to engage in tedious visual identification. A working prototype of this platform has helped us to streamline our 2D materials device research while collecting user feedback for continual refinements to our workflow. Moreover, using this platform, we are compiling physical and digital libraries of exfoliated 2D materials with the goal of democratizing access to high-quality materials for researchers. In this presentation, we describe the ongoing development of the hardware, software and control interface used in this impactful materials discovery platform.

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.

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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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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.

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

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

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

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

11:45am **NS2+2D-TuM-16 Quantitative Comparative Force Spectroscopy on Molecules***, 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.

Nanoscale Science and Technology
Room 206 A W - Session NS-TuA

Advanced Nanoscale Materials & Device Technologies

Moderators: Andrew Mannix, Standford University, **Taisuke Ohta**, Sandia National Laboratories

2:15pm **NS-TuA-1 Engineering at the Limits of the Nanoscale***, **Farnaz Niroui**,* Massachusetts Institute of Technology **INVITED**

Next-generation devices for computing, sensing, and information processing leverage the unique properties of emerging low-dimensional materials. However, integrating these materials into functional nanosystems is challenged by their incompatibility with conventional fabrication techniques. To unlock their full potential, new heterogeneous integration platforms are essential. By combining top-down fabrication with the precision of bottom-up processes, we present strategies that overcome these limitations, enabling precise and deterministic integration of low-dimensional materials with down to sub-10 nm resolution. Through these strategies, we have developed new device platforms for energy-efficient computing, enhanced sensing, and quantum photonic technologies, which will be discussed in this talk.

2:45pm **NS-TuA-3 Theoretical Insights into Ethylene Hydroformylation on Transition Metal Heterogeneous Catalysts***, **Shyam Kattel**,* University of Central Florida*; Sourav Ghoshal,* Florida A&M University

Traditional hydroformylation, an important oxo-synthesis route, is an industrial process to produce aldehydes by the reaction of synthesis gas, a mixture of CO(g) and H_2(g), with alkenes. Currently, hydroformylation represents one of the largest homogeneously catalyzed reactions in industry and is carried out using Rh and or Co-based transition metal complexes as a catalyst. However, the homogeneous nature of this reaction leads to difficulties in catalyst separation and recovery, active metal losses, metal species contamination in aldehydes, and corrosivity of catalytic solutions. The design of heterogeneous catalytic systems without sacrificing the activity and selectivity will avoid the drawbacks associated with homogeneous catalysts and be highly useful. However, a fundamental understanding of reaction mechanisms and key steps/descriptors that control the activity and selectivity of alkene hydroformylation on heterogeneous catalytic systems is limited.

Herein first-principles density functional theory (DFT) calculations were carried out to compute reaction energetics and kinetics of ethylene hydroformylation to C3 Oxygenates on (111) surface and small nanoparticles/clusters of eight face center cubic transition metals Cu, Ni, Rh, Pd, Ag, Pt, Ir, and Au. Our DFT and microkinetic simulations revealed that the metal surface model failed to capture the experimentally reported activity/selectivity trends, whereas the nanocluster model demonstrated excellent agreement with experimental results. The Rh nanoparticle showed a lower activation energy (0.87 eV) for the *CO and *C_2H_5 coupling reaction, a key reaction step for C-C coupling in hydroformylation reaction. Under experimental reaction conditions (~473 K, 1 atm), the results from microkinetic simulations illustrate that the selectivity of Rh nanoparticle for the formation of C_2H_5CHO (a C-C coupling product) is highest among all the metals studied in the present study for a temperature range of 450-900K. Thus, our results from DFT and microkinetic simulations provide atomistic insight into the reaction pathways of ethylene hydroformylation to C_2H_5CHO on transition metal catalysts and identify sites that promote the C-C coupling, a key reaction step in hydroformylation reaction. Finally, this work highlights the critical role of nanoparticle size and structure in tuning the selectivity of ethylene hydroformylation to a desired product.

3:00pm **NS-TuA-4 Van Der Waals 3D Assembly of 2D Nanomaterials for Scalable Electronics***, **Joohoon Kang**,* Yonsei University, Korea

Two-dimensional (2D) nanomaterials have been received a great attention as potential building blocks for use in fundamental elements of (opto)electronic applications due to their diverse and remarkable electronic and optical properties. However, such fundamental demonstrations cannot be directly applied to practical applications because of scalable synthesis of high-quality nanomaterials and their proper assembly. In this presentation, I will demonstrate wafer-scale van der Waals assembly of 2D materials, which are exfoliated via a molecular intercalation-assisted electrochemical exfoliation method. The resulting materials with distinct electronic properties including metal, semiconductor, and insulator, can be assembled into various (opto)electronic devices such as transistors, diodes, logic gates, and photodetectors. Also, such solution-based approach further enables inkjet printing-based device fabrications without a conventional lithography.

3:15pm **NS-TuA-5 Impact of External Screening on the Valence and Core-Level Photoelectron Spectra of One-Layer WS_2***, Alex Boehm, Chris Smyth, Andrew Rakyoung Kim, Don Bethke, Tzu-Ming Lu, Jose Fonseca Vega, Jeremy Robinson, **Taisuke Ohta**,* Sandia National Laboratories, USA

In a well-screened environment, transition metal dichalcogenides (TMDs) rearrange their charge carriers to screen the added charges, and reduce the electronic band gap. Consequently, when interfaced with dissimilar materials, a sheet of TMD would change its band gap adapted to its local external screening environment. Similarly, a well-screened environment stabilizes photo-holes or core-holes created in the photoemission process and, in turn, boosts the kinetic energy of photoelectrons resulting in the apparent smaller binding energy. Complication arises when determining the electronic band alignment of TMDs using photoelectron spectroscopy since the screening influences the material property of interest as well as its assessment approach concurrently. Using a sample that contains areas of suspended and gold-supported one-layer WS_2, we show how the electronic states of WS_2 under the contrasting effective or ineffective external screening environment align at the built-in junction. The photoelectron spectra point to the breakdown of rigid shifts between the valence states and core-levels with the core-levels shifting more than twice as much as the valence states. Additionally, effectively-screened WS_2 displays a valence state with a substantially larger photoemission linewidth than ineffectively-screened suspended WS_2. Altogether, our result provides key insights into how the local variation of the external screening environment creates essentially a heterojunction within a layer of WS_2.

The work was supported by the Laboratory Directed Research and Development program at Sandia National Laboratories and Base Programs and the Nanoscience Institute at the Naval Research Laboratory via the Office of Naval Research. A.R.K. acknowledges support from the U.S. Department of Energy, Office of Science, Division of Materials Sciences and Engineering (grant BES 20-017574). Samples were fabricated, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the US Department of Energy, Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly-owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S. Department of Energy or the United States Government.

4:00pm **NS-TuA-8 III-Nitride Ferroelectrics for Low-Power Computing Devices***, **Deep Jariwala**,* University of Pennsylvania

Since the demise of Dennard scaling, modern computer has largely relied on architectureal innovations such as multi-core processors and GPUs vs CPUs the address the evolving needs of computing paradigm. This above problem has been exacerbated since computing has largely evolved from arithmetic centric to data centric in the age of billions of internet-connected devices and artificial intelligence. Thus, dense and reliable data storage combined with fast and high bandwidth access in novel memory devices has become the frontier for research in modern computing hardware. In this regard there have been several advancements across a variety of technologies in the past three decades. Ferroelectric materials and devices are among the forefront of these technologies due to their low-power and fast switching abilities but suffer from integration challenges.

Therefore, in this talk, I will try to make the case of how novel III-nitride materials might present interesting avenues to overcome some of the above limitations being faced by Silicon hardware. I will start by presenting our ongoing and recent work on integration of 2D chalcogenide semiconductors emerging wurtzite structure ferroelectric nitride materials namely aluminium scandium nitride (AlScN). First, I will present on Ferroelectric Field Effect Transistors (FE-FETs) made from 2D materials when integrated with AlScN and make the case for 2D semiconductors in this application. I will then show our most recent results on scaling 2D/AlScN FE-FETs, achieving ultra-high carrier and current densities in ferroelectrically gated MoS_2 and also demonstrate negative-capacitance FETs by engineering the AlScN/dielectric/2D interface. Then, I will switch gears to introduce the ferroelectric diode (FeD) memory device and demonstrate multi-bit operation as well as compute in memory (CIM) using FeD devices made from AlScN.

4:15pm **NS-TuA-9 Chemical and Mechanical Modification of 2D Semiconductors for Electronic Devices***, **Andrew Mannix,*** Stanford University

Layered van der Waals materials, composed of discrete, atom-thin sheets, enable the deterministic assembly of heterostructures and precise placement of dopants and defects, offering a powerful route to tailor electronic and quantum properties. However, achieving scalable synthesis, controlled electronic interfaces, and low defect density remain major challenges for technological applications. This talk will highlight recent advances in overcoming these materials science barriers to enable next-generation (opto)electronic and quantum technologies based on 2D semiconductors and their heterostructures.

To accelerate chemically-tailored synthesis and compositional tuning of transition metal dichalcogenides (TMDCs) like WS_2 and WSe_2, we developed a hybrid metal-organic chemical vapor deposition process. Using solution-phase deposition of metal salt precursors and vapor-phase chalcogen delivery, this method provides high quality growth with precise doping, alloying, and growth chemistry modification [1]. Confined-space growth using this method enabled the selective formation of ferroelectric 3R-phase TMDC films on dielectrics [2], opening new possibilities for ferroelectric semiconductor devices and nonlinear optics.

Interfacing 2D semiconductors with electrodes remains a key challenge. We found that mechanical strain from top contacts, such as Ni on WS_2, can significantly enhance device performance—an often-overlooked effect [3]. For p-type WSe_2 transistors, we show that chloroform intercalation doping is a clean, reliable, and stable method to improve contact quality, even at low temperatures. These advances provide critical pathways toward scalable 2D semiconductor technologies.

[1] Z. Zhang, L. Hoang, et al., *ACS Nano* **18**, 25414 (2024).

[2] Z. Zhang, et al., *Nano Letters*, **24**, 12775 (2024).

[3] L. Hoang, et al., *Nano Letters*, **24**, 12768 (2024).

4:30pm **NS-TuA-10 Fabrication of Si Nanopillars Using Pmma Resist***,* ***Kareena Guness****, Zachary Kranefeld, T. Pan Menasuta, Basil. F Vanderbie, Thomas. E Vandervelde,* Tufts University

Poly-methyl methacrylate (PMMA) is the most commonly used e-beam resist. While it is cost effective, easily available, and offers the highest resolution among any polymeric resist, PMMA suffers from poor dry-etch resistance. For that reason, other resists like HSQ and ZEP are typically preferred. In this work, we report the fabrication of silicon nanopillars using PMMA, emphasizing on the process optimizations, particularly in reactive ion etch (RIE) chemistry, required to overcome key roadblocks. Electron beam lithography was used to write patterns in PMMA positive tone resist. To transfer the patterns to the substrate and achieve nanopillars of high-aspect ratios with smooth sides, RIE was employed with SF6 and O2. The hard mask was removed by soaking the wafer in remover-pg for several hours. The fabrication processes were characterized by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM).

4:45pm **NS-TuA-11 Nanoplastic Pillar Arrays for Chemical Sorption Assays***,* ***Sandra Gutierrez Razo****, Andrew Madison, Craig Copeland, Danuta Liberda-Matyja, John Pettibone, Daron Westly, Samuel Stavis,* NIST

Nanoplastic chemical sorption is of great interest and concern. Because of their scale, nanoplastic particles are difficult to detect and quantify. Many approaches involve optical microscopy and microspectroscopy, so we are fabricating pillar arrays on silicon wafers to produce novel nanoplastic standards. We spin coat low-density polyethylene (LDPE) films that are less than 100 nm thick. We then pattern the thin films using electron-beam lithography and oxygen etch. Control over pillar size, shape, and position enables useful calibrations. The arrays can also be used as substrates to study the sorption of chemicals onto LDPE. We begin with two florescent chemicals, rhodamine B, a common fluorophore, and and 4,4'-diamino-2,2'-stilbene disulfonic acid (DSD), an optical brightener added to laundry detergent. Further study of the correlation of fluorescence intensity and pillar volume will elucidate interactions of nanoplastic particles and chemical sorbents of environmental concern and technological interest.

The figure in the supplemental document shows LDPE films and pillars. (a-b, left) OPTIR spectra showing three absorption peaks consistent with LDPE at 2919, 2850, and 1456 cm-1 indicating that the composition does not change after patterning with electron-beam lithography and etching. (a, right) Optical micrograph showing nucleation sites and spherulite boundaries in an LDPE film before nanofabrication. (b, right) Optical micrograph showing features after patterning. (c) Atomic force micrograph showing pillars of similar height of approximately 76 nm and diameters varying from approximately 1000 nm to 100 nm, before chemical sorption. (d) Fluorescence micrograph of LDPE pillars after soaking in a rhodamine B solution. (e) Fluorescence micrograph of LDPE pillars after soaking in DSD solution. For both (c) and (d), the peak wavelength of fluorescence excitation is approximately 550 nm, and fluorescence emission is collected through a long-pass filter above 590 nm.

5:00pm **NS-TuA-12 Optimizing Nanocrystalline WO_3 Thin Films: The Role of Oxygen, Thickness, and Pressure in Highly Selective and Responsive NO Gas Sensing***,* ***Somdatta Singh,*** Indian Institute of Technology Roorkee, India*; Ravikant Adalati,* University of Mons, Belgium*; Prachi Gurawal, Raman Devi, Radhika Jain, Davinder Kaur, Ramesh Chandra,* Indian Institute of Technology Roorkee, India

WO_3 thin films have been deposited using the room temperature (RT) sputtered DC magnetron sputtering approach on n-type (100) silicon substrates at various O_2/Ar gas ratios, thicknesses, and pressure variations for NO gas detection. The structural characteristics of the film were examined using X-ray diffraction (XRD). X-ray photoelectron spectroscopy (XPS) confirms that all monoclinic-phase WO_3 thin films contain oxygen vacancies. The FESEM study revealed a nanocrystalline structure with a granular, porous morphology. This study discusses how the WO_3 thin film's stoichiometry affects the NO gas sensing capability. The sub-stoichiometric WO_3 thin film-based sensor improved performance in terms of high stability, selectivity, and fast response/recovery time. The sensor response (R_g/R_a) was approximately 52.53 for a 100 ppm NO concentration at 275°C, with a fast response time of about 26 sec and a recovery time of about 19 sec. WO_3 thin-film-based NO gas sensing has been evaluated across a range of operating temperatures (50–325°C) and gas concentrations (1–100 ppm), observing a change in sensor response. Additionally, the NO gas-detecting mechanism on WO_3's surface has been discussed. These results demonstrate the potential for creating high-performance, cost-effective gas sensors based on room-temperature sputtered nanocrystalline WO_3 thin films.

Keywords: WO_3; Thin films; Sputtering; Metal oxide; NO sensor.

5:15pm **NS-TuA-13 Effects of Anode Distance on Field Emitter Array Performance in Simulation***,* ***Youngjin Shin****, Kenneth Chap, Ellie Bultena, Akintunde Akinwande,* Massachusetts Institute of Technology

We present our exploration into channel electric field redistributions of field emitter arrays (FEAs) by simulating the electrostatics at various anode-to-emitter distances, L_{AE}. Silicon FEAs are cold cathode electron sources that have shown promise for high-power applications such as power switches. One of the limiting factors of FEAs as a power switch is its relatively low efficiency at lower voltages. Some of the factors that contribute to an FEA's efficiency are the on-voltage (V_{ON}=25V-30V), operating anode-to-emitter voltage (V_{AE}), and the gate leakage current. Typically, to achieve a higher efficiency (>99%), FEAs are utilized in high-voltage applications that require >10kV bias on the anode to maximize the ratio between V_{AE} and V_{ON} [1]. However, there are challenges in operating FEAs at high-voltages due to large amounts of leakage current when driving higher current densities. In prior works, it has been implied that electrons emitted at a non-vertical emission angle are collected by the gate electrode, increasing the leakage current [2]. L_{AE} has mainly been studied for its effects on space charge but have not yet discussed its impact on reducing the gate leakage current when the device is in saturation, improving the output power efficiency. In this study, we conduct electrostatic simulations in COMSOL to demonstrate how decreasing L_{AE} influences channel field redistribution to reduce leakage current at the gate aperture with flat and cusp anode geometries.

Our simulations show that changes in L_{AE} result in distinct local electric field distribution patterns along the gate aperture; at smaller L_{AE}, the electric field is mostly vertical, whereas at large L_{AE}, the non-uniform field has higher horizontal electric field components away from the center of the gate aperture. Fig.1 and Fig.2 show the electric field distributions across the gate apertures for a 3x3 FEA at V_{AE}=200V, V_{GE}=40V, and L_{AE}=2mm, 5mm, and 30mm for a flat and cusp anode, respectively. The field distribution at 30mm indicates that it is likely that a smaller proportion of electrons from the emitter are collected at the anode compared to the 2mm and 5mm configuration due to the electric field being almost entirely vertical across the entire gate aperture. The cusp anode shows the most dramatic difference between 2mm and 5mm, likely owing to its focused tip shape. Our results indicate that reducing L_{AE} increases the vertical electric field, encouraging the emitted electrons have a vertical trajectory towards the anode, preventing its collection at the gate. Future work will focus on experimental validation of these findings and analyzing how to prevent breakdown at L_{AE}<5mm.

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**.**

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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.

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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.

Electronic Materials and Photonics
Room 207 A W - Session EM2+AP+NS+TF-WeA

Advances in Materials and Devices for Energy Storage

Moderators: Claire Davis-Wheeler Chin, Sandia National Lab, **Alexander Kozen**, University of Vermont

3:15pm **EM2+AP+NS+TF-WeA-5 In-Situ Characterisation of Solid Electrolyte Interphase Formation on Lithium Metal for Energy Storage***, **Anthony Somers**,* Deakin University, Australia

The Solid Electrolyte Interphase (SEI) is a complex passivating layer that forms on the anode in the early stages of battery cycling. Ideally this layer should protect the anode from degradation while allowing the ions of interest to freely move through with high efficiency. To ensure long cycle life this layer also needs to be stable over hundreds of charge/discharge cycles. For the safe and successful operation of promising new battery technologies, such as lithium metal, information on how electrolyte composition effects the SEI is needed.

Most analysis of the SEI is ex-situ, making it difficult to identify the processes occurring during the initial formation phase. While there are a range of in-situ and operando techniques that have been used to investigate SEI formation, there is often a lack of cross-checking between techniques to confirm findings or determine all processes involved.

In this work a range of in-situ, operando and ex-situ techniques have been used to identify the mechanisms of SEI formation in relation to cycling performance for lithium metal batteries with ionic liquid containing electrolytes. To achieve this, techniques able to detect early subtle changes at the electrode, such as electrolyte rearrangement and organic adsorption, as well as the final reactions that lead to the formation of inorganic, passive layers have been used. Measurements such as operando FTIR spectra, in-situ differential capacitance and electrochemical quartz crystal microbalance and ex-situ XPS are used to form this more complete picture of the processes involved in SEI formation.

3:30pm **EM2+AP+NS+TF-WeA-6 Intercalation of Polyacrylonitrile Nanoparticles in Ti3C2 MXene Layersfor Improved Supercapacitance***, **Shanna Marie Alonzo**, Bishnu Bastakoti,* North Carolina A&T State University

We report the intercalation of polyacrylonitrile nanoparticles in $Ti_3C_2T_x$ MXene layers through simple sonication. The use of polyacrylonitrile, which was synthesized via radical polymerization, offered dual benefits: (1) It increased the interlayer spacing ofMXene, thereby exposing more surface area and enhancing ion transport channels during charge and discharge cycles, and (2) Integrating MXene with polyacrylonitrile enables the creation of a composite with conductive properties, following percolation principle. X-ray diffraction analysis showed an increase in the c-lattice parameter, indicative of the interlayer spacing, from 22.31 Å for the pristine MXene to 37.73 Å for the MXene–polyacrylonitrile composite. The intercalated polyacrylonitrile nanoparticles facilitated the delamination by weakening the interlayer interactions, especially during sonication. Electrochemical assessments revealed significant improvement in the properties of the MXene–polyacrylonitrile composite compared to the pristine MXene. The assembled asymmetric device achieved a good specific capacitance of 32.1 F/g, an energy density of 11.42 Wh/kg, and 82.2% capacitance retention after 10,000 cycles, highlighting the practical potential of the MXene–polyacrylonitrile composite.

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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 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.

Nanoscale Science and Technology

Room Ballroom BC - Session NS-ThP

Nanoscale Science and Technology Poster Session

NS-ThP-1 Single and Dual Sintering Techniques on Flexible Metal Nanoparticle Patterns*, **Md. Mahfujur Rahman**, Rajib Chowdhury, Seonhee Jang,* University of Louisiana

The application of metallic nanoparticle (NP) inks has become the center of developing flexible printed electronic devices such as solar cells, displays, wearables, and sensors. The approach of defining the mechanical, electrical, and material properties of printed patterns depends on the type of metallic NPs. The most utilized NPs are silver (Ag), gold (Au), and copper (Cu). Ag NPs are highly considered for their excellent electrical conductivity and resistance to oxidation. On the other hand, Cu NPs are highly preferred because of their affordability to Ag NPs, yet they are highly prone to oxidation. During printing of metallic NP inks for conductive patterns, a lack of electrical conductivity in the patterns is observed because of induced organic additives and stabilizing agents. Consequently, sintering is essential for removing these organic residues and enhancing the conductivity of the printed patterns.

This study focuses on utilizing two metallic inks of Ag NP ink (PSI-211, NovaCentrix) and Cu NP ink (CP-008, NovaCentrix) to fabricate the conductive patterns on flexible polyimide (PI) sheets. Either single or dual sintering processes were conducted to optimize the electrical conductivity. For the single sintering process, the printed metal NP patterns were subjected to either laser irradiation (LO) or thermal treatment (TO). During the LO sintering process, the Ag and Cu NPs underwent Nd:YAG laser irradiation at 600 and 800 mJ for 15 and 30 s, respectively. For the TO sintering process, Ag and Cu NPs were introduced in a formic acid (FA) vapor environment at 140 and 260 °C for 1.5 and 15 min, respectively. The dual sintering method involved thermal treatment followed by laser irradiation (TL) and laser irradiation followed by thermal treatment (LT).

After sintering, a microstructural analysis was conducted using scanning electron microscopy. The analysis confirmed that the LT condition for sintering of the Ag NP pattern showed improved particle agglomeration and necking. Atomic force microscopy (AFM) analysis revealed the highest roughness of 48 nm, indicating superior grain growth. With a resistance ratio (R/R_0) of 1.75 during the folding test, the Ag NP pattern sintered using the LT condition showed the lowest electrical sheet resistance. Through agglomeration and coalescence during sintering, the Cu NP pattern sintered with the TO condition displayed the most uniform grain growth. The Cu NP pattern sintered under the TO condition had the highest mechanical Vickers hardness of 55.36 N/mm^2 because of the improved connection between the NPs. Additionally, the Cu NP pattern showed the highest roughness value of 51.36 nm.

NS-ThP-2 Impacts of Hydrogen Adsorption on Carbon Nanotube–Metal Schottky Contacts*, Chuntian Huang, Nini Ye, Haijun Luo, Hezhu Shao, **Changkun Dong**,* Wenzhou University, China

Carbon nanotube (CNT)–metal Schottky contacts are widely employed in different types of electronic devices, including field effect transistors (FET) and gas sensors. CNTs are normally considered stable on electronic properties with gas adsorptions. In this work, performance changes of the multi-walled carbon nanotube (MWCNT)–metal junctions related to hydrogen adsorptions were illustrated. MWCNT/Pd and MWCNT/Au Schottky junctions based resistive sensors were constructed to investigate the low-pressure gas sensing performances for hydrogen in the range of 1e−7 to 1e−3 Pa. Two types of sensors presented opposite behaviors with hydrogen adsorptions, i.e., the sensor resistance rose for the MWCNT/Pd sensor but dropped for the MWCNT/Au sensor with increasing hydrogen pressure. The work function reductions of Pd and CNT are considered the key cause, which could change the Schottky barrier properties dramatically.

Such effects were investigated by the first-principles calculations. The work functions of Pd and MWCNT tend to decrease with the dissociated hydrogen adsorptions, while the electronic properties of Au remain constant. The work function of the Pd-CNT Schottky junction drops with hydrogen adsorptions on either CNT or Pd according to the analysis of the density of states (DOS) and charge density difference. It is expected that electrons transfer from Pd of lower work function to CNT after the H adsorption, leading to the resistance increase of the Schottky junction for the p-type MWCNTs. On the other side, the resistance of the Au-CNT Schottky junction would decrease for the electron transformation from CNT to Au. The results are consistent with the experimental investigation and provide important reference significance for applications of metal-CNT junctions.

NS-ThP-3 The Nanoscale Materials Characterization Facility (NMCF) at the University of Virginia*, **Catherine Dukes**, Diane Dickie, Graham Frazier, Helge Heinrich, Art Lichtenberger, Joe Thompson, Richard White,* University of Virginia

The **Nanoscale Materials Characterization Facility** and **Innovations in Fabrication** clean-room microfabrication/biomanufacturing facility are advanced user facilities within UVa's School of Engineering and Applied Science. Our instruments are available for researchers from academic and industrial institutions on a pay-for-time basis. We provide comprehensive services in materials preparation and processing, as well as a suite of advanced analytical techniques. Researchers are welcome to (1) visit the **NMCF** for collaborative sample science or (2) send specimens for remote analyses by one of five expert instrument scientists, ensuring personalized guidance and optimized results.

We operate two transmission electron microscopes: a 200kV Talos system and a 300 kV Themis with probe correction for sub-Å resolution and monochromated EELS. Both offer EDS for compositional analysis and mapping, as well as sample holders for in-situ cooling, heating, biasing, liquid-cell and gas-cell experiments. A Helios dual-beam FIB-SEM is used for surface, cross-sectional, and 3D imaging, EDS analysis, orientation mapping with electron-backscatter diffraction and TEM sample preparation. Additionally, two standalone scanning electron microscopes are available: a Quanta 650 FE-SEM with EDS and EBSD, and a Phenom XLG2 environmental SEM for electron imaging and EDS.

Four X-ray powder diffraction systems are available for analyzing bulk composition and phase orientation, with specialized stages for in situ heating and X-ray reflectivity. An X-ray fluorescence spectrometer provides highly sensitive elemental analysis for $Z > 10$. The facility also features an integrated Renishaw Raman spectrometer/Bruker AFM system for molecular identification, surface chemistry, and nano-scale topography, along with a Invenio-S FTIR for chemical fingerprinting and organic material identification.

For quantitative surface composition and chemistry, two X-ray photoelectron spectrometers are available: a Versaprobe III small-spot instrument with ion gun for depth profiling, hot-cold stage, and processing chamber; and a HiPP-Lab ambient-pressure XPS with *in-situ* high-temp liquid cell, plasma processing, glove box, sample prep chamber and gas reaction cell. Optical instrumentation includes a white-light profilometer for surface metrology, and a digital light microscope for 2D/3D imaging and videography.

A complete suite of metallurgical equipment for cutting, mounting, polishing, sputter coating, etching, and plasma cleaning, as well as Rockwell and Vickers hardness testing, is also available.

Contact: https://engineering.virginia.edu/NMCF

NS-ThP-4 Exciton-Polariton Devices from Two-Dimensional Chalcogenide Semiconductors*, **Deep Jariwala**,* University of Pennsylvania

The isolation of stable atomically thin two-dimensional (2D) materials on arbitrary substrates has led to a revolution in solid state physics and semiconductor device research over the past decade. A variety of other 2D materials (including semiconductors) with varying properties have been isolated raising the prospects for devices assembled by van der Waals forces. Particularly, these van der Waals bonded semiconductors exhibit strong excitonic resonances and large optical dielectric constants as compared to bulk 3D semiconductors..

First, I will focus on the subject of strong light-matter coupling in excitonic 2D semiconductors, namely chalcogenides of Mo and W. Visible spectrum band-gaps with strong excitonic absorption makes transition metal dichalcogenides (TMDCs) of molybdenum and tungsten as attractive candidates for investigating strong light-matter interaction formation of hybrid states. We will present our recent work on the light trapping in multi-layer TMDCs when coupled to reflective substrates. Next, I will show the extension of these results to superlattices of excitonic chalcogenides, multilayer halide perovskites as well as metal organic chalcogenolates. These hybrid multilayers and materials offer a unique opportunity to tailor the light-dispersion in the strong to ultra-strong coupling regime. Finally, if time permits, I will discuss the physics of strong light-matter coupling and it's applications in phase modulator devices, photovoltaic devices as well as control of light in magnetic semiconductors.

NS-ThP-5 Scalable Photonics with Low-Dimensional Superlattices*, Jason Lynch*, *Deep Jariwala,* University of Pennsylvania

Superlattices of III-V semiconductors have long been used in state-of-the-art photodetectors, light emitting diodes, and lasers while plasmonic superlattices promise to surpass the diffraction limit of light and confine light on the nanometer scale. However, both cases typically use three-dimensional media which do not leverage the advantages of improved electro-optical properties, flexibility, and stability found in low-dimensional media. Recent research has demonstrated superlattices with monolayer semiconductors, but they normally use exfoliated flakes which limit their lateral areas to several square microns. As the growth of large-area, low-dimensional materials becomes more common, integrating low-dimensional media into superlattices promises to improve the performance of commercially available photonic devices. In this poster, we highlight two of our recent works that use 2D layers to improve the tunability and stability of centimeter-scale superlattices. First, we stack monolayer transition metal dichalcogenides (TMDCs) into a superlattice to increase the light-matter interaction strength without sacrificing their ideal monolayer properties. By electrostatically doping the TMDC layers, the system is actively modulated between the strong and weak coupling regime of exciton-polaritons which drastically alters reflected light. Using spectroscopic ellipsometry, the TMDC superlattice is observed to produce a full 2π phase shift in the reflected light. Second, we improve the thermal stability in a TiN-dielectric hyperbolic superlattice by replacing the three-dimensional Al_2O_3 with two-dimensional hBN. The new mixed-dimensional interface prevents atoms from diffusing across the TiN-hBN interface. This results in the superlattice maintaining its stratified geometry upon annealing at high temperatures (800 °C) for at least 10 hours. Both works study centimeter-scale superlattices whose fabrication techniques (wet-transfer and sputtering) can be implemented commercially. Therefore, our work promises to bring the improved qualities of low-dimensional media to practical, large-area photonic systems.

NS-ThP-6 Optical Readout Approaches for Photonic Thermometry*, Kevin Douglass,* *Michal Chojnacky, Thinh Bui, CH S S PAVAN Kumar, Nikolai Klimov,* National Institute of Standards & Technology

NIST is developing a fully packaged photonic-based temperature sensor with the aim of replacing resistance-based thermometry.One of the major deliverables of our photonic thermometry project is creating readout methodologies tailored to the measurement need from highest accuracy metrology applications to real world temperature sensing with fit-for-purpose accuracy in a robust deployable system.Over the past year we have developed and tested various photonic readout strategies to achieve these various goals. These approaches will be described in detail with supporting data to compare their respective advantages and disadvantages.

NS-ThP-7 A Comprehensive Investigation of Raman Laser-Induced Structural Modification in CVD-Grown Monolayer MoS_2*, Sieun Jang,* *Seonha Park, Songkil Kim,* Pusan National University, Republic of Korea

Molybdenum disulfide (MoS_2) has been extensively explored to be utilized as an electronic material in a variety of device applications. In particular, the tunability of MoS_2 enhances its electrical properties making it an intriguing candidate for field-effect transistors (FETs), while also extending beyond electrical properties to structural phase engineering. Raman laser irradiation offers a straightforward method to induce modifications via thermal processes without the intervention of other chemical substances. However, most studies on the modification of MoS_2 have focused on multi-layered structures or have been conducted under low-power laser conditions, leaving the feasibility of phase transition in monolayer MoS_2 elusive. In this study, we fundamentally elucidated the effects of high-power Raman laser irradiation on the surface of chemical vapor deposition (CVD)-grown monolayer MoS_2 under ambient conditions and uncovered the underlying mechanisms of laser-induced modifications by applying intense photon energy with highly interactive reactions. Our results revealed both etching and deposition phenomena in two discernible regions, and it can be demonstrated by intensity threshold based on the spatial distribution of laser irradiance within the laser spot. Furthermore, phase transition was found to be inhibited due to the promoted oxidation and the deposition of hydrogenated amorphous carbon, and p-type doping was observed, likely occurring in the region beneath the hydrogenated amorphous carbon deposition as substitutional doping on the 2H phase of MoS_2. To compare the thermal effects, MoS_2 modifications were further analyzed using simplified heat transfer estimations. These findings deepen our understanding of how Raman laser irradiation modifies MoS_2 under ambient conditions, providing guidelines for optimizing its modification processes.

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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