2D Materials
Room Ballroom A - Session 2D-ThP
2D Materials Poster Session

2D-ThP-1 Electrochemical Lithium Intercalation Cycling-Induced Phase Transition of 2H-MoS_2 to 1T and delayed Reversion to the 2H Phase, ***Yerin Hong***, *Juhwan Lim, Jinhong Min,* University of Michigan, Ann Arbor, Republic of Korea*; Nishkarsh Agarwal,* University of Michigan, Ann Arbor, India*; Robert Hovden,* University of Michigan, Ann Arbor*; Ageeth Bol,* University of Michigan, Ann Arbor, Netherlands*; Yiyang Li,* University of Michigan, Ann Arbor

In this study, we investigated the phase transition behavior of molybdenum disulfide (MoS_2) during and after repeated lithium intercalation and deintercalation cycles, motivated by its potential for energy storage and electronic applications. MoS_2 undergoes a phase transition from the 2H (trigonal prismatic) to the 1T (octahedral) phase upon lithium insertion. After cycling with galvanostatic cycling with potential limitation (GCPL) and using Raman spectroscopy, we confirmed that the 1T phase persisted even after most lithium was removed. Interestingly, a spontaneous reversion of the 1T phase to the 2H phase was observed over time. Raman spectroscopy results showed a significant decrease in 1T phase peaks for cycled MoS2, with the phase converted to 2H after resting periods for several days. Additionally, electrochemical cycling of the cycled MoS_2 flakes revealed lithium potential profiles was comparable to pristine MoS_2, reinforcing the evidence of spontaneous phase reversion. These results demonstrate the metastable nature of the 1T phase and structural evolution of MoS_2 upon and after lithium intercalation cycling. In addition, these findings can provide key insights into the potential strategies of the precise phase control for energy storage and electronic applications, or to synthesize endotaxial structure with distinct quantum states.

2D-ThP-2 Controlling Sputtering Energy Threshold in TMD Plasma Processing via Surface Functionalization and Cryo Temperatures, ***Yury Polyachenko***, *Sofiia Yarytska,* Princeton University*; Yuri Barsukov, Shoaib Khalid, Igor Kaganovich,* Princeton University Plasma Physics Lab

Transition metal dichalcogenides (TMDs) are a novel class of quasi-2D materials with potential applications in smaller semiconductor chips, nanoscale piezoelectric biosensing, and more. However, their manufacturing consists of many steps and poses various currently unsolved challenges.

In this study [1], we perform a computational investigation of a TMD manufacturing stage with low-energy plasma-assisted desorption and etching of MoS_2. First, we systematically select an appropriate level of theory and employ a combination of equilibrium and non-equilibrium ab initio molecular dynamics (AIMD) simulations to identify the geometric regions of MoS_2 that exhibit the highest susceptibility to damage induced by plasma particles. We provide energy thresholds for sputtering and investigate their dependence on the incident angle. We show how oxidation and fluorination of MoS_2 into MoS_2O and MoS_2F can lower the sputtering energy thresholds from ~30eV to ~10eV. Such functionalizations expand the energy range where plasma is expected to desorb the target TMD top layer without damaging the metal scaffold. Additionally, the threshold values for MoS_2O and MoS_2F exhibit distinct dependencies on temperature and impact angle, indicating that variation of these parameters could enable precise and selective etching.

We predict a previously unobserved temperature-dependent behavior of the sputtering threshold in MoS_2O at cryo temperatures ~100-200K. We propose a multistage sputtering mechanism to explain this newly observed trend by its connection to threshold sensitivity to impact angle: from ~14eV for a normal $\theta \approx 0°$impact to ~7eV for a $\theta \approx 20°$impact. We validate the underlying hypothesis through numerical AIMD simulations. We further demonstrate that the proposed mechanism is not restricted to MoS_2 but is also operative in $MoSe_2$, WS_2, and WSe_2.

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[1] Yury Polyachenko, Yuri Barsukov, Shoaib Khalid, Igor Kaganovich; J. Phys. Chem. Lett. 2026, 17, 18, 5207–5214 , https://doi.org/10.1021/acs.jpclett.6c00348

2D-ThP-3 Graphene/MoS_2 Au Nanoparticle Floating-Gate Memristor Arrays for Low-Power Neuromorphic Systems, ***Sabeen Hong***, *Woo Jong Yu,* Department of Electrical and Computer Engineering, Sungkyunkwan University, Republic of Korea

Recent progress in neuromorphic computing has highlighted the need for device platforms capable of performing memory and computation in an energy-efficient manner. In conventional von Neumann architectures, the physical separation of memory and processing units causes data-transfer bottlenecks and considerable energy waste, ultimately limiting computational speed. As an alternative approach, memristive devices have attracted attention because their tunable conductance states can emulate synaptic weight modulation. In this work, we demonstrate a low-power neuromorphic system based on gold nanoparticle floating-gate memristors (AuNp-FGMs).

The AuNp-FGM is designed using graphene as the floating gate and MoS_2 as the channel material. By inserting gold nanoparticles between the floating gate and tunneling oxide, a two-terminal memristor structure was fabricated. The device operates within the ±3 V range, and its conductance modulation is governed by changes in the Fermi energy level (E_f) of graphene. Owing to this floating-gate-based charge modulation mechanism, the AuNp-FGM exhibits reliable memory behavior and analog switching characteristics suitable for neuromorphic applications.

The fabricated device shows an on/off ratio exceeding 10^6, data retention for over 9 hours, and endurance over 80,000 cycles. In addition, the device exhibits low cycle-to-cycle variability, with a Cv of 3.6% measured from 90 cycles, where Cv = σ/μ, σ is the standard deviation, and μ is the mean value. The synaptic update characteristics were further evaluated through multi-level potentiation and depression. For 100-level potentiation using +4 V pulses with a duration of 0.5 s, the non-linearity factor ranges from 0.1 to 0.6. For 100-level depression using −3 V pulses with a duration of 0.2 s, the non-linearity factor ranges from 2.3 to 4.6, measured from 15 devices. Similar modulation behavior was also observed when the number of input pulses was varied to 50, 100, 200, 300, and 400.

To evaluate the applicability of the AuNp-FGM to system-level neuromorphic operation, a neuromorphic array composed of 2 neurons and 32 synapses was constructed. The array was tested using three input patterns: horizontal, vertical, and diagonal. Through 40 learning simulations, the total energy consumption was calculated to be 70 μJ. This corresponds to a 97% reduction in energy consumption compared with previous experiments. These results indicate that graphene/MoS_2-based AuNp-FGM arrays provide a promising platform for low-power neuromorphic systems by combining reliable floating-gate memory characteristics with efficient synaptic weight modulation.

2D-ThP-4 Inhibition of Alumina Atomic Layer Deposition on Modified 2D van der Waals Material $CrPS_4$, ***Marissa Piña***, *Andrew Teplyakov,* University of Delaware

$CrPS_4$ is a 2D van der Waals material in the ternary transition metal chalcogenide (TTMC) class of compounds. As an A-type antiferromagnetic semiconductor, thin $CrPS_4$ flakes a few layers thick can display net or zero magnetization depending on whether there is an odd or even number of layers. The combination of 2D magnetic materials such as $CrPS_4$ with topological insulators such as atomic layer deposition (ALD)-grown alumina has potential as a magnetic tunnel junction in spintronics devices including magnetic RAM, but has seldom been studied to date.

We have analyzed the atomic layer deposition of alumina on mechanically exfoliated $CrPS_4$ flakes before and after modification with acetylacetone (acacH) at room temperature and at 140 °C. The modifications seem to result in inhibited alumina growth, which was very unexpected considering alumina grows rapidly on most surfaces. In both cases, the alumina grown on the modified $CrSP_4$ surface may experience a growth delay of over 1 nm [determined by ToF-SIMS depth profiling after 60 cycles of water and trimethylaluminum (TMA) at 130 °C] and a smoother surface compared to alumina grown on the unmodified surface.

The difference in unmodified versus modified alumina growth is likely related to defects which provide nucleation sites for ALD growth. The defects are potentially passivated by the acacH modification. The acac-containing fragments, including $Cr(acac)^+$, that indicate a successful modification appear uniformly across the $CrPS_4$ flakes in ToF-SIMS ion images. Additionally, AFM of the $CrPS_4$ flakes after these modifications and after alumina ALD reveal a nearly atomically smooth surface, possibly indicating uniform coverage.

The alumina growth could be more efficient on unmodified surfaces because TMA decomposes or builds up at the defects, as we observed clusters of CH^- and AlO_2^- fragments on the $CrPS_4$ surface by ToF-SIMS that become larger after higher numbers of ALD cycles. This means that the acacH modification could result in a more perfect interface and a better alumina film. This process also has potential applications in area-selective ALD, since alumina growth on $CrSP_4$ can be slowed with a simple modification, especially when you couple the current findings with the fact that the number of $CrPS_4$ layers can be controlled by an atomic layer etching (ALE) process.

2D-ThP-6 Strain-Tunable Mid-Infrared Optical Absorption in Bilayer Silicon for Silicon-Compatible Photonics, ***Kumar Vishal,*** Wright University

Two-dimensional bilayer silicon (BLSi) offers a silicon-compatible platform for extending integrated photonics into the mid-infrared, but its optical response remains strongly governed by strain-induced structural and electronic transitions. In this work, density functional theory calculations are used to evaluate the strain-dependent optical properties of AA-stacked BLSi under biaxial in-plane tensile strain, with optical absorption and refractive index calculated for in-plane polarization by including interband and intraband transitions.The results show that tensile strain drives a structural transition from a low-buckled bilayer lattice to a buckle-free honeycomb configuration at approximately 5.17% strain. This transformation removes the out-of-plane buckling and produces an abrupt increase in the refractive index, demonstrating the strong coupling between atomic geometry and optical response. In the buckle-free phase below the large-strain bandgap-opening threshold, the optical absorption edge remains pinned near 1.14 μm, indicating a strain-resistant transition at the M point. When the strain exceeds approximately 12.26%, both direct and indirect energy bandgaps open, and the direct-gap-associated interband transition moves into the mid-infrared. By increasing strain, the absorption peak redshifts across a broad wavelength range from about 1.5 to 11.5 μm, while the refractive index increases sharply and exhibits mid-infrared dispersion linked to these interband transitions.These findings identify strain as an effective tuning parameter for controlling the mid-infrared optical behavior of bilayer silicon. The predicted broadband tunability, silicon compatibility, and strong strain-dependent absorption suggest that BLSi could provide a pathway toward CMOS-compatible mid-infrared photodetectors and integrated silicon photonic components without relying on heterogeneous III-V or II-VI absorber integration.

2D-ThP-7 Nanoscale Friction in Exfoliated SnSe and $SnSe_2$ Two-Dimensional Materials, ***Mehmet Ozdogan,*** *Thomas Iken, Deniz Cakir, Nuri Oncel,* University of North Dakota

Two-dimensional layered materials are promising candidates for solid-state lubrication because weak interlayer van der Waals interactions can enable low-resistance sliding at micro- and nanoscale contacts. While graphene and transition-metal dichalcogenides have been widely studied in this context, the tribological response of layered tin chalcogenides remains comparatively unexplored. Here, we investigate the nanoscale frictional properties of mechanically exfoliated SnSe and $SnSe_2$ nanoflakes using atomic force microscopy-based lateral-force microscopy, supported by X-ray photoelectron spectroscopy and first-principles calculations.

SnSe and $SnSe_2$ flakes were exfoliated onto SiO_2 substrates and measured under ambient conditions using calibrated lateral-force microscopy. Graphene flakes of comparable thickness were measured under the same conditions as a reference solid lubricant. Friction maps and load-dependent lateral-force measurements show that both SnSe and $SnSe_2$ exhibit low friction coefficients, with values of 0.023 ± 0.004 and 0.027 ± 0.019, respectively, compared with 0.042 ± 0.060 for graphene. These results indicate that Sn-based layered chalcogenides can provide frictional performance comparable to or better than commonly studied two-dimensional lubricants under ambient conditions.

To understand the microscopic origin of the measured friction trends, density functional theory calculations were performed for pristine and oxygen-modified SnSe and $SnSe_2$ surfaces. Potential-energy-surface calculations indicate that pristine $SnSe_2$ should possess lower intrinsic sliding barriers than SnSe, consistent with its weaker interlayer interaction. However, XPS analysis reveals the presence of thin native oxide layers on both materials after air exposure. Incorporating oxygen-induced surface distortion into the calculations reverses the predicted friction trend, producing higher sliding barriers for oxidized $SnSe_2$ than for oxidized SnSe. This result explains the experimentally observed lower friction of SnSe relative to $SnSe_2$ and highlights the strong influence of surface chemistry on the tribological behavior of two-dimensional materials.

These findings establish SnSe and $SnSe_2$ as low-friction layered chalcogenides and show that the measured ambient friction response is strongly influenced by native surface oxidation. The intrinsic calculations further suggest that $SnSe_2$ could exhibit even lower friction when surface oxidation is suppressed, making surface control essential for evaluating its true lubricating potential [1].

[1]. *ACS Appl. Nano Mater.* ***2025****, 8, 14713−14719.*

2D-ThP-8 Influence of Sapphire Annealing Conditions on Terrace Formation and TMD Nucleation and Growth Kinetics, ***Morteza Sheibani Karkhaneh,*** Boise State University

The controlled synthesis of high-quality two-dimensional transition metal dichalcogenides (2DTMDs) is essential for the development of next-generation electronic, optoelectronic, andcatalytic devices. In order to grow high quality monolayer TMD thin films, many researchershave demonstrated the need to control the surface properties of the substrate. Specifically,terrace formation and the resulting step heights of c-plane sapphire has been shown to be acritical component of growing unidirectional TMD crystals and achieving thin films with minimalto no grain boundaries. However, while many papers have shown various ways to achievedifferent terrace formations, there is a need to understand how different processing conditionsimpact terrace formation, step heights, and ultimately the kinetics of TMD crystal growth.In this study, c-plane cut sapphire substrates were annealed at various temperatures,processing gases, pressures, and ramp/dwell conditions to obtain different terrace formationswith varying step heights using AFM. We demonstrate how these different factors impact thereordering of the sapphire surface and then explore how CVD growth conditions may inducereordering of the surface, even after pretreatment of the sapphire and ultimately impacting TMDcrystal growth.In this regard, we utilized pretreated sapphire to show how different surface properties impactTMD nucleation and growth. To understand the impact of the sapphire surface on TMD growth,we characterize the TMD samples using various techniques including Raman spectroscopy,TERS, photoluminescence, XPS, and AFM.The results demonstrate that substrate annealing plays a critical role in controlling TMDnucleation and growth kinetics. These findings provide important insights into substrate engineering for the scalable growth of high-quality TMDs that may expand to other 2D materials,offering a practical route toward wafer-scale integration of TMD-based devices.

2D-ThP-9 A New Metric to Assess the Rashba Spin-Orbit Coupling in Undulated 2D Materials, *Zhicheng Li, Favian Sun,* ***Sunny Gupta,*** *Boris Yakobson,* Rice University

Wrinkles and undulations are ubiquitous in two-dimensional (2D) materials. By breaking mirror symmetry, such topographical deformations can enable spin-orbit coupling and Rashba spin splitting, allowing spin precession with important implications for spintronic devices. The Rashba parameter, α_R, is commonly used to quantify the strength of Rashba spin splitting, with larger α_R generally associated with shorter spin-precession lengths. However, using first-principles electronic-structure calculations, we show that α_R can be an inadequate metric for materials with non-parabolic bands and higher-order Rashba spin-orbit interactions. To address this limitation, we propose a new dimensionless metric, L_{pr}, where L_{pr} is the spin-precession length and κ is the curvature of undulation. This metric directly captures device-relevant spin-precession behavior and enables more meaningful comparison and ranking of materials by Rashba-effect strength. Finally, using transport calculations, we demonstrate current modulation arising from spin precession in undulated 2D materials and show how this effect can be controlled in realistic device geometries.

2D-ThP-11 Multifunctional GO-Based 2D Materials for Auranofin Combination Therapies, ***Diego La Mendola,*** *Lorenzo Chiaverini, Luca Famlonga,* University of Pisa, Italy*; Cristina Satriano,* University of Catania, Italy*; Tiziano Marzo,* University of Pisa, Italy

Graphene oxide (GO) has emerged as a promising two-dimensional nanomaterial for drug delivery due to its large surface area, biocompatibility, and versatile surface chemistry. GO can efficiently load therapeutic agents through π–π stacking, hydrogen bonding, and electrostatic interactions, enabling high drug-loading capacity and controlled release. These properties make GO-based nanocarriers attractive for applications in cancer therapy, anti-inflammatory treatments, and multifunctional nanomedicine.

In this work, graphene oxide was investigated as a two-dimensional platform for the loading and delivery of Auranofin (AF), a gold-containing compound originally developed for rheumatoid arthritis and currently

attracting significant interest for its anticancer, anti-inflammatory, and redox-modulating properties. In particular, GO nanosheets were employed for the development of AF-based combination systems, including AF–NAC (Auranofin-N-acetylcysteine) and AF-NPX (Auranofin-Naproxen).

The study focused on the physicochemical interactions between GO and the different therapeutic agents, exploiting the high adsorption capability and oxygen-containing functional groups of graphene oxide. The resulting hybrid nanostructures were subjected to comprehensive physicochemical characterization, including UV–Vis spectroscopy, Fourier-transform infrared spectroscopy, dynamic light scattering, zeta potential analysis, and atomic force microscopy, in order to evaluate structural, morphological, and surface properties. In addition, drug-loading efficiency and stability in physiological conditions were assessed to correlate structural features with functional performance. The developed systems were further analyzed in terms of loading efficiency, stability, and potential synergistic effects associated with oxidative stress modulation and anti-inflammatory activity. Special attention was devoted to the AF–NAC system for the investigation of redox-regulation mechanisms, while the AF–NPX formulation was designed to combine the pharmacological activity of Auranofin with the anti-inflammatory properties of Naproxen.

Preliminary findings indicate that graphene oxide represents a promising 2D nanocarrier for improving drug stability, controlled release, and multifunctional therapeutic performance. These results further support the potential of GO-based platforms in advanced nanomedicine and combination drug delivery strategies, although challenges related to toxicity, biodegradation, and long-term biosafety still require careful investigation for future clinical translation.

2D-ThP-13 Nanoscale Imaging of Layer-Parity and Twist-Dependent Magnetism in CrSBr, ***Aalok Tiwari***[1], Carnegie Mellon University, USA; *Shubhada Patil,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Ravi Kumar Bandapelli,* Carnegie Mellon University, USA; *Alevtina Smekhova,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Wenhao Liu,* University of Texas at Dallas; *I-Hsuan Kao, Zhenhong Cui, Brandon Tran,* Carnegie Mellon University, USA; *Zixin Zhai,* University of Texas at Dallas; *Raghvendra Posti, Sandy Adhitia Ekahana,* Carnegie Mellon University, USA; *Alexander X. Gray,* Temple University; *Bing Lv,* University of Texas at Dallas; *Florian Kronast Kronast,* Helmholtz-Zentrum Berlin für Materialien und Energie, Germany; *Simranjeet Singh, Jyoti katoch,* Carnegie Mellon University, USA

Van der Waals (vdW) antiferromagnetic semiconductors offer the potential for innovative energy-efficient spintronics at atomic thickness. The advent of twist engineering further enables tailored arrangement of spins yielding emergent magnetic ground states via competing interactions. Chromium sulfide bromide (CrSBr) serves as an ideal platform for understanding the interplay between atomic thickness and twist-angle-dependent emergent spin texture at micrometer length scales. We carry out x-ray magnetic circular and linear dichroism (XMCD/XMLD) combined with photoemission electron microscopy (PEEM) to resolve the magnetic order at nanoscale resolution in atomically thin and 90° twisted CrSBr. We demonstrate layer-parity-dependent magnetic order persisting from bulk through monolayer limit. The remanent state shows strong temperature and layer number dependent coercivity. By twisting two CrSBr ferromagnetic monolayers with in-plane magnetic easy axes by 90°, we observe a superlattice effect in the twisted region leading to new emergent order.

2D-ThP-14 Impact of Air Exposure on the Stability and Resistivity of TaS_2 and $TaSe_2$ Films, ***Tinsae Alem***, *Michael Hann, Kory Burns, Stephen McDonnell,* University of Virginia

Transition metal dichalcogenides (TMDs) are promising for next-generation electronic, optoelectronic, and flexible device applications due to their tunable bandgaps, optical anisotropy, and mechanical flexibility. However, most TMDs, particularly Ta- and Nb-based thin films, are limited in practical use due to environmental instability; this is because ambient exposure can degrade their structural and electronic properties via oxidation and surface adsorption. In this study, we investigate the air stability of molecular beam epitaxy (MBE)-grown TaS_2 and $TaSe_2$ thin films (~5-10nm) by examining oxidation during sequential air exposure. Oxide-layer formation was estimated using X-ray reflectivity (XRR), while electrical resistivity measurements and X-ray photoelectron spectroscopy (XPS) tracked changes in resistivity and chemical composition. We compare degradation behavior between sulfide and selenide films, as well as the influence of substrate choice (SiO_2/Si and sapphire). Our results show that the TaS_2 grown on SiO_2/Si exhibits minimal changes in resistivity, outperforming both TaS_2 grown on sapphire and $TaSe_2$ grown on SiO_2/Si under identical ambient conditions. We further observe a gradual increase in resistivity with exposure time in $TaSe_2$, culminating in a complete transition from selenide to oxide after ~437hr of sequential air exposure. These findings correlate oxidation evolution with electrical transport degradation, providing insight into stability trends and degradation mechanisms in Ta-based TMD thin films. Understanding the oxidation rate and its relationship with resistivity could provide insight into improving the reliability and integration of TMD thin films for potential environmental sensing applications.

2D-ThP-15 Functional Agents for Functional Materials, ***Bogdan Dryzhakov***, *Emily Herron,* Oak Ridge National Laboratory

Two-dimensional materials and heterostructures exhibit rich spatially varying optical responses, but interpreting hyperspectral spectroscopy datasets from these systems often requires expert-driven feature assignment and time-intensive comparison to prior literature. CHUNKS, or Cross-modal Hypothesis Understanding for Nanoscale Knowledge in Spectroscopy, is a domain-aware, retrieval-augmented agentic workflow that addresses this challenge by connecting experimental spectra to materials-science literature context. By integrating raw hyperspectral data to materials science corpus of >119K full text articles, CHUNKS generates actionable insights, including hypotheses, spectral feature classifications, and parameter initialization for downstream analysis. This workflow supports rapid, informed decision-making during initial materials characterization and provides a pathway toward experiment automation by making spectral interpretation more systematic and knowledge-guided. Here, we demonstrate CHUNKS on a hyperspectral scanning electron microscope cathodoluminescence dataset from a 2D heterostructure stack.

2D-ThP-16 Synthesis of Graphene Quantum Dots by Alkali Metal Intercalation and Exfoliation of Anthracite Coal, *George Bepete,* Concordia University, Canada; ***Gothamie Ratnayake***, *David Emanuel Sanchez, Zhuohang Yu, Edgar Dimitrov, Andres Fest Carreno,* The Pennsylvania State University; *Maykol Christian Damasceno Oliveira, Bartolomeu Cruz Viana, Francisco Eroni Paz Santos,* Federal University of Piauí, Brazil; *Mauricio Terrones,* The Pennsylvania State University

Leveraging the abundance and low cost of anthracite coal, a sustainable and scalable synthesis route is developed to produce graphene quantum dots (GQDs). Through this approach GQDs are collected as powders or slurries and redispersed in common solvents, enabling integration into diverse solution–processed platforms. Briefly, the process involves intercalating naturally sourced anthracite coal with potassium metal and exfoliating it in N-methyl-2-pyrolidone (NMP) to yield reduced GQDs of 2.5-3.5 nm in diameter. This method offers a practical path towards scalability with an isolated yield of ~ 28% GQDs based on the starting anthracite coal mass. Notably, the resulting GQDs feature a 3.4 eV direct bandgap, excitation–dependent photoluminescence, and thermo–optical properties (thermal diffusivity of $(6.4 \pm 0.3) \times 10^{-8}$ m^2/s and nonlinear refractive index of -4.69×10^{-9} cm^2/W). These intriguing thermo-optical properties along with improved scalability of the synthesis of GQDs motivate their use in future photothermal and nonlinear optical systems. Overall, this work reframes coal as a sustainable, low-cost precursor for quantum nanomaterials with applications in sensing, energy, and thermal management.

2D-ThP-18 Self-Intercalated Ti Reveal Stacking Order in Bilayer $TiSe_2$ Films, ***Nicolas Paulo Pereira Vasconcelos***, University of South Florida

Alternatively stacked transition metal dichalcogenides (TMD) may give rise to properties distinct from those of their conventional structures. Different layer stacking can also originate distinct point defects. Proper identification of defects is therefore important for the understanding of the properties of these materials. Here, scanning tunneling microscopy was used to identify native defects in MBE-grown ultrathin TiSe2 and to investigate the coexistence of an alternative stacking configuration. In monolayers surface and sub-surface Se-vacancies dominate. In bilayers, two additional point defects are observed that are separated into domains and are interpreted as Ti self-intercalation defects. The conventional 1T-TiSe2 stacking cannot account for both defect configurations, suggesting the existence of an alternative stacking. Rotating the top layer 180° about an axis passing through a Se atom at the bottom of the top layer. results in the alternative stacking. In both stacking configurations self-intercalated Ti atoms can occupy the preferred octahedral site, but express different symmetries allowing for discrimination between the stacking in STM images. Finally, sequential thermal annealing revealed a local structural transformation

[1] **JVST Highlighted Poster**

associated with increase of Ti intercalation, forming an irreversible 2x2-like periodic superstructure.

2D-ThP-19 Why Does Selective Area van der Waals Epitaxy (SAVE) Work?, ***Maxim Wunder***, Stockton University*; Madison Ramsey, Stephanie Law,* Pennsylvania State University

Selective area van der Waals epitaxy (SAVE) enables site-controlled growth of Bi_2Se_3 on SiO_x-patterned c-plane sapphire substrates, but the origin of selectivity between exposed sapphire and the surrounding SiO_x mask remains unclear. Here, we examine three possible contributions to SAVE selectivity: surface wettability, adatom diffusion across the mask, and surface-dependent nucleation.

Contact-angle measurements showed that SiO_x-coated sapphire remained more wettable and had a higher calculated surface energy than bare sapphire, both before and after UHV annealing. This trend is opposite to that expected if preferential wetting of sapphire were responsible for selective Bi_2Se_3 growth, indicating that macroscopic wettability alone does not explain SAVE selectivity.

To test whether adatom diffusion across the SiO_x mask contributes to selectivity, patterned samples with different feature spacings were analyzed by atomic force microscopy. A computational AFM analysis workflow was used to estimate average mask coverage across a large set of scans. This metric was used for comparative analysis rather than chemical identification of individual features. No clear relationship between feature spacing and average mask coverage was observed for the feature sizes and shapes measured, weakening a spacing-dependent diffusion model.

Finally, Bi_2Se_3 deposition on unpatterned sapphire and unpatterned SiO_x-coated sapphire was compared under identical growth conditions. Substantially greater growth was observed on bare sapphire, while the SiO_x-coated surface remained largely free of deposited material. Together, these results are most consistent with surface-dependent adsorption, desorption, and nucleation behavior as the dominant mechanism underlying SAVE selectivity.

This work was supported by the Coherent / II-VI Foundation and the National Science Foundation Nanomanufacturing of Emerging 2D Materials and Devices REU Program (EEC-2244201).

2D-ThP-21 Surface Electron Accumulation and Spatially Separated Bipolar Transport in WSe_2 Revealed by ARPES, ***Cheng-Maw Cheng***, National Synchrotron Radiation Research Center, Taiwan*; Hemanth Kumar Bangolla,* Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taiwan*; Chi-Yang Chen, Kuei-Yi Lee, Liang-Chiun Chao,* Graduate Institute of Electro-Optical Engineering, National Taiwan University of Science and Technology, Taiwan*; Rajesh Kumar Ulaganathan,* Centre for Nanotechnology, Indian Institute of Technology Roorkee, India*; Raman Sankar,* Institute of Physics, Academia Sinica, Taiwan*; Abhishek Ghosh,* Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan*; Ruei-San Chen,* Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology, Taiwan

Two-dimensional transition-metal dichalcogenides (TMDCs) have attracted considerable attention for next-generation electronic and optoelectronic applications because of their tunable electronic structures and van der Waals surfaces. Among them, WSe_2 is particularly promising because of its p-type characteristics and ambipolar transport behavior. However, the microscopic origin of its carrier polarity and the role of surface electronic states remain incompletely understood. Here, we investigate the origin of bipolar transport in nanostructured and bulk WSe_2, with particular emphasis on its surface electronic structure revealed by angle-resolved photoemission spectroscopy (ARPES). ARPES measurements provide direct evidence for pronounced surface electron accumulation (SEA), demonstrating that the near-surface region is heavily n-type, whereas the inner bulk remains lightly p-type. The surface electron concentration reaches approximately 10^{20} cm^{-3}, about four orders of magnitude higher than the bulk hole concentration. This electronic inhomogeneity gives rise to spatially separated bipolar transport, with electrons dominating near the surface and holes governing transport in the bulk, accounting for the observed thickness-dependent conductivity and carrier activation energy. The SEA is attributed primarily to selenium vacancies at the WSe_2 surface, while interactions with ambient molecules can modify or passivate these defects and alter the surface carrier density. These results highlight the crucial role of surface electronic structure in the macroscopic transport properties of WSe_2 and demonstrate the power of photoelectron spectroscopy in disentangling surface and bulk electronic contributions in van der Waals materials.

References

1. Hemanth Kumar Bangolla *et al.,* Nanoscale 18, 5941 (2026).

2D-ThP-22 Selective Area Epitaxy of van der Waals Materials, ***Ryan Trice***, *Stephanie Law, Madison Ramsey, Sarah Olandt,* Penn State University

Two-dimensional (2D) van der Waals (vdW) materials are of interest for a variety of applications ranging from optoelectronics and photocatalysis to energy storage and topological devices. However, vdW materials synthesized using common techniques such as chemical or physical vapor deposition often exhibit a high density of growth-related defects: ranging from grain boundaries and twin defects to 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 wet chemistry 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 causes significant damage to the surfaces or edges of the materials. To address these issues, we used selective area van der Waals epitaxy (SAVE) to grow Bi_2Se_3 thin films. SAVE is a technique in which thin films nucleate and grow in defined areas on a wafer. This is done through the use of a patterned mask where growth conditions are selected such that the film will only nucleate inside the exposed pattern.

In this poster, we will describe SAVE growth of Bi_2Se_3 on Al_2O_3 (001) substrates using a SiO_2 mask. The mask was deposited onto a 10x10mm substrate by atomic layer deposition. Patterning of the SiO_2 mask was done through e-beam lithography with dry etching to achieve nano-scale patterned samples with holes of various shapes and sizes. The processed substrates were then loaded into a molecular beam epitaxy chamber for growth of the Bi_2Se_3 film. First, we examine the effects of different substrate temperatures on the selective growth of the Bi_2Se_3 thin films. Second, we will discuss the different growth orientations and processes in the nano-scale features. Third we will investigate the geometric influence of variously shaped patterns on the crystal quality of the selectively grown films.

2D-ThP-23 Atomic Layer Deposition of Electrical Contacts to 2D Semiconductors, ***Sebastian Cimino***[1], University of Central Florida*; Justin Chiu, Maxim Wunder, Eric Welp, Ziheng Chen, Suzanne Mohney, Stephanie Law, Saptarshi Das,* Penn State University

Two-dimensional (2D) semiconductors have captivated researchers for decades. As scientists continue to investigate the electronic properties of two-dimensional (2D) transition metal dichalcogenides (TMDs), engineers envision a path to augment current silicon technologies using integration. In this investigation, thermal atomic layer deposition (ALD) was used to study a candidate electrical conductor, aluminum zinc oxide (AZO), for electrical contacts to the 2D semiconductor MoS_2. Thermal ALD was chosen for its ability to form conformal films in situations not amendable to line-of-sight deposition, such as recessed edges of a 2D semiconductor layer. Furthermore, only modest temperatures are needed to deposit AZO using supercycles of diethyl zinc and water and of trimethyl aluminum and water. AZO grown with a 20:1 ratio of $ZnO:Al_2O_3$ yielded the lowest resistivity, and the resistivity was thickness-dependent for films thinner than 50 nm grown on HfO_2/Si. Growth at 175 °C yielded AZO layers with lower resistivity than growth at 150 °C or 200 °C. We used atomic force microscopy to study selectivity of the deposition process on edges of MoS_2. Although prior work showed selective growth of ZnO on the edges of MoS_2[1], we did not observe the same selectively in our study of AZO, possibly due to the use of a higher growth temperature (200 °C vs. 125 °C). Further work will consider the limits of selectivity of AZO deposition and its suitability as an electrical contact to MoS_2.

[1] T. N. Walter et al., Atomic Layer Deposition of ZnO on MoS_2 and WSe_2, *Appl. Surf. Sci.* 480 (2019) 43.

[1] **JVST Highlighted Poster**

2D-ThP-24 Electrically Controllable Single-Photon Emitters in Monolayer WSe_2 with negligible Stark Shift, ***Seon Namgung***[1], Physics, Republic of Korea

Single-photon emitters (SPEs) based on two-dimensional (2D) materials offer compelling advantages, including mechanical flexibility, high quantum yield, and seamless chip integration; however, electrical modulation at the single-photon level remains challenging. Here, we demonstrate a novel approach to engineering electrically controllable, purified SPEs in monolayer WSe_2 using a silicon nanopyramid substrate. The nanopyramid architecture induces localized strain to isolate SPEs while simultaneously serving as a gate platform for electrical modulation. Notably, the emitter demonstrates robust voltage-controlled single-photon emission without unwanted spectral shifts—exhibiting a negligible Stark effect owing to a gap formed between the WSe_2 and the nanopyramid surface.Under electrical modulation, single-photon purity is enhanced down to $g^2(0) = 0.06\pm0.03$.

2D-ThP-28 Two-dimensional 1T-HfSe2: Surface Structure and Air Stability, *Christopher M. Smyth,* Sandia National Laboratories*; Joslin S. Prasanna, Hui Zhu,* The University of Texas at Dallas*; Zaibing Guo,* King Abdullah University of Science and Technology, Saudi Arabia*; Joy S. Lee,* The University of Texas at Dallas*; Juan Pablo Oviedo,* Baylor University*; Jian Wang, Julia W.P. Hsu,* The University of Texas at Dallas*; Husam N. Alshareef,* King Abdullah University of Science and Technology, Saudi Arabia*; Moon J. Kim, Jiyoung Kim, Robert M. Wallace,* ***Rafik Addou****,* The University of Texas at Dallas

The two-dimensional semiconductor $HfSe_2$ is a promising candidate for future electronic, optical, and sensing applications due to its moderate bandgap (~1.1 eV) and the spontaneous formation of a native high-κ dielectric in ambient conditions. In this study, a range of experimental techniques was employed to investigate the intrinsic surface properties of bulk $HfSe_2$ grown by chemical vapor transport and to directly track oxidation in air. Scanning tunneling microscopy reveals a high defect density across the $HfSe_2$ surface caused by Se vacancies and impurities, confirmed by XPS, inductively coupled plasma mass spectrometry, and high-resolution Rutherford backscattering spectrometry. Furthermore, XPS highlights the highly reactive nature of the $HfSe_2$ surface in air, where the formation of HfO_x is detected after a 1 min exposure to air, resulting in changes to the electronic properties, such as the work function and the valence band offset. Understanding the intrinsic surface properties, air stability, and material quality will facilitate the integration of 1T-$HfSe_2$ in novel devices.

This work was partially supported by the Jonsson School Research Initiative at the University of Texas at Dallas.

[1] **JVST Highlighted Poster**

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