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.

References

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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.

1. K.O.E. Henriksson et al, Journal of Physics: Condensed Matter, 25(44), 445401

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2D-ThP-9 Discretized Atomic Layer Deposition Recipe for Wafer-scale Synthesis of MoS_2*, 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***[1]*,* Western Michigan University*; Chen Chen, Isaiah Moses, Wesley Reinhart, Joan Redwing,* The Pennsylvania State University*; Steven Durbin,* University of Hawai'i 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***[2]*,* 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.

2D-ThP-12 Band Gap Opening in AB-Stacked Bilayer Silicon*,* ***Kumar Vishal****, Hong Huang, Yan Zhuang,* Wright State University

Despite their potential as of being the excellent candidates for advancing CMOS technology to its physical limits, the presence of an opened energy bandgap in either single- or bilayer- silicene poses a significant challenge, hindering its applications in the main stream semiconductor industry. Previous attempts, including applying external electric field, surface decoration, nanopatterning, and applying uniaxial strain along designate directions, have proven insufficient in meeting the stringent demands of CMOS technology concerning operational reliability, processing environment sensitivity, product yield, and achievable processing standards. Recently a number of research reported that applying of the biaxial in-plane strain leads to energy bandgap opening in AA-stacked bilayer silicene, however the maximum energy bandgap opening is limited to 16 meV.

In this work, we present a theoretical study of the opening of energy bandgap in AB-stacked bilayer silicene. Employing the Density Functional Theory (DFT), our investigations have taken into account of the effects of both ferromagnetism and antiferromagnetism, alongside external biaxial in-plane strain/stress and vertical biasing effects. Within a strain range spanning from -5.17% to 10.35%, we observed a strain-tunable energy bandgap opening with a maximum of 380 meV at a strain level of 7.76%. Notably, beyond this strain range, the energy bandgap remains closed. In addition, under compressive strain, the energy band diagram presents spin-

[1] **JVST Highlighted Poster**

[2] **JVST Highlighted Poster**

generated features, with discernible energy band splitting. On the contrary, tensile strain leads to a break of the spin generation, except at specific high symmetry points such as . We further observe a degeneration of the energy band diagram at these high symmetry points upon the application of gate voltage along the vertical direction. The coupling of the ferromagnetism and antoferromagnetism between the two silicene layers results in a transition from metallic material to semiconductor. The potential of the opened bandgap makes the AA-stacked bilayer silicene a very promising candidate material to be applied in the CMOS technology, while the strain-induced tunable bandgap opening offers immediate potential for applications in the infrared (IR) spectrum. In addition, the spin-induced band diagram degeneration may holds promise for integrated spintronics applications.

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