

## Poster Abstracts

### Poster 1

---

#### **2D Crystal Consortium-Materials Innovation Platform**

email: 2DCC@psu.edu

web: mip.psu.edu

#### *OUR RESEARCH FOCUS*

The 2DCC-MIP is focused on advancing the synthesis of 2D materials within the context of a national user facility. The 2DCC is developing custom deposition tools with in-situ and real time characterization and facilities dedicated to epitaxial and bulk growth of chalcogenide single crystals. Unique capabilities are also available to simulate growth kinetics through first principles and reactive potential approach.

### Poster 2

---

#### **Graphene Stabilization of Two-dimensional Gallium Nitride**

Zakaria Y. Al Balushi<sup>1,2,\*</sup>, Ke Wang<sup>3</sup>, Ram Krishna Ghosh<sup>2,4</sup>, Suman Datta<sup>2,3,4</sup>, Joshua A. Robinson<sup>1,2,3</sup> and Joan M. Redwing<sup>1,2,3,4</sup>

<sup>1</sup> Dept. of Materials Science and Engr., The Pennsylvania State University, University Park, PA USA

<sup>2</sup> Center for 2-Dimensional and Layered Materials, University Park, PA USA

<sup>3</sup> Materials Research Institute, University Park, PA USA

<sup>4</sup> Dept. of Electrical Engr., The Pennsylvania State University, University Park, PA USA

The spectrum of two-dimensional (2D) and layered materials “beyond graphene” has been continually expanding, however, the synthesis of wide bandgap 2D crystals remain limited. Along similar lines to initial theoretical discovery and subsequent experimental synthesis of “beyond graphene” 2D materials (i.e. silicene and germanane), theoretical studies have suggested that wurtzite indium nitride (InN), gallium nitride (GaN), and aluminum nitride (AlN) take on a hexagonal 2D graphitic structure with thickness tunable energy bandgaps (~0.7 – 7.0 eV) as a result of quantum confinement. The experimental synthesis of stable wide bandgap 2D nitrides “beyond hexagonal boron nitride (hBN)” on technologically relevant substrates, however, still remains elusive. We have developed a novel alternative growth route, known as migration enhanced encapsulated growth (MEEG)<sup>1</sup>, which utilizes the mechanism of intercalation *via* defects in graphene to stabilize few layers of new wide bandgap 2D materials that are not layered in bulk crystals<sup>1</sup>.

Here we show the mechanism of 2D nitride formation and discuss graphene’s ability to provide sufficient thermodynamic stabilization of the (direct bandgap ~5 eV) 2D buckled structure of GaN that exhibits

unique properties from that of bulk crystals. In the case of 2D GaN, a layer of gallium intercalates between the hydrogenated quasi-free standing epitaxial graphene (QFEG) and SiC substrate interface. This intercalated layer of gallium is subsequently converted to bilayer 2D GaN *via* nitrogen intercalation and ammonolysis using  $\text{NH}_3$ . We demonstrate that the 2D GaN atomic structure grown *via* MEEG is not a simple 2D planar structure as predicted by theory, but rather a combination of two different buckled structures. This atomic arrangement can considerably impact the electronic structure as we demonstrate using density functional theory (DFT), in which we verify our findings by directly identifying the positions of the nitrogen and gallium atomic columns in the bilayer 2D GaN structure using aberration corrected scanning TEM (STEM) in annular bright field (ABF) mode. While the deconvolution of individual layers is very difficult, we utilize various experimental techniques (UV reflectance and low loss electron energy loss spectroscopy) to verify that the 2D GaN exhibits a bandgap of  $\sim 5$  eV, demonstrating for the first time that the electronic properties of stoichiometric atomic layers of GaN is significantly impacted by quantum confinement. Our graphene intercalation approach provides a novel pathway towards stabilizing new 2D materials (group III-nitrides and other compound semiconductors) that are not layered in bulk crystals, which may open up new avenues of research in 2D novel electronic and optoelectronic devices.

[1] Graphene stabilization of two-dimensional gallium nitride Al Balushi et al. arXiv:1511.01871

### Poster 3

---

## Evaluation of Two Dimensional Metallic Transition Metal Dichalcogenides as Next Generation Interconnects

A. Arnold, D. Schulman, A. Razavieh, S. Das

**Abstract:** As semiconductor devices continue to scale, the copper wires interconnecting them become thinner, narrower and longer leading to significantly increased parasitic resistance and capacitance which ultimately limit the on-chip performance. Consequently, alternative materials are being explored. 2D materials show great scaling potential due to their minimal thickness. Preliminary investigations of semi-metallic graphene have shown promising characteristics but still fall slightly below the best results shown for copper. Another class of 2D materials, metallic transition metal dichalcogenides (TMDs) have shown bulk resistivity values, comparable to and in some cases less than those of graphite, but have received comparably little attention. If the lower bulk resistivity of some metallic TMDs translates into improved performance of nanoribbon interconnects, metallic TMDs could be a viable alternative to copper.

*Poster 4*

---

## Growth of Vertical MoS<sub>2</sub> flowers on graphite paper for Hydrogen Evolution Reactions (HERs)

Ganesh Rahul Bhimanapati  
The Pennsylvania State University

**Abstract:** Layered materials, especially the transition metal dichalcogenides (TMDs), are of interest for a broad range of applications. Among the class of TMDs, molybdenum disulfide (MoS<sub>2</sub>) is perhaps the most studied because of its use in optoelectronics, energy storage and energy conversion applications. Understanding the fundamental structure property relations is key for better optimization of these materials. In the current work, a controlled synthesis of MoS<sub>2</sub> flower-like structures via powder vaporization is shown. This flower morphological growth is readily achieved on multiple substrates such as graphite, silicon and silicon dioxide. The resulting flowers are highly crystalline and stoichiometric. Contact angle measurements indicated that MoS<sub>2</sub> flowers exhibit the highest reported contact angle of  $\sim 156 \pm 10^\circ$ , making it super hydrophobic material. As MoS<sub>2</sub> is an ideal candidate for hydrogen evolution reactions (HERs), the presence of vertical flakes would further improve the performance for HERs. Electrochemical measurements showed that the as grown MoS<sub>2</sub> flowers had a Tafel slope of 185 mV/dec. Further enhancement to the HERs was done by treating the surface with UV-Ozone. This surface treatment allowed us to tune the wettability of the surface by changing the edge chemistry of the flowers, which was further confirmed by improved HERs performance (Tafel slope was reduced to 54 mV/dec).

*Poster 5*

---

## Effects Of Uniaxial And Biaxial Strain On Few-Layered Terrace Structures Of MoS<sub>2</sub> Grown By Vapor Transport

Amber McCreary<sup>1,2,3</sup>, Rudresh Ghosh<sup>4</sup>, Matin Amani<sup>1,†</sup>, Jin Wang<sup>5</sup>, Karel-Alexander N. Duerloo<sup>6</sup>, Ankit Sharma<sup>4</sup>, Karalee Jarvis<sup>7</sup>, Evan Reed<sup>6</sup>, Avinash M. Dongare<sup>5</sup>, Sanjay K. Banerjee<sup>4</sup>, Mauricio Terrones<sup>3,8,9</sup>, Raju Namburu<sup>2</sup> & Madan Dubey<sup>1</sup>

<sup>1</sup>Sensors & Electron Devices Directorate, U.S. Army Research Laboratory; <sup>2</sup>Computational and Information Sciences Directorate, U.S. Army Research Laboratory; <sup>3</sup>Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University; <sup>4</sup>Microelectronics Research Center, The University of Texas at Austin; <sup>5</sup>Department of Materials Science and Engineering and Institute of Materials Science, University of Connecticut; <sup>6</sup>Department of Materials Science and Engineering, Stanford University; <sup>7</sup>Texas Materials Institute, The University of Texas at Austin; <sup>8</sup>Department of Materials Science & Engineering, The Pennsylvania State University; <sup>9</sup>Department of Chemistry, The Pennsylvania State University.

**Abstract:** One of the most fascinating properties of molybdenum disulfide (MoS<sub>2</sub>) is its ability to be subjected to large amounts of strain without degrading the material. The potential of MoS<sub>2</sub> mono- and few-layers in electronics, optoelectronics, and flexible devices requires the fundamental understanding of their properties as a function of strain. While previous reports have studied mechanically exfoliated flakes, tensile strain experiments on chemical vapor deposition (CVD)-grown few-layered MoS<sub>2</sub> has not

been examined hitherto, although CVD is the state of the art synthesis technique with clear potential for scale-up processes. In this report, we used CVD-grown terraced MoS<sub>2</sub> layers to study how the number and size of the layers affects the physical properties under uniaxial and biaxial tensile strain.

Interestingly, we observed significant shifts in both the Raman in-plane mode (as high as -5.2 cm<sup>-1</sup>/% strain) and photoluminescence (PL) energy (as high as -88 meV/% strain) for the few-layered MoS<sub>2</sub> under uniaxial strain when compared to monolayers and few-layers of MoS<sub>2</sub> studied previously. We also observed slippage between the layers which results in a hysteresis of the Raman and PL spectra during further applications of strain. This work demonstrates that CVD-grown few-layered MoS<sub>2</sub> is a realistic, exciting material for tuning its properties under tensile strain.

## *Poster 6*

---

### **Contacts to Transition Metal Dichalcogenides**

T. N. Walter, M. Abraham, A. C. Domask, Y. Zeng, R. Gurunathan, H. Simchi, and S. E. Mohney  
The Pennsylvania State University

**Abstract:** The resistance of electrical contacts to transition metal dichalcogenides (TMDs) remains an obstacle for the optimization of TMD-based field effect transistors. We are studying the role of pre-metallization surface preparation and annealing on the electrical characteristics of contacts through analysis of sets of back-gated transistors with varying channel lengths. We are also performing materials characterization of the contacts using transmission electron microscopy and other techniques, and predicting the reactivity of annealed contacts using thermodynamics (for MoS<sub>2</sub>, WS<sub>2</sub>, and WSe<sub>2</sub>).

## *Poster 7*

---

### **Studying the Spin and Valley Physics in 2D Transition Metal Dichalcogenides**

Zefang Wang  
Shan/Mak Group, The Pennsylvania State University

**Abstract:** The newly emerged two-dimensional (2D) transition metal dichalcogenides (TMDs) with nonequivalent K and K' valleys have provided an ideal laboratory for exploring the valley degree of freedom of electrons, as well as their potential applications for electronics and optoelectronics. We develop optical microscopy techniques to investigate the valley and spin dependent optical and transport properties in 2D semiconductor TMDs. Examples include the valley Hall effect and the interaction effects in atomically thin TMDs.

## Poster 8

---

### Exploring Electronic Phases in Atomically Thin NbSe<sub>2</sub>

Egon Sohn

Shan/Mak Group, The Pennsylvania State University

**Abstract:** Atomically thin van der Waals materials have emerged as a frontier for both fundamental physics and device applications. We investigate atomically thin metals such as group-V transition metal dichalcogenide NbSe<sub>2</sub>. Using transport, magnetotransport and Raman scattering measurements, we observe superconductivity and charge-density-wave order in NbSe<sub>2</sub> down to the monolayer limit. The 2D nature, the strong spin-orbit interaction and the underlying symmetry in this class of materials give rise to unique properties in the electronic phases and provide means to control these phases.

## Poster 9

---

### Nonlocal Transport Measurement in H-shaped Graphene Devices

Hua Wen<sup>1</sup>, Jing Li<sup>1</sup>, Jun Zhu<sup>1,2</sup>

<sup>1</sup>*Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA*

<sup>2</sup>*Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, Pennsylvania 16802, USA*

**Abstract:** Single layer graphene has been experimentally demonstrated to exhibit high mobility and long spin lifetimes, making it promising as spin transport channel. However, small intrinsic spin-orbit coupling in graphene ( $\sim 10 \mu\text{eV}$ ) hampers spin manipulating via electrical approach which is vital for spintronics applications. Theoretical calculations show that adatom-decorated graphene manifests a sizeable spin-orbit coupling ( $\sim 10 \text{ meV}$ ). Furthermore, this spin-orbit coupling can be probed electrically by Spin Hall Effect (SHE) and Inverse Spin Hall Effect (ISHE) in an H-bar shaped device. Recently such experiments have been carried out on H-shaped graphene with chemisorbed (hydrogen and fluorine) and physisorbed (gold and iridium) adatoms. Controversy results have been reported on the interpretation of the signal, whether it is from spin-orbit coupling or non-spin origin. Here we present our study on such H-shaped graphene devices with variable device dimensions and temperatures. Our results reveal that non-diffusive transport plays an important role in the observed signal when electron mean free path is comparable to device dimension. Additionally, charge inhomogeneity can substantially influence the observed signal, pointing to the complex origin of signals observed in such H-shaped graphene devices.

*Poster 10*

---

**Magnetoresistance and Anti-Ferromagnetic Coupling in FM-Graphene-FM Trilayers**

Enrique D. Cobas, Olaf M. J. van 't Erve, Shu-Fan Cheng and Berend T. Jonker  
 US Naval Research Laboratory

**Abstract:** Both high-magnetoresistance(MR) minority spin filtering[1] and anti-ferromagnetic (AFM) coupling[2-3] have been predicted for FM|Graphene|FM vertical heterostructures. Our previous experiments[4-5] demonstrated ordinary magnetoresistance in NiFe-Graphene-Co heterostructures and no evident AFM coupling. Here we present experimental results that confirm both MR minority spin filtering and AFM coupling in high-quality FM|Graphene|FM heterostructures. Multi-layer graphene was synthesized by chemical vapor deposition directly on the bottom ferromagnetic electrode consisting of a sputtered quasi single-crystalline NiFe(111) film on sapphire. A top ferromagnetic layer was deposited by e-beam evaporation to avoid plasma damage to the graphene. The stack was patterned into symmetric cross-bar structures using Ar ion milling. Measurements show negative magnetoresistance in excess of 10 percent, confirming spin-filtering, and weak anti-ferromagnetic coupling throughout the temperature range 15K to 300K. The temperature dependence of the MR was studied and found consistent with thermal excitation of spin waves in the ferromagnetic electrodes. Junction resistance-area products are in the range of 10  $\Omega\text{cm}^2$ . These heterostructures provide a fast and low-power magnetic field sensor in the sub-100 Oe range and are a step towards high-MR low RA-product MRAM junctions.

- [1] Karpan, et al. Phys. Rev. Lett 99, 176602, 2007.
- [2] Li et al., App. Phys. Lett 98 (13), 133111, 2011.
- [3] Kim, D. et al., App. Phys. Lett 102 (11), 112403, 2013
- [4] Cobas et al., Nano Lett. 12, 3000, 2012.
- [5] Cobas et al., IEEE Trans. Mag., 49 (7), 4343, 2013.

*Poster 11*

---

**Tuning the Trion Polarization in Monolayer WS<sub>2</sub>**

A. T. Hanbicki<sup>1</sup>, M. Currie<sup>1</sup>, K. M. McCreary<sup>1</sup>, C. S. Hellberg<sup>1</sup>, A. L. Friedman<sup>1</sup>, G. Kioseoglou<sup>2</sup>, and B. T. Jonker<sup>1</sup>

<sup>1</sup>Naval Research Laboratory, Washington, DC 20375

<sup>2</sup>University of Crete and Foundation for Research and Technology Hellas (FORTH), Heraklion Crete, 71003, Greece

**Abstract:** Monolayer transition metal dichalcogenides, MX<sub>2</sub> (M = Mo, W and X = S, Se), are direct-gap semiconductors with some interesting properties. First, the low-dimensional hexagonal structure leads to two inequivalent K-points, K and K', in the Brillouin zone. Second, this valley index and spin are intrinsically coupled, and spin-dependent selection rules enable one to independently populate and interrogate a unique K valley with circularly polarized light. Consequently, one can selectively populate each valley independently with circularly polarized light, and determine the valley populations via the

polarization of emitted light. Optical emission is dominated by neutral and charged excitons (trion), and changes in emitted polarization provide insight into the fundamental processes of intervalley scattering. We prepare single-layer WS<sub>2</sub> films such that the photoluminescence is from the negatively charged trion and observe a room temperature optical polarization in excess of 40% for the trion. Using an applied gate voltage, we can modulate the electron density and subsequently the polarization continuously from 20-40%. Both the polarization and the emission energy monotonically track the gate voltage with the emission energy increasing by 45 meV. We discuss the role electron capture of the trion has on suppressing the intervalley scattering process.

**Acknowledgement:** This work was supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research #AOARD 14IOA018-134141.

## *Poster 12*

---

### **Optical Polarization and Intervalley Scattering in Single Layers of MoS<sub>2</sub> and MoSe<sub>2</sub>**

B.T. Jonker<sup>1</sup>, G. Kioseoglou<sup>2</sup>, A.T. Hanbicki<sup>1</sup>, M. Currie<sup>1</sup> and A.L. Friedman<sup>1</sup>

<sup>1</sup>Naval Research Laboratory, Washington, DC 20375

<sup>2</sup>Department of Materials Science and Technology, University of Crete, Heraklion Crete, 71003, Greece

**Abstract:** We probe the valley population dynamics in MoSe<sub>2</sub> and MoS<sub>2</sub> by selectively populating the K and K' valleys with circularly polarized light while systematically varying the laser excitation energy. For both systems, the difference in the excitation energy and photoluminescence emission energy,  $dE = E_{pump} - E_{PL}$ , governs the depopulation of carriers in each valley. Adding more energy above a distinct threshold characteristic of the longitudinal acoustic (LA) phonon for each material enables inter-valley scattering and produces a sharp decrease in the observed circular polarization. LA phonons in these two systems have different energies (30 meV for MoS<sub>2</sub> and 19 meV for MoSe<sub>2</sub>), and we show that the threshold for the excess energy required to initiate the depolarization process clearly reflects the material specific phonon energy. In addition, our results show that independent of how many carriers are excited, i.e. whether you create neutral or charged excitons, the scattering process is the same. We find that the key parameter for the depolarization process is the extra kinetic energy of the exciton – depolarization is due to intervalley scattering that begins to occur when the exciton energy exceeds a threshold corresponding to twice the LA phonon energy.

**Acknowledgement:** This work was supported by core programs at NRL, and by the Air Force Office of Scientific Research #AOARD 14IOA018-134141.

## Poster 13

---

### Substrate Effects in CVD Synthesized Monolayer WS<sub>2</sub>

K.M. McCreary<sup>1\*</sup>, A.T. Hanbicki<sup>1</sup>, G. Kioseoglou<sup>2</sup>, M. Currie<sup>1</sup>, and B.T. Jonker<sup>1</sup>

<sup>1</sup>Naval Research Laboratory, Washington, DC 20375

<sup>2</sup>University of Crete, Heraklion Crete, 71003, Greece

\* kathleen.mccreary@nrl.navy.mil

**Abstract:** The unique electronic band structure in single layer WS<sub>2</sub> provides the ability to selectively populate a desired valley by exciting with circularly polarized light. The valley population is reflected through the circular polarization of photoluminescence (PL). We investigate the circularly polarized PL in WS<sub>2</sub> monolayers synthesized on SiO<sub>2</sub>/Si substrates using chemical vapor deposition (CVD). The resulting polarization is strongly dependent on the sample preparation. As-grown CVD WS<sub>2</sub> (still on the growth substrate) exhibits PL emission from the neutral exciton and polarized emission that is unaffected by laser power. Removing WS<sub>2</sub> from the growth substrate and repositioning on the same substrate significantly impacts the optical properties. In transferred films, the excitonic state is optically controlled via high-powered laser exposure such that subsequent PL is from either the charged exciton state or the neutral exciton state. Additionally, the neutral excitonic emission exhibits low polarization whereas the trion polarization can exceed 25% at room temperature, demonstrating the ability to optically control the degree of circularly polarized emission. The removal process may modify the strain, sample-to-substrate distance, and chemical doping in the WS<sub>2</sub> monolayer, and work is underway to determine how these factors influence the valley populations.

**Acknowledgement:** This work was supported by core programs at NRL and the NRL Nanoscience Institute, and by the Air Force Office of Scientific Research #AOARD 14IOA018-134141.

## Poster 14

---

### Tunable Growth, Transfer, Atomic Structure Analysis, and Heterostructure of Two-dimensional (2D) Hexagonal Boron Nitride (h-BN) Crystals

Mohammed Abu AlSaud<sup>1</sup>, Amin Azizi<sup>1</sup>, Fu Zhang<sup>1</sup>, and Nasim Alem<sup>1</sup>

<sup>1</sup> Department of Materials Science and Engineering, Materials Research Institute, and Center for Two Dimensional and Layered Materials, The Pennsylvania State University, University Park, Pennsylvania 16802, USA

**Abstract:** Two-dimensional (2D) hexagonal boron nitride (h-BN) crystals has some outstanding properties such as high mechanical strength, atomic-thick electron tunneling barrier, high thermal conductivity, and high optical transparency. Also, h-BN offers atomically smooth surfaces for graphene device applications. It can also be stacked with other 2D crystals, i.e. graphene and transition metal dichalcogenides (TMDs), to create novel van der Waals Heterostructures with unique properties. In this work, we show how the morphology and h-BN size can be controlled using low-pressure chemical vapor deposition (LPCVD) technique. We also demonstrate a consistence method of transferring h-BN crystals

to different substrates. Atomic and chemical structure of grown h-BN crystals are studied using scanning electron microscopy (SEM), ultra-high-resolution aberration-corrected transmission electron microscopy (TEM), selected-area electron diffraction (SAED), and Electron energy-loss spectroscopy (EELS). Furthermore, we demonstrate the synthesis of graphene and hexagonal boron heterostructure using low-pressure chemical vapor deposition technique.

## Poster 15

---

### Broadband Femtosecond Transient Absorption Spectroscopy for CVD MoS<sub>2</sub> Monolayer

S. H. Aleithan<sup>1</sup>, M. Livshits<sup>2,3</sup>, S. Khadka<sup>1</sup>, J. Rack<sup>2,3</sup>, M. Kordesch<sup>1</sup> and E. Stinaff<sup>1</sup>

<sup>1</sup> Department of Physics and Astronomy, Ohio University, Athens, Ohio, OH 45701, USA

<sup>2</sup> Department of Chemistry, Ohio University, Athens, Ohio, OH 45701, USA

<sup>3</sup> Department of Chemistry and Chemical Biology, University of New Mexico, Albuquerque, NM 87131, USA

**Abstract:** Two-dimensional atomic crystals of transition metal dichalcogenides (TMD) are considered promising candidates for optoelectronics, valleytronics, and energy harvesting devices. These materials exhibit excitonic features with high binding energy as a result of confinement effect and reduced screening when the material is thinned to monolayer. Studies have shown that the uv-vis absorption spectrum of the material has at least three peaks commonly labeled as A, B, and C. A and B are the two direct transitions between the conduction band and the spin-orbit split valance band around  $K$  ( $K'$ ) point in the Brillouin zone, while C is associated with the band nesting region between  $K$  and  $\Gamma$ . In this work samples of MoS<sub>2</sub> were grown by chemical vapor deposition (CVD), pumped with femtosecond laser, and probed by femtosecond white light resulting in broadband differential absorption spectra with three distinct features related to the three dominant absorption peaks in the material. Interestingly, for pump wavelengths both resonant and non-resonant with the A and B excitons, we observe a ground state bleach around C (2.9 eV), with decay components similar to A and B. This observation indicates significant k-space delocalization and overlap among the three excitonic wave functions (A, B, and C). Comparison of time dynamics for all features in resonance and non-resonance excitation is consistent with this finding.

## Poster 16

---

### Computational Discovery of Two-Dimensional Group IV-Group V Materials

M. Ashton, S.B. Sinnott, and R.G. Hennig

**Abstract:** First-principles calculations are used to predict the stability and properties of two-dimensional (2D) group IV-V MX (M = Si, Ge, Sn, P; X = P, As, Sb, Bi) compounds in two crystal structures: a low symmetry  $Cm$  layer inspired by the layered bulk structures of SiP, SiAs, GeP and GeAs, and a high symmetry  $P\bar{6}m2$  structure previously predicted to be stable for 2D SiP. The compositions we investigate are generally more stable in the  $Cm$  structure than the  $P\bar{6}m2$  structure, although the energy differences

between the two are quite small in most cases. The electronic properties of the two structures, however, are quite different- the  $Cm$  band gaps are systematically larger by close to 15% for most compounds, and their band edges are higher by 0.1-0.4 eV due to the reduced dipole moments at the  $Cm$  surfaces. Therefore, we predict that all of these compounds in the  $Cm$  crystal structure will form Type I heterojunctions in contact with their  $P\bar{6}m2$  polymorphs. Additionally, Pourbaix diagrams show that several of these compounds are also stable in moisture and possibly even in aqueous conditions.

## Poster 17

---

### Chemical Vapor Deposition Growth and Transmission electron Microscopy of Freestanding Van Der Waal Heterostructures

F. Zhang<sup>1,2</sup>, A. Aizi<sup>1,2</sup>, and N. Alem<sup>1,2</sup>

<sup>1</sup> Department of Materials Science and Engineering and Materials Research Institute, The Pennsylvania State University, University Park, PA 16802, USA.

<sup>2</sup> Materials Research Institute, The Pennsylvania State University, University Park, PA 16802, USA.

**Abstract:** Transitional-metal dichalcogenides (TMDs), emerging as post-graphene materials, are desirable candidates for electronic and optoelectronic devices as well as low cost catalysts. Van der Waals (vdW) heterostructures based on transitional-metal dichalcogenides (TMDs) can open up pathways to generate novel materials via a bottom-up approach. This study demonstrates a new approach for the direct growth of freestanding TMDs/graphene heterostructure and TMDs/hBN heterostructure. Aberration-corrected transmission electron microscopy (TEM) imaging and spectroscopy, coupled with Raman and photoluminescence studies will be used to investigate the atomic, chemical, and electronic structure of the heterostructures and their resulting optoelectronic response. In this study we also determine the nucleation and growth of vdW heterostructures and the role of substrate defects in the epitaxial growth of TMDs. Such direct growth technique enables us to investigate the heterostructure nucleation and growth mechanisms at the atomic level by TEM, which can be utilized to study a wide spectrum of van der Waals heterostructures.

## Poster 18

---

### 2D Layers Where You Want Them: Tuning Substrate Surfaces for Selective-Area Growth

B. Bersch, S. Eichfeld, G. Bhimanapati, K. Zhang, A. Piasecki, N. Glavin, A. Voevodin, and J. Robinson

**Abstract:** In recent years, there has been a concentrated effort toward developing large-area chemical vapor deposition (CVD) of two-dimensional transition metal dichalcogenides (TMDs) such as molybdenum disulfide ( $\text{MoS}_2$ ). Moreover, continued improvement in materials integration has led to the realization of high-performance transistors and next-generation electronics based on these novel 2D semiconductors. While there has been substantial effort in achieving uniform and large-domain TMDs, there have been few reports on selective-area growth of these materials. The selective and controllable growth of TMDs on device-ready substrates bypasses the need for destructive and non-scalable film

transferring techniques and top-down lithographic patterning techniques post-synthesis. Not only does this process open up the possibility of realizing advanced lateral and vertical direct-grown van der Waals heterostructures with ultra-clean interfaces, it also provides a blueprint for realizing structural engineering and ultra-scaled edge effects within these 2D materials. Utilizing an ultra-thin polymer surface functionalization (PFL) achieved through standard lithographic patterning prior to growth, we demonstrate a facile bottom-up process to selectively grow TMDs films with geometrically defined form factors and pristine edges. As a result of this patterning process, we are able to tune the substrate surface energy which ultimately leads to the preclusion of TMD nucleation and growth in PFL-coated regions. We have demonstrated that our selective-area growth process is compatible with various growth techniques (including metal-organic chemical vapor deposition and oxide powder vaporization) using a variety of different precursors and with multiple UV and electron sensitive resist polymers. Lastly, we have investigated the electrical properties of field-effect transistors (FETs) fabricated on selectively grown MoS<sub>2</sub> channels. In doing so, we have discovered a significant substrate impact on mobility of MoS<sub>2</sub> films directly grown on sapphire substrates, and we propose methods for decoupling MoS<sub>2</sub> films from their growth substrates for improved transistor performance on sapphire.

## Poster 19

---

### Synthetic Heterostructures Based on Two-Dimensional van der Waals Solids

\*Y.-C. Lin<sup>1</sup>, S. M. Eichfeld<sup>1</sup>, R. Addou<sup>2</sup>, N. Lu<sup>2</sup>, R. K. Ghosh<sup>3</sup>, S. Datta,<sup>3</sup> J. Li<sup>4</sup>, R.M. Feenstra<sup>4</sup>, M. J. Kim<sup>2</sup>, R. M. Wallace<sup>2</sup>, and J. A. Robinson<sup>1</sup>

1. Department of Materials Science and Engineering and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, PA 16802 USA

2. Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA

3. Department of Electrical Engineering, The Pennsylvania State University, University Park, PA 16802 USA

4. Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213 USA

**Abstract:** Recently, layered materials became important for ultimate scaling process because of their prominent electrical and optical properties presented in their two-dimensional (2D) limits. Their applications cover the spectrums from Ultraviolet to near Infrared utilized in our daily life. In order to place the electronics made of these exotic materials in reality, synthetic structures that integrate different type of 2D layers need to be developed. On this poster, a series of heterostructures based on graphene, hexagonal boron nitrides (hBN), and semiconducting transition metal dichalcogenides (TMD) atomically thin layers derived from direct growth would be introduced. Epitaxial graphene has been utilized as a template for atomically thin sulfur- and selenium-based TMD and hBN grown by thin film deposition techniques, such as powder vaporization and metal-organic chemical vapor deposition. It provides a surface that is chemically inert and atomically flat that enable van der Waals (vdW) epitaxy that allows different 2D crystals that are largely lattice-mismatched register to each other. Their chemistry and structures are likely unchanged after the process at elevated temperatures. The properties of as-grown vdW heterostructures are fundamentally different to those from the constituent materials due to their

electrical couplings. Depending on their purposes, a vdW heterostructure can serve as photodetectors (various semiconducting monolayer TMD-graphene) and electrical diodes ( $\text{MoS}_2\text{-WSe}_2$  and  $\text{WSe}_2\text{-MoSe}_2$  grown on graphene), where graphene is used as a bottom electrode. The good performances of these devices attribute to the good quality of the as-grown layers as well as clean interfaces between each layer. In addition, by tuning the doping type of underlying graphene electrode, the electron properties of these diodes can also be tuned. These results opened up the possibility of making sophisticated vdW heterostructures for lasers, communications, and high-speed electronics all via direct synthesis.

## Poster 20

---

### Growth, Characterization, Dielectric Integration and Radiation Response of $\text{WSe}_2$

Roger C. Walker II, Sarah M. Eichfeld, Joshua A. Robinson

**Abstract:** Tungsten diselenide ( $\text{WSe}_2$ ) is a layered material existing at the scalable limit of atomically thin, two-dimensional sheets. This semiconductor with a direct, sub-visible band gap ( $E_g = 1.65$  eV) has been proposed for future “post-silicon” opto-electronics. Ultra-thin monolayer  $\text{WSe}_2$  supports space applications due to the minimized interaction probability with cosmic radiation. To achieve this, a suitable growth technique such as metal-organic chemical vapor deposition (MOCVD) must be. In addition to growth of nano-scale  $\text{WSe}_2$  film, an appropriate dielectric material must be selected for device application. It must be electronically compatible with  $\text{WSe}_2$  and be able to grow film morphology on the quasi-inert interface provided by the layered material.  $\text{HfO}_2$ , with a band gap of  $\approx 5$  eV and band offsets  $>1$  eV with  $\text{WSe}_2$ , is a promising candidate material based on its properties and can be grown in films using atomic layer deposition (ALD). To this end, we are exploring the growth of  $\text{WSe}_2$  using MOCVD, its stability to various forms of radiation, and the chemical nature of  $\text{WSe}_2\text{-HfO}_2$  heterostructures. For our experiments,  $\text{WSe}_2$  is grown via MOCVD using tungsten hexacarbonyl and either dimethylselenium or hydrogen selenide as precursors. Key parameters such as precursor ratio, total flow of ambient gas, growth temperature and the substrate surface are used to tune the material growth. Surface characterization techniques such as XPS, AFM and SEM are combined to analyze sample quality and determine optimal growth conditions. Dielectric integration via ALD is carried out at  $110^\circ\text{C}$  using tetrakis(dimethylamido)hafnium and water as precursors.

Our  $\text{WSe}_2$  growth results show that the key parameters allowing for the formation of thin films are the growth temperature and the substrate. At a growth temperature of  $600^\circ\text{C}$ , we are able to obtain nanocrystalline film growth on SiC substrates regardless of surface treatment. In contrast, higher temperatures lead to the growth of individual flakes. Growths on these substrates are being used for ongoing investigations on laser and high-energy ion beam impact on this material. Preliminary results exploring the impact of X-rays and low-energy ion plasma impact are showcased here. We find that long-term exposure to soft X-rays in vacuum leaves the  $\text{WSe}_2$  chemically intact, only creating a small surface potential (i.e. a few volts) in semiconducting or insulating substrates. X-ray-assisted removal of surface oxygen creates a smaller potential (i.e. 100 mV), but can occur on any substrate. Low-energy oxygen ion plasma can be used to rapidly convert  $\text{WSe}_2$  into a layered  $\text{WSe}_2\text{-WO}_x$  hybrid. This appears to be due to a combination of vacancy formation and ion implantation, followed by oxidation upon exposure to

atmosphere. In an unexpected result, selenium oxide was also produced as a byproduct. Preliminary dielectric integration results show that the WSe<sub>2</sub> is not apparently chemically modified during the ALD process. Dielectric layers start as islands nucleating out of surface defects on WSe<sub>2</sub> flakes and then coalesce into films over time. XPS analysis over time shows variation in the film chemistry as it grows, as well as persistent carbon contamination from the hafnium precursor.

## Poster 21

---

### Substrate Coupling and Decoupling in Epitaxial MoS<sub>2</sub> Monolayers

Kehao Zhang<sup>1,2</sup>, Brian M. Bersch<sup>1,2</sup>, Baoming Wang<sup>3</sup>, Ke Wang<sup>4</sup>, Ganesh R. Bhimanapati<sup>1,2</sup>, Aman Haque<sup>3</sup>, Joshua A. Robinson<sup>1,2</sup>

1. *Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA, 16802, United States;*
2. *Center for Two-Dimensional and Layered Materials, The Pennsylvania State University, University Park, PA, 16802, United States;*
3. *Department of Mechanical & Nuclear Engineering, The Pennsylvania State University, University Park, PA, 16802, United States;*
4. *Materials Characterization Laboratory, The Pennsylvania State University, University Park, PA, 16802, United States*

**Abstract:** In recent decades, 2D materials have attracted tremendous interests due to its unique electronic, optoelectronic, optical and piezoelectric properties.<sup>1-3</sup> However, the performance of 2D materials on the electronic devices such as field effect transistors (FETs) is much lower than the theoretical prediction.<sup>4,5</sup> Most MoS<sub>2</sub> based FETs are fabricated on exfoliated MoS<sub>2</sub> and transferred CVD-grown MoS<sub>2</sub>. No FETs with appropriate mobility has been reported on as-grown MoS<sub>2</sub> monolayers on sapphire. The low performance of as-grown MoS<sub>2</sub> is believed to be caused by the strong film-substrate coupling.<sup>6</sup> In this study, we explain the relationship between the epitaxial MoS<sub>2</sub> and the sapphire pre-treatment. Decreasing the surface energy of sapphire after the annealing results in better alignment. The strong film-substrate coupling is visualized by Raman spectroscopy by observing the significant A<sub>1g</sub>/E<sub>2g</sub> ratio change. The PV grown epitaxial MoS<sub>2</sub> exhibits strong local charge transfer in single domains, which results in heavily n-type doped MoS<sub>2</sub>. The extra electrons are considered to be the scattering center and reduce the FET mobility significantly. To remove the film-substrate coupling, water steaming and liquid nitrogen quench is conducted. Both methods are able to remove the extra electrons caused by the film-substrate charge transfer and tune the MoS<sub>2</sub> monolayer to be less n-doped. As a result, the FET mobility is increased by ~100x after the decoupling.

#### Reference:

- (1) Wang, Q. H.; Kalantar-Zadeh, K.; Kis, A.; Coleman, J. N.; Strano, M. S. *Nat. Nanotechnol.* **2012**, 7 (11), 699–712.
- (2) Wu, W.; Wang, L.; Li, Y.; Zhang, F.; Lin, L.; Niu, S.; Chenet, D.; Zhang, X.; Hao, Y.; Heinz, T. F.; Hone, J.; Wang, Z. L. *Nature* **2014**, 514 (7523), 470–474.
- (3) Li, H.; Yin, Z.; He, Q.; Li, H.; Huang, X.; Lu, G.; Fam, D. W. H.; Tok, A. I. Y.; Zhang, Q.; Zhang, H. *Small* **2012**, 8 (1), 63–67.

- (4) Kang, K.; Xie, S.; Huang, L.; Han, Y.; Huang, P. Y.; Mak, K. F.; Kim, C.-J.; Muller, D.; Park, J. *Nature* **2015**, 520 (7549), 656–660.
- (5) Lee, H. S.; Baik, S. S.; Min, S.; Jeon, P. J.; Kim, J. S.; Choi, K.; Ryu, S.; Choi, H. J.; Kim, J. H.; Im, S. *arXiv.org* **2014**, 27.
- (6) Ma, N.; Jena, D. *Phys. Rev. X* **2014**, 4 (1), 011043.

## Poster 22

---

### Electron Beam Nanosculpting of Few-nm-Wide Black Phosphorus Nanoribbons and Nanopores

P. Masih Das, G. Danda, A. Cupo, W.M. Parkin, L. Liang, N. Kharche, X. Ling, S. Huang, M. Dresselhaus, V. Meunier, and M. Drndic

**Abstract:** Black phosphorus (BP) is a highly anisotropic allotrope of phosphorus with great promise for fast functional electronics and optoelectronics. We demonstrate the controlled structural modification of few-layer BP along arbitrary crystal directions with sub-nm precision for the formation of few-nm-wide armchair and zigzag BP nanoribbons. The nanoribbons are fabricated, along with nanopores and nanogaps, using a combined mechanical-liquid exfoliation procedure along with in situ transmission electron microscope (TEM) and scanning TEM nanosculpting. We predict that the few-nm-wide BP nanoribbons realized experimentally possess clear one-dimensional quantum confinement, even for few layer systems. The demonstration of this procedure is key for the development of BP-based electronics, optoelectronics, thermoelectrics, and other applications in reduced dimensions.

## Poster 23

---

### Phosphorene Nanoribbons and Nanopores

Andrew Cupo<sup>1</sup>, Paul Masih Das<sup>2</sup>, Gopinath Danda<sup>2,3</sup>, William M. Parkin<sup>2</sup>, Liangbo Liang<sup>4</sup>, Neerav Kharche<sup>1</sup>, Xi Ling<sup>5</sup>, Shengxi Huang<sup>5</sup>, Mildred Dresselhaus<sup>5</sup>, Marija Drndic<sup>2</sup>, and Vincent Meunier<sup>1</sup>

<sup>1</sup>*Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York, 12180, USA*

<sup>2</sup>*Department of Physics and Astronomy, University of Pennsylvania, Philadelphia, Pennsylvania, 19104, USA*

<sup>3</sup>*Department of Electrical and Systems Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, 19104, USA*

<sup>4</sup>*Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

<sup>5</sup>*Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology, Cambridge, Massachusetts, 02139, USA*

**Abstract:** Single atomically-layered black phosphorus (phosphorene) is promising for nanoelectronic applications due to its direct band gap of 2 eV and carrier mobility of about  $1,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ . Theoretical studies have shown that phosphorene nanoribbons (PNRs) can be used for next generation transistors.

However, obtaining monolayers is difficult due to strong interlayer forces. Our band structure calculations show that the electronic properties of nanoribbons resulting from in-plane confinement are preserved in the phosphorene to bulk transition, justifying the use of multi-layered samples. Furthermore, nanopores in phosphorene can be used for DNA sequencing with spatial resolution comparable to single atomic layers, while preventing noise from high frequency sampling due to the presence of a band gap. Experiments indicate preferential expansion of nanopores in few-layer black phosphorus along the zigzag direction under symmetric irradiation. We demonstrate that the energy barrier for removing atoms from the most stable known zigzag edge of phosphorene is greater than that for the armchair edge, which predicts a comparatively faster recession of the armchair edge and therefore confirms the formation of a relatively longer zigzag edge in experiments.

## Poster 24

---

### Study of Noble Gases adsorption on Single-Walled Carbon Nanotubes

J. R. Alves da Cunha,<sup>\*,†,‡,¶,⊥</sup> Néstor Perea-Lopez,<sup>†,‡</sup> Ana Laura Elías,<sup>†,‡</sup> Victor Carozo,<sup>†,‡</sup> Paulo T. Araujo,<sup>%</sup> M. C. dos Santos,<sup>#</sup> and Mauricio Terrones<sup>\*,†,§,⊥,∥</sup>

<sup>†</sup> Department of Physics, The Pennsylvania State University, University Park, PA 16802, USA

<sup>‡</sup> Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, PA 16802, USA

<sup>¶</sup> Faculdade de Ciências Exatas e Naturais, Universidade Federal do Pará, Campus Universitário de Tocantins, PA 68.400-000, Brazil

<sup>%</sup> Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, AL 35487, USA

<sup>#</sup> Instituto de Física, Universidade de São Paulo, SP 05508-090, Brazil

<sup>§</sup> Department of Chemistry, The Pennsylvania State University, University Park, PA 16802, USA

<sup>⊥</sup> Department of Materials Sciences and Engineering, The Pennsylvania State University, University Park, PA 16802, USA

<sup>∥</sup> Institute of Carbon Science and Technology, Shinshu University, 4-17-1 Wakasato, Nagano-city 380-8553, Japan

**Abstract:** The adsorption of noble gases on carbon nanotubes (CNTs) is still a very active research field. Carbon nanostructures are suitable substrates to study different phases of noble-gas adsorbents. In this work, we investigate the adsorption of Argon (Ar), and Xenon (Xe) to the surfaces of Single-Walled Carbon Nanotubes (SWCNTs). Our strategy is to observe the shift of phonons frequencies observed in the Raman spectra of Ar and Xe adsorbed on (SWCNTs) bundles. Measurements were performed at 20 K using the laser lines 488 nm, 514.5 nm and 785 nm. At 20K, the Raman frequencies are up shifted due the gas solidification in the external grooves sites and external surfaces. The shifts obtained are consistent with physical adsorption where the interactions adsorbate-SWCNTs arise from “van der Waals” forces. The small up shift of the G<sup>+</sup> band would seem to rule out charge transfer under our experimental conditions.

*Poster 25*

---

## **DNA Translocation Through Tungsten Disulfide Nanopores**

G. Danda, P. Masih Das, Y.C. Chou, J. Mlack, C. Naylor, N. Perea-Lopez, Z. Lin, J.P. Thiruraman, C.C. Chien, L.B. Fulton, M. Terrones, A.T.C. Johnson, and M. Drndić

**Abstract:** Advances in solid-state nanopore sensor systems for DNA detection and analysis have been supported by using increasingly thinner materials to the point of utilizing atomically thin two-dimensional materials such as graphene. The recent fabrication and operation of nanopores in MoS<sub>2</sub> have opened up the possibility of using transition metal dichalcogenides (TMDs) as nanopore sensor materials. We first fabricate suspended WS<sub>2</sub> nanopore devices with sub-10 nm pore diameters using a novel nanomaterial transfer method. We also perform DNA translocation experiments to better understand the performance of TMD-based nanopore sensors.

*Poster 26*

---

## **Synthesis of Large-Scale Atomic Layer SnS<sub>2</sub> Through Chemical Vapor Deposition Method**

Gonglan Ye  
Rice University

**Abstract:** Two-dimensional layers of metal dichalcogenides have attracted much attention because of their ultrathin thickness and potential applications in electronics and optoelectronics. Monolayer SnS<sub>2</sub>, with a band gap of ~ 2.6 eV, has an octahedral lattice made of two atomic layers of sulfur and one atomic layer of tin. So far, there are limited reports on the growth of large scale and high quality SnS<sub>2</sub> atomic layers and study of their properties as semiconductor. Here, we report a chemical vapor deposition (CVD) growth of atomic layer SnS<sub>2</sub> with large crystal size and uniformity. In addition, layer number can be controlled from monolayer to few layers and to bulk by changing the growth time. Scanning transmission electron microscopy (STEM) was used to analyze the atomic structure and demonstrate the 2H stacking order of different layers. The resultant SnS<sub>2</sub> film is used as a photodetector with external quantum efficiency as high as 150%, suggesting promise for optoelectronic applications.

*Poster 27*

---

## **Substrate Screening Induced Renormalization of Excited-States in 2D Materials**

N. Kharche and V. Meunier

*Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, United States*

**Abstract:** Two-dimensional (2D) materials offer an emerging platform for exploring novel electronic phenomena in reduced dimensionality systems. Owing to their atomic scale thickness, the excitation energy levels in 2D materials are strongly renormalized due to the screening by the surrounding environment. This effect is expected to have strong impact when the 2D materials are integrated into functional devices. Accounting for such long-range screening requires methods beyond density functional theory (DFT), such as the GW approach, which are computationally too expensive for large-scale calculations including realistic substrates. To address this important issue, we develop an integrated first-principles computational approach combining DFT, the GW approximation, and a semi-classical image-charge model to compute the electronic band gaps in planar 2D systems in weak interaction with the underlying substrate, including long-range screening effects, in a computationally tractable manner. This methodology is general for any planar 2D system and we apply it here to the specific case of graphene nanoribbons (GNRs) since accurate experimental data exist. We find that the band gap of substrate-supported GNRs is reduced by several tenths of an eV compared to their isolated counterparts, with a width- and orientation-dependent renormalization. The predicted band gaps are in good agreement with the range of available experimental data on substrate-supported armchair GNRs. Our results indicate that the band gaps in GNRs can be tuned by controlling the electronic screening at the interface and suggest the interesting possibility of using spatially varying dielectric environment to engineer the screening effects and induce band offsets into 2D materials without any chemical modification.

*Poster 28*

---

## **Elucidating the Electronic Properties of Solution-Synthesized Colloidal 2D Tin(II) Sulfide**

A.J. Biacchi, S.T. Le, B.G. Alberding, J.A. Hagmann, S.J. Pookpanratana, S. Chowdhury, E.J. Heilweil, C.A. Richter, and A.R. Hight Walker

**Abstract:** 2D nanostructures are an important class of materials that has seen an explosion of interest in recent years due to their unique optoelectronic properties in conjunction with their morphology, which lends itself well for incorporation into nanoscale devices. To date, the vast majority of nanoscale 2D materials are synthesized by mechanical exfoliation or gas phase deposition techniques. Alternatively, colloidal-based solution syntheses offer a scalable and cost-efficient means of producing nanomaterials in high yield. While much progress has been made in engineering nanostructured materials in solution, it still remains a substantial challenge to fully characterize their electronic properties. This is largely due to their small dimensions, which usually require the formation of polycrystalline colloidal assemblies or films prior to performing carrier transport measurements. However, such a strategy does not allow for the

deconvolution of the intrinsic carrier transport within individual crystals from the transfer between separate colloids. Here we present the synthesis of 2D post-transition metal chalcogenide nanomaterials and a thorough investigation of the inherent electronic properties of individual crystals. First, we detail the development of a novel solution chemistry-based synthetic approach to produce nearly-monodisperse tin(II) sulfide (SnS) nanoribbons and nanosheets. Next, we describe the chemical and structural characterization of these nanomaterials, and how they are processed from solution to fabricate back-gated, single-crystalline, solid-state devices. Finally, we interrogate their electronic properties by a combination of multi-point contact probe transport measurements and time-resolved terahertz spectroscopy. These studies allow for the direct determination of the materials' carrier concentration, carrier mobility, resistivity, and the majority carrier type, which have been rarely reported for individual colloiddally-synthesized nanostructures.

## Poster 29

---

### **Analysis of Strain In Graphene-based Systems by Tip-Enhanced Raman Mapping**

E. L. Wood<sup>1</sup>, Y. Yang<sup>1</sup>, W. Gannett<sup>2</sup>, G. A. Shaw<sup>1</sup>, R. E. Elmquist<sup>1</sup>, M. W. Keller<sup>2</sup>, A. R. Hight Walker<sup>1</sup>

<sup>1</sup>*National Institute of Standards and Technology, Gaithersburg, MD, USA*

<sup>2</sup>*National Institute of Standards and Technology, Boulder, CO, USA*

erin.wood@nist.gov

**Abstract:** Understanding the effects of localized strain on the electronic, magnetic and optical properties in graphene is of paramount importance to designing robust devices. Confocal Raman spectroscopy has been the tool of choice for rapid, non-destructive characterization of graphene, both in relaxed and strained states, however this technique is diffraction limited to spot sizes of roughly 1 micron. Conversely, atomic force microscopy (AFM) has been used to investigate plastic deformation and has offered great insight to the deformation mechanics beyond the diffraction limit, but offers only limited chemical information. Utilizing special AFM tips comprised of a Raman-enhancing dielectric matrix, we are able to exploit the strengths of both techniques and gain sub-diffraction, chemical information with the sensitivity of Raman spectroscopy simultaneously with the topographical mapping of AFM, also known as tip-enhanced Raman spectroscopy or TERS. In this poster, we first demonstrate the spatial resolution increase using a strained silicon engineered test structure, which is enabled by our capability of working in a 180° backscattering configuration owing to our tuning-fork-based AFM. We then apply strain in as-grown graphene on various substrates, through indentation methods and investigate it with TERS, monitoring the shift in G' band within and around the plastic zone. We confirm that areas in which the substrate has been plastically deformed by the indentation the position of the G' band has shifted to lower wavenumber, indicating tensile strain. However, we also monitor that the strain, as indicated by Raman shift, extends beyond the plastic zone. We also show that the increase in spatial resolution affords better agreement between the topography and Raman strain mapping, validating TERS as a technique for sub-micron strain analysis.

*Poster 30*

---

## **Transfer Characteristics and Low-Frequency Noise In Single- and Multi- Layer MoS<sub>2</sub> Field-Effect Transistors**

D. Sharma<sup>1-3</sup>, A. Motayed<sup>1-4</sup>, P.B. Shah<sup>5</sup>, M. Amani<sup>5</sup>, M. Georgieva<sup>5</sup>, A.G. Birdwell<sup>5</sup>, M. Dubey<sup>5</sup>, Q. Li<sup>3</sup>, and A.V. Davydov<sup>1</sup>

<sup>1</sup>Material Measurement Laboratory, NIST, Gaithersburg, MD

<sup>2</sup>Theiss Research, Inc., La Jolla, CA

<sup>3</sup>Department of Electrical and Computer Eng., George Mason University, Fairfax, VA

<sup>4</sup>IREAP, University of Maryland, College Park, MD

<sup>5</sup>Sensors and Electron Devices Directorate, ARL, Adelphi, MD

**Abstract:** Leveraging nanoscale field-effect transistors (FETs) in integrated circuits depends heavily on its transfer characteristics and low-frequency noise (LFN) properties. Here, we report the transfer characteristics and LFN in FETs fabricated with molybdenum disulfide (MoS<sub>2</sub>) with different layer (L) counts. 4L to 6L devices showed highest I<sub>ON</sub>-I<sub>OFF</sub> ratio ( $\approx 10^8$ ) whereas LFN was maximum for 1L device with normalized power spectral density (PSD)  $\approx 1.5 \times 10^{-5}$  Hz<sup>-1</sup>. For devices with L  $\approx 6$ , PSD was minimum ( $\approx 2 \times 10^{-8}$  Hz<sup>-1</sup>). Further, LFN for single and few layer devices satisfied carrier number fluctuation (CNF) model in both weak and strong accumulation regimes while thicker devices followed Hooge's mobility fluctuation (HMF) model in the weak accumulation regime and CNF model in strong accumulation regime, respectively. Transfer-characteristics and LFN experimental data are explained with the help of model incorporating Thomas-Fermi charge screening and inter-layer resistance coupling.

*Poster 31*

---

## **Effect of Photo-Generated Carriers on Electronic Transport Properties of Multi-Layer Molybdenum Disulphide Nano-Sheet MOSFETs**

A. Razavieh<sup>1</sup> and S. Das<sup>1</sup>

<sup>1</sup>Department of Engineering Science and Mechanics, Pennsylvania State University, State College, PA 16802

**Abstract:** Layered 2-D materials have attracted a great deal of attention due to their unique electronic and optical properties. Although, there has been a lot of effort to explore their excellent potential for optical sensing applications beyond conventional approaches, less attention has been paid to electronic transport properties of 2-D photo-transistors. This work investigates the effect of photo-generated carriers on electronic transport properties of multi-layer MoS<sub>2</sub> MOSFETs through a combination of experiments and simulations. Specifically, the effect of photo-generated electrons and holes on device current is studied for different bias and transport conditions. While experimental and simulation data are consistent the current increase in the on-state and pseudo DIBL effects in the off-state of the experimental data can be precisely explained by modeling the photo-generated electron and hole current components in the vicinity of source and drain Schottky barriers. This work also investigates the above phenomena in long and short channel transistors.

*Poster 32*

---

## **Understanding the Formation of Monolayer Transition Metal Dichalcogenide Films Via a Substrate-Assisted Electrochemical Process**

Daniel Schulman, Dan May-Rawding, Saptarshi Das

**Abstract:** A recent report demonstrated a self-limiting, electrochemical process to create single-layer 2D transition metal dichalcogenides (TMDs) from mechanically exfoliated materials at dimensions approaching mm scale. The critical TMD-titanium nitride (TiN) substrate-assisted process is yet to be fully explained. Here, we report on how factors such as TiN deposition technique, post-deposition processing, and stoichiometric composition control the effectiveness of this process. Potentiostatic and potentiodynamic voltammetry elucidate on different aspects of the electro-ablation process and allow us to understand the detail chemical pathways associated with this process. In addition, high resolution XPS, Raman, photoluminescence and AFM mapping are used to study the monolayer formation and quality for a variety of TMD materials and substrates. These recent results are compared with previously reported DFT and Adaptive Bias Force simulation results supporting a  $H_2O_2$  mediated etching process. Finally, novel applications for the monolayer TMDs obtained through the EA process are proposed.

[1] Das, S. et al “A Self-Limiting Electro-Ablation Technique for the Top-Down Synthesis of Large-Area Monolayers of 2D Materials”, under review, *Nature Scientific Report*, 2016.

*Poster 33*

---

## **Thermodynamic Calculation and Practical Pathways In Controlled Oxidation, Etching and Sulfurization of Transition Metal Dichalcogenides**

Hamed Simchi, Timothy Walter, Frances Kwok and Suzanne E. Mohny

**Abstract:** Transition metal dichalcogenides (TMDs) have attracted a lot of interest in recent years due to their unique electrical, optical, and thermal properties resulting from their distinctive structure. Still, processing of these materials for electronic devices is immature. In this study, thermodynamic calculations were used as a tool for predicting processing conditions for a) oxidation and etching of TMDs and b) sulfurization of selected transition metals (V, Nb, Ta, Mo, W, Re). Thermodynamic predictions have helped guide experiments for the controlled processing and synthesis of TMDs. Samples have been analyzed using light microscopy, scanning electron microscopy, atomic force microscopy, and X-ray photoelectron spectroscopy. Good agreement between predictions and experiments has mostly been observed.

*Poster 34*

---

## Mapping Near-Field Environments of Plasmonic and 2-D Materials With Photo-Induced Force Imaging

T. U. Tumkur<sup>1</sup>, C. Doiron<sup>1</sup>, B. Li<sup>2</sup>, D. Swearer<sup>3</sup>, B. Cerjan<sup>4</sup>, X. Yang<sup>4</sup>,  
P. Nordlander<sup>4,1,2</sup>, N. H. Halas<sup>1,2,3,4</sup>, P. M. Ajayan<sup>2,3</sup>, E. Ringe<sup>2,3</sup>, I. Thomann<sup>1,2,3</sup>

<sup>1</sup>Department of Electrical and Computer Engineering, <sup>2</sup>Department of Materials Science and Nanoengineering, <sup>3</sup>Department of Chemistry, <sup>4</sup>Department of Physics, Rice University, Houston, Texas, USA.

Isabell.thomann@rice.edu

**Abstract:** We demonstrate the ability to map photo-induced gradient forces in materials, using a setup akin to atomic force microscopy. This technique allows for the simultaneous characterization of topographical features and optical near-fields in materials, with a high spatio-temporal resolution. We show that the near-field gradient forces can be translated onto electric fields, enabling the mapping of plasmonic hot-spots in gold nanostructures, and the resolution of sub-10 nm features in photocatalytic materials. We further show that the dispersion-sensitive nature of near-field gradient forces can be used to image and distinguish atomically thin layers of 2-D materials with high contrast.

*Poster 35*

---

## A Silicon-Based Two-Dimensional Chalcogenide: Growth of Si<sub>2</sub>Te<sub>3</sub> Nanoribbons, Nanoplates and Nanocrystals

Sean Keuleyan<sup>2</sup>, Mengjing Wang<sup>1</sup> (presenter) and Kristie J. Koski<sup>1</sup>

1. Department of Chemistry, Brown University, Providence, RI, 02912, USA

2. Voxel Nano, Beaverton, Oregon, USA

**Abstract:** We report the synthesis of high-quality single crystal two-dimensional, layered nanostructures of silicon telluride, Si<sub>2</sub>Te<sub>3</sub>, in multiple morphologies through VLS and colloidal methods. Morphologies include nanoribbons formed by VLS growth from Te droplets, vertical hexagonal nanoplates through vapor–solid crystallographically oriented growth on amorphous oxide substrates and flat hexagonal nanoplates formed through large-area VLS growth in liquid Te pools. Morphologies of nanorods can also be formed by colloidal reactions between Te and hexachlorodisilane. We show that the material may be modified after synthesis, including both mechanical exfoliation to as few as five layers and intercalation of metal ions including Li<sup>+</sup> and Mg<sup>2+</sup>, which suggests applications in energy storage materials. The material exhibits an intense red color corresponding to its strong and broad interband absorption extending from the red into the infrared. Si<sub>2</sub>Te<sub>3</sub> enjoys chemical and processing compatibility with other silicon-based material including amorphous SiO<sub>2</sub>, which suggests applications in silicon-based devices ranging from fully integrated thermoelectrics to optoelectronics.

*Poster 36*

---

**Observation of Interlayer Phonons in Transition Metal Dichalcogenide Atomic Layers and Heterostructures**

Gaihua Ye<sup>1</sup>, Zhipeng Ye<sup>1</sup>, Chun Hung Lui<sup>2</sup>, and Rui He<sup>1</sup>

<sup>1</sup>*Department of Physics, University of Northern Iowa, Cedar Falls, Iowa 50614, USA*

<sup>2</sup>*Department of Physics, University of California, Riverside, 900 University Avenue, Riverside, California 92521, USA*

**Abstract:** Interlayer phonon modes in atomically thin transition metal dichalcogenide (TMD) heterostructures were observed for the first time [1]. We measured the low-frequency Raman response of MoS<sub>2</sub>/WSe<sub>2</sub> and MoSe<sub>2</sub>/MoS<sub>2</sub> heterobilayers. We discovered a distinctive Raman mode (30 - 35 cm<sup>-1</sup>) that cannot be found in any individual monolayers. By comparing with Raman spectra of bilayer (2L) MoS<sub>2</sub>, 2L MoSe<sub>2</sub> and 2L WSe<sub>2</sub>, we identified the new Raman mode as the layer breathing mode (LBM) arising from the perpendicular vibration between the two TMD layers. The LBM only emerges in bilayer regions with atomically close layer-layer proximity and clean interface. In addition, the LBM frequency exhibits noticeable dependence on the relative orientation between the two TMD layers, which implies a change of interlayer separation and interlayer coupling strength with the layer stacking.

We also investigated the ultralow-frequency Raman response of atomically thin ReS<sub>2</sub>, a special type of TMD with unique distorted 1T structure [2]. We found that the two shear modes in bilayer ReS<sub>2</sub> are nondegenerate and clearly resolved in the Raman spectrum, in contrast to the doubly degenerate shear modes in other two-dimensional materials. By carrying out comprehensive first-principles calculations, we can account for the frequency and Raman intensity of the interlayer modes and determine the stacking order in bilayer ReS<sub>2</sub>. Few-layer ReS<sub>2</sub> exhibits rich Raman peaks at frequencies below 50 cm<sup>-1</sup>, where a panoply of interlayer shear and breathing modes are observed.

References

- [1] C. H. Lui, Z. Ye, C. Ji, K.-C. Chiu, C.-T. Chou, T. I. Andersen, C. Means-Shively, H. Anderson, J.-M. Wu, T. Kidd, Y.-H. Lee, and R. He, "Observation of interlayer phonon modes in van der Waals heterostructures," *Physical Review B* 91, 165403 (2015).
- [2] R. He, *et al.*, "Coupling and stacking order of ReS<sub>2</sub> atomic layers revealed by ultralow-frequency Raman spectroscopy," *Nano Letters* 16, 1404 (2016).

*Poster 37*

---

## Activation Energies of Rotational Defects in 2D Transition Metal Dichalcogenides

Anthony Yoshimura and Vincent Meunier

Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, New York 12180, United States

**Abstract:** Owing to their outstanding electrical and optical properties, two-dimensional (2D) transition metal dichalcogenides (TMDs) are promising for a wide array of applications in electronics, photonics, and energy harvesting. As with any material, 2D TMDs are subject to structural defects, which can modify their physical properties. It is therefore important to understand the conditions in which these defects can occur. Here we examine two types of defects in the pristine trigonal-prismatic TMD lattice: chalcogen vacancies and bond rotations. Chalcogen vacancies are one of the most common defects in any TMD lattice, as the removal of a chalcogen atom has a low energy barrier. A unique cluster of these vacancies enables a more complicated rotational defect to occur. This defect arises from a 60-degree rotation about the surface normal of the bonds on a metal atom centered in a six-vacancy cluster. The resulting structure is a three-fold symmetric set of three 8-membered rings subtended by the central metal atom. This extended defect has been recently observed in WSe<sub>2</sub>, WS<sub>2</sub> and MoSe<sub>2</sub>. Using density functional theory (DFT), we calculate the activation energy for these defects in several TMDs: MoS<sub>2</sub>, MoSe<sub>2</sub>, MoTe<sub>2</sub>, WS<sub>2</sub>, WSe<sub>2</sub>, and WTe<sub>2</sub>. We find that the activation energy for both chalcogen vacancies and rotational defects depends primarily on the chalcogen species, with sulfur having the largest and tellurium the smallest activation energy. Furthermore, we find that the chalcogen species also determines the thermodynamic stability of the rotational defect, with tellurium being the most stable and sulfur being the least.

*Poster 38*

---

## Influence of Substrate and Growth Conditions on Metalorganic Chemical Vapor Deposition of Tungsten Diselenide Thin Films

Xiaotian Zhang<sup>1</sup>, Sarah M. Eichfeld<sup>1,2</sup>, Joshua A. Robinson<sup>1,2</sup> and Joan M. Redwing<sup>1</sup>

1. Department of Materials Science and Engineering, The Pennsylvania State University, State College, PA, 16801, USA

Center for 2-Dimensional and Layered Materials, Materials Research Institute, The Pennsylvania State University, State College, PA, 16801, USA

**Abstract:** The development of electronic and optoelectronic devices based on transition metal dichalcogenides (TMDs) requires the ability to form large area, uniform films of monolayer or few layer thickness. We previously demonstrated the use of metalorganic chemical vapor deposition (MOCVD) for the scalable synthesis of WSe<sub>2</sub> thin films on a variety of substrates including sapphire and epitaxial graphene. In this work, we focus on understanding the effects of precursor chemistry, growth conditions and substrate type on the film growth and properties. WSe<sub>2</sub> films and monolayers were grown by

MOCVD using tungsten hexacarbonyl ( $W(CO)_6$ ) and dimethyl selenium ( $(CH_3)_2Se$ ) as precursors on sapphire and oxidized silicon substrates in a cold wall vertical reactor. The developed process is able to prepare samples ranging from  $WSe_2$  domains that exhibit vibrational modes and strong room temperature photoluminescence ( $PL:E_{2g}=8.5$ ) consistent with monolayer material to fully-coalesced 15 nm thick  $WSe_2$  films that are highly c-axis oriented on sapphire. Additionally, impacts of substrate temperature and total gas flow rate have also been investigated. The deposition of  $WSe_2$  starts at substrate temperatures of 400°C, where films exhibit a nanocrystalline form. In contrast, highly c-axis oriented and large grain size  $WSe_2$  films are produced at substrate temperatures of 800°C. A high total gas flow rate which reduces the gas phase supersaturation of precursors leads to a reduction in secondary nucleation on the monolayers but also decreases the grain size of the  $WSe_2$  domains. Finally, we find that  $WSe_2$  domains show vertical orientation on thermal oxide silicon substrate at high temperature while they remain lateral growth on sapphire substrate.

## Poster 39

---

### Synthesis and Characterization of Cvd-Grown Multilayer Graphene Nanoribbons

Kazunori Fujisawa<sup>1</sup>, Yu Lei<sup>2</sup>, Cheon-Soo Kang<sup>3</sup>, Ana Laura Elias<sup>1,4</sup>,  
Hiroyuki Muramatsu<sup>3</sup>, Takuya Hayashi<sup>3</sup>, and Mauricio Terrones<sup>1,2,4,5</sup>

<sup>1</sup>(Department of Physics, The Pennsylvania State University, University Park, Pennsylvania 16802, USA)

<sup>2</sup>(Department of Materials Science and Engineering & Materials Research Institute, The Pennsylvania State University, University Park, Pennsylvania 16802, USA)

<sup>3</sup>(Faculty of Engineering, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan)

<sup>4</sup>(Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, Pennsylvania 16802, USA)

<sup>5</sup>(Department of Chemistry, The Pennsylvania State University, University Park, Pennsylvania 16802, USA)

**Abstract:** Electronic structure of carbon material changes depending on its morphological structure. For example diamonds behave as insulator, graphene behave as conductor, and some carbon nanotubes behave as semiconductor. Graphene nanoribbon (GNR) is a ribbon shaped 1D graphene and both of semiconducting and metallic behaviors are predicted. GNR have been prepared by lithography assisted top-down cutting of graphene, oxidation-assisted chemical unzipping of carbon nanotubes and chemical synthesis. Here we report novel synthesis of multilayer GNR with around 10 nm of width. The CVD technique have been used for bulk production of carbon nanotubes, thus this technique is promising for bulk production of GNR. The synthesized GNR was characterized by Raman spectroscopy and high resolution transmission electron microscopy (HR-TEM). HR-TEM revealed that the layers of GNRs are randomly stacked rather than AB stacking. The prominent 2D peak in Raman spectra indicate that the GNR exhibit Dirac cone and the 4-fold higher D band than G band corresponds to exposed edge structure. This edge exposed multilayered GNR can be a promising material for electronics or catalyst support.

*Poster 40*

---

## Ultrasensitive Molecular Sensor Using N-doped Graphene through Enhanced Raman Scattering

Simin Feng<sup>1</sup>, Maria Cristina dos Santos<sup>2</sup>, Bruno R. Carvalho<sup>1,3</sup>, Ruitao Lv<sup>4</sup>, Kazunori Fujisawa<sup>1</sup>, Ana Laura Elias<sup>1</sup>, Yu Lei<sup>1</sup>, Nestor Perea Lopez<sup>1</sup>, Marcos A. Pimenta<sup>3</sup> and Mauricio Terrones<sup>1,5,6\*</sup>

<sup>1</sup>*Department of Physics and Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, University Park, PA 16802, USA*

<sup>2</sup>*Instituto de Física, Universidade de São Paulo, São Paulo, SP, Brazil*

<sup>3</sup>*Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais, 30123-970, Brazil*

<sup>4</sup>*Key Laboratory of Advanced Materials (MOE), School of Materials Science and Engineering, Tsinghua University, Beijing, 100084, P. R. China*

<sup>5</sup>*Department of Chemistry, Department of Material Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA*

<sup>6</sup>*Research Center for Exotic Nanocarbons, Shinshu University, Wakasato 4-17-1, Nagano-city 380-8553, Japan*

**Abstract:** As a novel and efficient surface analysis technique, graphene enhanced Raman scattering (GERS) has attracted increasing research attention in recent years. In particular, chemically doped graphene demonstrates much enhanced GERS effects than pristine graphene (PG) and it can be used to efficiently detect trace amount of molecules. However, the GERS mechanism is still an open question. Here, we present a comprehensive study on the GERS effect of PG and nitrogen-doped graphene (NG). By controlling the N-doping in NG, the Fermi level of graphene shifts, and if this shift aligns with the lower unoccupied molecular orbital (LUMO) of a molecule, charge transfer is enhanced, thus significantly amplifying the molecule vibrational Raman modes. We confirmed these findings using different organic fluorescent molecules: Rhodamine B (RhB), Crystal Violet (CRV) and Methylene Blue (MB). Interestingly, Raman signals from these dye molecules can be detected even for concentrations as low as  $10^{-11}$  mol/L, thus providing excellent molecular sensing capabilities. In order to explain our results, these NG-molecule systems were modeled using dispersion corrected density functional theory. Furthermore, we demonstrated that when using different laser excitations, it is possible to determine the gaps between the higher occupied and the lower unoccupied molecular orbitals (HOMO-LUMO) of different molecules. This work clearly demonstrates that N-doped graphene has enormous potential when detecting low concentrations of molecules and could also effectively identify their HOMO-LUMO gaps.

## Poster 41

---

### **Electric Field Directed Self-Assembly of 2D TMDs**

**Donna Deng**<sup>‡</sup>, Zhong Lin<sup>†</sup>, Chanjing Zhou, Jie Li<sup>\*</sup>, Ana L. Elias<sup>†</sup>, Nestor Perea<sup>†</sup>, Kehao Zhang<sup>‡</sup>, Jeffrey Mayer<sup>\*</sup>, Theresa S. Mayer<sup>\*</sup>, Mauricio T. Terrones<sup>†</sup> – <sup>\*</sup>Department of Electrical Engineering, <sup>†</sup>Department of Physics, <sup>‡</sup>Department of Materials Science and Engineering – *Penn State University*

**Abstract:** Manipulation of 2D materials onto a substrate for post-processing have been dominated by exfoliation or direct transfer methods, both of which are time consuming and impractical for fabricating arrays of TMDs necessary for large scale device circuitry. An alternative method is electric-field assisted directed self-assembly of monolayer TMDs from a suspension onto a substrate by utilizing dielectrophoretic forces. This method produces a large-area dense array of flat, wrinkle free monolayer TMDs. Not only does self-assembly provide a way to control positioning of the sheets, a clear orientation preference is observed when the sheets have clearly defined polygon shapes, and is confirmed using semi-analytical calculations for triangular monolayers. We confirm through optical characterization that this method does not damage the monolayers.

## Poster 42

---

### **Strain-Lattices in Graphene and a New Path to Silicene Synthesis: Presenting our Recent Work in the Exploration of 2D Materials with STM and STS**

Ehsan Monazami, Cameron Volders, Gopalakrishnan Ramalingam and Petra Reinke  
*Department of Materials Science and Engineering, University of Virginia*

**Abstract:** In this presentation we will show two different lines of inquiry we are currently pursuing, and which hold considerable promise for graphene manipulation on one hand, and advancing the integration and synthesis of silicene on the other hand. Both experiments were performed in-situ and we used Scanning Tunneling Microscopy and Spectroscopy to assess geometric and electronic structure.

Graphene is one of the most intriguing materials for understanding and manipulating charge carrier transport in Dirac system. Despite numerous theoretical predictions, that local deformation of the graphene layer can be used to modulate charge carrier transport, the experimental realization of deformation fields on the nanoscale has proven very difficult. We introduce here a new approach, which is based on the intercalation of fullerene molecules at the graphene-substrate (Cu(001) in our experiment) interfaces to introduce local deformations in a controlled manner (Nanoletters **15**, 7421 (2015)). The intercalation can be controlled and amorphous and crystalline intercalated structures can be made, where the crystalline structure has a square symmetry. We will illustrate how the interplay between graphene-substrate and graphene-molecule interactions influence the local deformation, and will discuss all aspects of intercalant structure geometry. The crystalline intercalant structure shows a superlattice peak in the electronic structure, which is critical for charge carrier transport manipulation.

Silicene is much less studied than its carbon counterpart, and while a silicene-based transistor has recently been demonstrated, the integration of silicene in device structures and assessment of its electronic structure remains challenging. The vast majority of silicene growth has been pursued on Ag-single crystal substrates, which hinders many aspects of silicene research. We have discovered a new pathway for silicene synthesis, which uses the (0001) surface of hexagonal  $\text{MoSi}_2$ . This surface has a silicene-like reconstruction (SLR), and we will illustrate with detailed analysis of the surface structure, that this reconstruction is indeed identical to a low-buckled silicene. The SLR is produced by synthesis of the  $\text{MoSi}_2$  crystallites on a Si(001) surface and subsequent annealing - the Si-surface layer relaxes to a full silicon termination and a low buckling structure dominates for crystallites larger than about 15 nm. We will discuss possible approaches to obtain a large continuous layer, and offer this new route of silicene synthesis as an alternative approach to silicene integration.

## Poster 43

---

### 2D Materials Theory and Computation

Arunima K. Singh (NIST); Francesca Tavazza (NIST); Albert V. Davydov (NIST); Benjamin P. Burton (NIST); Richard G. Hennig (UF); Lincoln J. Lauhon (NU)

**Abstract:** The discovery of graphene has led to an explosion in research efforts towards other two-dimensional (2D materials). 2D materials not only represent the ultimate scaling in the vertical direction, but also show a variety of novel and useful electronic, optical, and mechanical properties. In this poster, using a variety of examples, we highlight the strength of *ab-initio* simulations in not only supplementing experimental efforts but also in providing invaluable guidance to discovery, characterization and synthesis of 2D materials.

First, we present a density-functional theory based discovery of the pyrite-structure of monolayer  $\text{PdS}_2$  and  $\text{PdSe}_2$ , and characterization of their energetic, dynamic, electronic and spectroscopic properties [1]. Second, using density-functional theory simulations we identify  $\text{Al}_2\text{O}_3$  as a suitable substrate and a dielectric for  $n$ -layer  $\text{MoS}_2$  [2]. Thirdly, we develop a python based open-source tool for high-throughput screening of substrates for synthesis and functionalization of 2D materials [3]. Fourth, we predict entropy stabilized incommensurate phases in the system  $\text{MoS}_2$ - $\text{MoTe}_2$  [4]. Lastly, in conjunction with experimental measurements, we demonstrate the success of atom probe tomography in identifying Ag dopants in layered 2D material  $(\text{PbSe})_5(\text{Bi}_2\text{Se}_3)_3$  [5], thereby significantly advancing the knowledge of structure-property relationships in 2D materials.

[1] Arunima K. Singh, Richard G. Hennig, The pyrite structure of  $\text{PdS}_2$  and  $\text{PdSe}_2$  monolayers, APS March Meeting (2016). [2] Arunima K. Singh, Richard G. Hennig, Albert V. Davydov, and Francesca Tavazza. " $\text{Al}_2\text{O}_3$  as a suitable substrate and a dielectric layer for  $n$ -layer  $\text{MoS}_2$ ." *Applied Physics Letters* 107, no. 5: [053106 \(2015\)](#). [3] Arunima K. Singh, Kiran Mathew, Albert V. Davydov, Richard G. Hennig, and Francesca Tavazza. "High-throughput screening of substrates for synthesis and functionalization of 2D materials." In *SPIE Nanoscience+ Engineering*, pp. [955316-955316](#). International Society for Optics and Photonics, (2015). [4] Benjamin P. Burton, and Arunima K. Singh. "Prediction of entropy stabilized incommensurate phases in the system  $\text{MoS}_2$ - $\text{MoTe}_2$ ." *arXiv preprint arXiv:1508.01423* (2015). [5] Xiaochen Ren, Arunima K. Singh, Lei Fang, Albert Davydov, Francesca Tavazza, Mercuri G. Kanatzidis and Lincoln J. Lauhon; Atom Probe Tomography Analysis of Doping in 2-D Materials, MRS Fall Meeting (2015)