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 $Cv = \sigma/\mu$, 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-5 Investigation of Phase Separation of Mixture of Oil and Water in Monte Carlo Simulation, ***Mehabaw Fikrie***, Gondar, Ethiopia; *Tibebe Birhanu,* Catholic University of Korea, Ethiopia

Phase separation, the spontaneous segregation of a homogeneous mixture into distinct phases with different physical and chemical characteristics, is a fundamental phenomenon in soft matter physics, materials science, and energy-related technologies. Understanding the microscopic dynamics of immiscible fluid systems such as oil-water mixtures is increasingly important for advancing enhanced oil recovery (EOR), chemical processing, and emerging computational material design. In this study, Monte Carlo (MC) simulation techniques were employed to investigate phase separation behavior in mixed oil-water particle systems under varying thermodynamic and spatial conditions. Simulations were performed for particle systems ranging from 500 to 2,500 particles with interval 500 within square simulation domains of side lengths 25–40 units with 5 unit interval. Critical parameters including box size, particle density, interaction strength, and simulation time were systematically analyzed to evaluate their effects on phase evolution and stability. The findings reveal that a system with box size L = 30 and particle number N = 2000 exhibits the clearest and most stable phase-separated structure. Increased particle interactions and larger system sizes significantly enhance the transition from homogeneous dispersion to well-defined phase domains. Furthermore, extended equilibration times improved the sharpness and stability of interfaces, with optimal separation observed at MCstep = 10^6. The results provide valuable computational insights into molecular-scale phase dynamics, wettability control, and interfacial phenomena. This work demonstrates the growing role of computational modeling and simulation in emerging trends of science and technology, particularly in energy optimization, advanced materials research, and intelligent fluid-system engineering.

Keywords: Oil-water mixture; Phase separation; Monte Carlo simulation; Box size; Particle number

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-10 Ultra-Thin ALD-Based Conformal Coatings for Corrosion and Moisture Protection in High-Density Advanced Packaging, ***Rakesh Kumar****,* Specialty Coating Systems, Inc.*; Shuichi Sawada,* Daisan Kasei Co., Ltd, Chiba, Japan

The continued evolution of advanced packaging, encompassing high-density substrates, fine-pitch interconnects, microvias, and microBGA architectures, is enabling increasingly complex, high-performance electronic systems. Yet as feature sizes shrink and packaging densities rise, ensuring long-term reliability against corrosion and moisture ingress becomes a critical manufacturing challenge. This creates a compelling need for ultra-thin conformal coatings capable of delivering near-hermetic protection without compromising the dimensional and electrical tolerances demanded by advanced packaging designs.

Atomic Layer Deposition (ALD), introduced in the late 1990s, offers a uniquely precise solution: nanometer-scale films of metals and metal oxides deposited with exceptional conformality and thickness control. However, its broader adoption in electronics manufacturing has historically been limited by elevated processing temperatures incompatible with sensitive substrates and assembled components.

This paper presents a room-temperature ALD-based conformal coating process directly applicable to printed circuit boards, advanced packaging substrates, and sensitive electronic assemblies. The coating can be deployed as a standalone layer or in conjunction with Parylene, enabling flexible integration into existing packaging workflows. Corrosion resistance was evaluated through 21-day mixed flow gas (MFG) testing using Cl_2, H_2S, NO_2, and SO_2, conditions representative of harsh field environments. Results confirm robust protection in aggressive corrosive atmospheres, alongside strong substrate adhesion and excellent electrical insulation. Critically, when combined with Parylene C, the ALD coating improves the water vapor transmission rate by 63–100 times, establishing it as a high-impact materials solution for the reliability and protection requirements of next-generation advanced packaging

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-12 Transport and Dielectric Interface Engineering in ALD-Grown MoS_2 Transistors, ***Alberto Martinez****,* University of Granada, Spain*; Francisco Gamiz,* Univeristy of Granada, Spain*; Carlos Marquez,* University of Granada, Spain

The electrical performance of MoS_2 transistors is strongly determined by how the 2D semiconductor is grown and coupled to surrounding dielectrics. Plasma-enhanced atomic layer deposition (PE-ALD) is attractive for CMOS-oriented integration because it enables direct, conformal growth over large areas and can be followed by dielectric deposition without transfer steps. However, ALD-grown MoS_2 is not a direct equivalent of CVD-grown material. Its nanocrystalline morphology, small grain size, grain-boundary density, and growth-dependent stoichiometry can promote ambipolar or weakly polarity-selective operation, defect-assisted conduction, and hopping-like transport. Understanding these mechanisms is essential for reliable encapsulation and gate-stack design.

Here, we investigate ALD-grown MoS_2 field-effect transistors with emphasis on transport mechanisms, contact effects, and dielectric integration. Back-gated devices are used as diagnostic structures to evaluate the intrinsic channel response. Their transfer characteristics show no systematic preference for n-type or p-type operation, suggesting localized states, grain-boundary conduction, and hopping-assisted transport through defects.

To separate channel and contact contributions, we analyze device arrays with different geometries and extract sheet and contact resistance. These parameters allow us to assess how ALD growth and dielectric processing affect both the MoS_2 channel and the metal/MoS_2 interface. The results indicate that the dielectric environment strongly influences channel conductivity and device variability, highlighting the role of surface states, trapped charge, and dielectric-induced doping.

We then evaluate in situ dielectric encapsulation using Al_2O_3- and Si_3N_4-based layers deposited directly on MoS_2. Encapsulation is considered not only as passivation, but also as a functional interface for front-gate devices. Electrical measurements, bias-stress experiments, and low-frequency characterization are used to probe charge trapping, interface stability, and dielectric coupling, providing insight into how deposition conditions influence hysteresis, noise, drift, and robustness.

Finally, selected dielectric stacks are extended to front-gated MoS_2 transistors, where the encapsulation layer also acts as the gate insulator. By comparing back-gate and front-gate operation, we evaluate the transition from diagnostic test structures to local-gate architectures. Overall, this work connects ALD growth, defect-assisted transport, resistance extraction, and dielectric interface engineering, providing guidelines for scalable ALD-grown MoS_2 transistors compatible with CMOS-oriented fabrication.

2D-ThP-13 Nanoscale Imaging of Layer-Parity and Twist-Dependent Magnetism in CrSBr, ***Aalok Tiwari***, 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 Natinal 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-17 Al–Pd Dual-atom Sites on N-doped Defective Graphene for CO_2 Activation: A DFT Study of 2D Catalytic Surfaces, ***Radhey Bhattarai***, *Yirong Mo,* University of North Carolina at Greensboro

Two dimensional materials provide a powerful platform for surface-site engineering because of their fully exposed atomic planes, tunable defect chemistry, and strong electronic sensitivity which enable precise control of adsorption and catalytic reactivity. The solid carbon materials have emerged as a promising option as these are affordable and have high surface area allowing them to capture small molecules like CO_2 and release it as other chemically valuable products using less heat, particularly when controlled with nitrogen structure. To make carbon capture much cheaper, easier and designing catalyst that generates most controllable active sites, two metal atom system containing main group elements and transition metal elements are paired which will be dispersed on the 2D carbon material. The density functional theory (DFT) is used to investigate Al-Pd dual-atom catalysts system where metal atoms are anchored on defective N-doped graphene as model 2D catalytic surfaces for electrochemical CO_2 reduction. To understand how defect structure and heteronuclear site geometry influence catalysts stability, charge redistribution, and surface intermediates binding, two local coordination environments are examined.

The data obtained from the calculation shows that Al-Pd pair generates an asymmetric active site on the graphene surface which shows cooperative bifunctional role where Al promotes polarization of CO_2 while Pd modulates charge transfer and the binding strength of reaction intermediates. From the electronic structure analysis, including charge redistribution and projected density of states, confirms that both the 2D support and the local coordination environment strongly leads the reactivity of this catalysts system. The free energy analysis and transition state analysis further gives insight into CO_2 reduction selectivity and its competition with hydrogen adsorption.

This work demonstrates how cheap, affordable, versatile, and defect engineered graphene can host atomically dispersed bimetallic sites and how the first principle surface science can guide the design of low-dimensional catalytic 2D materials for carbon conversion.

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