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

2D-ThP-1 Molecular Beam Epitaxy Synthesis and Characterization of 2D InSe, ***Emily Toph***, *Eric Vogel,* Georgia Institute of Technology; *Brent Wagner,* Georgia Tech Research Institute

InSe, a monochalcogenide two-dimensional (2D) semiconductor[1] with a large room-temperature electron mobility of approximately 10^3 cm^2 V^{-1} s^{-1}, is a promising material for high-sensitivity Hall sensors[2], ballistic transistors,[3] and non-volatile memory applications.[4]The In-Se system contains many different stable phases[5] including selenium rich In_2Se_3 and selenium deficient In_4Se_3 phases. The synthesis of InSe is challenging due to the narrow stability range of its stoichiometry on the phase diagram and the need for a surface morphology with large grain lateral growth. Therefore, synthesizing high-quality InSe requires a detailed understanding of how the synthesis parameters affect the structure and stoichiometry of In_xSe_y thin films near and within the narrow range of stability for InSe.

The growth of 2D InSe thin films has been achieved using a novel molecular beam epitaxy (MBE) two-step method involving an indium precursor layer, which effectively suppresses the formation of unwanted phases and allows for high-quality films.[6] This work builds upon this novel approach by investigating how synthesis parameters, including substrate temperature, precursor flux, and deposition time influence the structural and stoichiometric properties of InSe thin films deposited on sapphire substrates. The chemical bonding, crystalline structure, and morphology of the thin films are characterized by X-ray Photoelectron Spectroscopy, Raman spectroscopy, X-ray diffraction and Atomic Force Microscopy. By understanding how these synthesis parameters impact film quality, the optimal synthesis conditions for InSe thin film deposition can be further refined, enhancing the potential for device applications.

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

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

2D-ThP-3 Charge Transfer States at the Monolayer WS_2/HAT-CN Interface, ***Xu He***, *Antoine Kahn,* Princeton University

Understanding how WS_2 interacts electronically with organic molecules is very important for hybrid optoelectronics and energy harvesting applications, where charge separation at the interface governs device function. In this work, we investigate a heterojunction between monolayer WS_2 and 1,4,5,8,9,11-hexaazatriphenylene hexacarbonitrile (HAT-CN) to study energy level alignment and interfacial charge transfer.

The combined ultraviolet photoelectron spectroscopy and inverse photoemission spectroscopy (UPS/IPES) measurements show that the pristine monolayer WS_2 has an ionization energy (IE) of 6.00 eV and an electron affinity (EA) of 3.44 eV with a 2.56 eV electronic gap, while films of pristine HAT-CN show an IE of 9.48 eV and EA of 5.66 eV with a 3.82 eV electronic gap. These values suggest a type-II energy level configuration at the interface, providing an energetic driving force for electrons to transfer from WS_2 into HAT-CN.

Raman and Photoluminescence (PL) spectroscopies, and X-ray photoelectron spectroscopy (XPS) were performed on 1L-WS_2 with 0, 3.75, 7.5, and 15nm HAT-CN thicknesses. The Raman signature of WS_2 remains consistent across different thicknesses of HAT-CN, suggesting that the WS_2 lattice remains intact despite HAT-CN presence. XPS confirms HAT-CN adsorption on WS_2. PL spectra reveal a >90% quenching of the intrinsic WS_2 emission at around 633nm after HAT-CN deposition without visible PL peak shift. This significant PL quenching indicates the formation of a charge transfer (CT) state at the interface. The large difference in electronic gaps of 1L-WS_2 and HAT-CN suggests that it is not a Frenkel energy transfer. A device with mechanically transferred 1L-WS_2 and HAT-CN is being constructed and tested for photocurrents. We expect to see an external quantum efficiency (EQE) spectra whose absorption in the energy range below the electronic gap of both 1L-WS_2 and HAT-CN will provide direct evidence for the formation of CT states at the interface.

A systematic study on the evolution of the WS_2 VBM and HAT-CN LUMO positions is performed with combined UPS/IPES by evaporating 0, 0.5, 1, 2, 5, and 10nm HAT-CN on 1L-WS_2 on p-Si. This series of energy alignment studies show that the 1L-WS_2/HAT-CN interface shows a slight relaxation of the CT gap, which aligns well with the loss of electrons from WS_2 into HAT-CN layer.

This work demonstrates how tailoring the energy level alignment in hybrid 2D/organic heterojunctions can enable interfacial charge transfer. Our findings underscore the potential of engineering van der Waals interfaces between TMD monolayers and molecular semiconductors for novel excitonic devices and energy conversion applications.

2D-ThP-4 Enhanced Etching and Surface Cleaning of MoS_2 via Pre-Fluorination and Plasma-Activated Desorption, ***Shoaib Khalid,*** *Yuri Barsukov, Stephane Ethier, Igor Kaganovich,* Princeton University Plasma Physics Lab

Transition metal dichalcogenides (TMDs) are a class of layered materials that have garnered significant attention for their unique electronic, optical, and mechanical properties. Their tunable bandgap, high carrier mobility makes them ideal candidates for applications in next-generation electronics, optoelectronics, and energy storage devices. This study, based on ab initio molecular dynamics (AIMD) calculations, suggest that pre-fluorinating the MoS_2 surface before Ar plasma bombardment significantly enhances the etching yield and improves surface smoothness. Additionally, we propose a strategy to remove excess fluorine adsorbed on sulfur using low-energy electrons from the plasma. Our results show that F^- ions migrate much faster than neutral F atoms, facilitating their desorption. We also find that when H atoms are adsorbed on the surface, F^- ions diffuse until they encounter an H adatom, leading to the desorption of stable HF molecules. This approach of utilizing low-energy reactive species from plasmas offers an effective method for surface transport and cleaning of electronegative adsorbates, such as halogens, from the MoS_2 surface.

This research was supported by the Princeton Plasma Physics Laboratory under U.S. Department of Energy Prime Contract No. DE-AC02-09CH11466.

2D-ThP-5 2d Topological Phases, β-Sn Transformation, and Implications for Topological Superconductivity, ***Cheng-Maw Cheng,*** National Synchrotron Radiation Research Center, Taiwan; *Ye-Shun Lan,* National Tsing Hua University, Taiwan; *Shu-Hua Kuo,* National Synchrotron Radiation Research Center, Taiwan; *Yen-Hui Lin,* National Tsing Hua University, Taiwan; *Jing-Yue Huang,* National Synchrotron Radiation Research Center, Taiwan; *Pin-Jui Hsu, Horng-Tay Jeng,* National Tsing Hua University, Taiwan

Two-dimensional topological materials offer unique electronic properties that are promising for next-generation quantum and spintronic devices. In particular, 2D topological insulators (TIs) host robust spin-polarized edge states protected by a bulk band gap induced by spin-orbit coupling, while topological nodal line semimetals (TNLSMs) feature one-dimensional band degeneracies protected by crystalline symmetries. Despite theoretical predictions, experimental realization of 2D TNLSMs remains scarce. In this work, we report the synthesis and characterization of a monolayer cubic β-Sn phase grown on a Cu(111) substrate via sequential deposition. Starting from low-temperature growth of α-Sn (stanene), we observed a well-defined honeycomb lattice using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), consistent with prior reports. Subsequent Sn deposition led to a structural phase transition into a high-coverage, single-layer β-Sn with a body-centered tetragonal structure. This transition was confirmed by STM and angle-resolved photoemission spectroscopy (ARPES), revealing a dramatic change in the electronic structure. Combined with first-principles density functional theory (DFT) calculations, we demonstrate that monolayer β-Sn hosts two distinct types of nodal lines—coexisting in a single 2D mono-elemental material. This observation marks the first realization of a 2D topological semimetal featuring dual nodal line types. Given β-Sn's known superconductivity in bulk form, our findings establish ultrathin β-Sn as a promising platform for exploring 2D topological superconductivity and potentially hosting Majorana fermions.

2D-ThP-6 Transition of Exohedral Fullerenes Fe+C60 to Endohedral Fullerenes Fe@C60 Upon Its Deposition on the Surface of an Iron Crystal Using Md Simulations*, **Danila Alyabev,*** Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan*; Dmitriy Bazarov,* Digital Technologies and Artificial Intelligence Research Institute, Tashkent, Uzbekistan

To date, following the discovery and isolation of fullerenes, there have been a large number of both experimental and theoretical studies on their research. A specific group includes the so-called endofullerenes—fullerenes with encapsulated atoms or molecules inside their cavities, such structures are of both theoretical and practical interest. In the current study, the possibility of transition of exohedral fullerene Fe+C_{60} to endohedral fullerene Fe@C_{60} through scattering of Fe+C_{60} on the surface of an iron crystal is explored by methods of molecular dynamics.

In this study, we used the LAMMPS software package in combination with a selected Tersoff potential for modeling purposes [1]. To conduct the model experiment, we created two models: a system consisting of Fe and C_{60} exofullerenes heated to 900 K, i.e. Fe+C_{60} model (T = 900K), and an iron crystal heated to 300 K (T = 300K). We then isolated a region on the surface of the iron crystal where exofullerenes were deposited normally at a vertical velocity of 4200 m/s (7.15eV, 400 impact points, process time – 5 ps, timestep – 0.0001 ps)

The primary objective of this study was to isolate those fullerenes where the iron atom was encapsulated within the fullerene structure. Dynamic data was acquired and processed as follows: 12 carbon atoms on the lower hemisphere of each fullerene were selected; Vectors were constructed between the iron atom and each of these selected carbon pairs, and the angles formed by these vectors were measured – a total of 66 angle measurements were taken for each of 400 instances. a 400 × 67 data array was generated, where the potential energy value of the iron atom was recorded in a separate column after 5ps model time.

The output data was analyzed using cluster analysis methods, which allowed the classification of fullerenes into groups based on their characteristic geometries. One of the isolated groups included fullerenes with geometries similar to those with endohedral structures, the bond lengths of these fullerenes were compared to those in the study [2]. Based on the simulation results, it is expected that 21-30% of the exofullerenes will transition to endofullerenes under the given initial conditions.

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

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

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

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

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

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

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

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2D-ThP-9 Discretized Atomic Layer Deposition Recipe for Wafer-scale Synthesis of MoS₂*, Sachin Shendokar,* ***Shyam Aravamudhan,*** North Carolina A&T State University

Monolayer MoS_2, a 2D material, holds enormous promise for transcending the fundamental limits of silicon-based electronics and continuing the downscaling of transistors and logic circuits for energy-efficient computing. However, major research efforts are needed to overcome many fabrication and integration challenges including wafer-scale growth control, doping, contacts, gate stack, and reliability. In this work, we attempt to address one of the challenges, namely wafer-scale synthesis of MoS2. Atomic Layer Deposition (ALD) is one of the most promising techniques for wafer-scale growth of MoS2 due to its conformal, self-limiting, and low-temperature characteristics. We present here a novel discretized ALD recipe for wafer-scale deposition of uniformly thick MoO3, further, to sulfurized to stoichiometric MoS2. This is an alternative approach for ALD to determine temperature and time based on the Arrhenius equation and first -order reaction kinetics. Wafer-scale uniformity, film morphology, composition and crystallinity were measured using a comprehensive set of characterization techniques including ellipsometry, AFM, XPS, Raman, XRD and Photoluminescence measurements.

2D-ThP-10 Modeling Synthesis Pathways for Transition Metal Dichalcogenide Monolayers with Quantum and Statistical Learning Techniques*,* ***Andrew Messecar,*** Western Michigan University*; Chen Chen, Isaiah Moses, Wesley Reinhart, Joan Redwing,* The Pennsylvania State University*; Steven Durbin,* University of Hawaiʻi at Mānoa*; Robert Makin,* Western Michigan University

The ability for machine learning technologies to estimate patterns from information has made them a top approach for optimizing the growth and characterization of a broad range of material systems, including few and single atomic layer materials such as transition metal dichalcogenides (TMDs). In this work, we have applied both quantum and classical machine learning approaches to investigate and model the metal–organic chemical vapor deposition (MOCVD) of TMD thin films as grown with dihydrogen chalcogenide gas and transition metal hexacarbonyl precursors. Several hundred discrete records of MOCVD–grown TMD samples synthesized in a single laboratory have been organized into material–specific data sets. For each growth trial, Raman spectra characterizing the resulting sample have been utilized to assess monolayer coverage. The distance between the A_{1g} and E_{2g} Raman mode peaks in each spectrum was measured and associated with the respective growth record as an output variable within the data set. The MOCVD synthesis parameter data was subsequently mapped to the measured A_{1g} and E_{2g} Raman mode peak distance using supervised learning techniques. A combination of p–value calculations, Pearson's correlation coefficients, SHAP values, and regression tree splitting rules were used to analyze the statistical importance of each MOCVD operating parameter for influencing the expected value of the distance between the A_{1g} and E_{2g} Raman mode peaks. Various quantum as well as classical supervised machine learning approaches – including k–nearest neighbors, tree–based models, and quantum support vector machines, were fit to the data and compared for generalization performance. In the case of MoS_2, generalizing beyond the training data indicates that maximizing both the $Mo(CO)_6$ injector hydrogen gas flow during the growth step and the value of the $Mo(CO)_6$ flow during the reaction temperature ramp up step is forecasted to result in a minimization of the A_{1g} and E_{2g} Raman mode peak distance. This predicted reduction of the peak distance between the A_{1g} and E_{2g} vibrational modes in Raman spectra acquired of MoS_2 thin films corresponds with improved monolayer coverage. This methodology is applicable to additional TMD materials and characterization features of interest.

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2D-ThP-11 Investigating Optical Properties of Moiré Excitons in Twisted Transition Metal Dichalcogenide (TMDC) Homobilayers*,* ***Dheeraj Koneru,*** Stevens Institute of Technology

Over the past decade, atomically thin 2D van der Waals (vdW) materials have become powerful systems to study light-matter interaction and electronic confinement. In monolayer transition-metal dichalcogenides (TMDCs), optical absorption is dominated by tightly bound excitons due to reduced screening and enhanced Coulomb interactions. I present the optical study of moiré excitons in twisted WSe2 homobilayers, where a small interlayer twist generates a periodic potential landscape that traps excitons at specific locations in real space.

To isolate and study these moiré-localized excitons (MXs), I detail the fabrication process of monolayer WSe2 on SiO2, followed by tear-and-stack assembly to produce a clean interface between the twisted homobilayers. Through power-dependent, polarization-resolved, and magneto-optical spectroscopy, I demonstrate that the narrow, quantum dot-like spectral lines originate from localized MXs. These results reveal how structural symmetry, twist angle, and magnetic fields impact valley physics in moire superlattices. The findings offer new opportunities for creating quantum emitter arrays for integrated quantum photonics.

Author Index

Bold page numbers indicate presenter