

Tuesday Afternoon, November 5, 2024

2D Materials

Room 122 - Session 2D+LS+NS+SS-TuA

Electronics Properties

Moderators: Masa Ishigami, University of Central Florida, Slavomir Nemsak, Advanced Light Source, Lawrence Berkeley National Laboratory

2:15pm **2D+LS+NS+SS-TuA-1 NanoARPES for the Study of 2D Materials, Aaron Bostwick**, Advanced Light Source, Lawrence Berkeley National Laboratory **INVITED**

Angle-resolved photoemission spectroscopy (ARPES) is the premier technique for the determination of the electronic bandstructure of solids, and has found wide application for many classes of materials, such as oxides, semiconductors, metals, and low-dimensional materials and surfaces. Among the important topics it addresses are the underlying many-body interactions that determine the ground and excited state functionalities of all materials. Recently the development of nanoARPES using microfocused x-ray beams has opened ARPES to a wider class of samples and enabled the measurement of 2D devices *in-situ* with applied electric fields, currents, strain and femtosecond laser pulses to the samples. In this talk I will give an introduction to the ARPES technique, the MAESTRO facility and share some of our recent work on the bandstructure and many-body interactions in 2D heterostructures of chalcogenides, graphene, and boron nitride and light induced metastable phases in 1T-TaS₂.

2:45pm **2D+LS+NS+SS-TuA-3 Observation of Interlayer Plasmon Polaron in Graphene/WS₂ Heterostructures**, S. Ulstrup, Aarhus University, Denmark; Y. Veld, Radboud University, Netherlands; J. Miwa, A. ones, Aarhus University, Denmark; K. McCreary, J. Robinson, B. Jonker, Naval Research Laboratory; S. Singh, Carnegie Mellon University, USA; R. Koch, E. Rotenberg, A. Bostwick, C. Jozwiak, Advanced Light Source, Lawrence Berkeley National Laboratory; M. Rosner, Radboud University, Netherlands; Jyoti Katoch, Carnegie Mellon University, USA

Van der Waals heterostructures offer us exciting opportunity to create materials with novel properties and exotic phenomena such as superconductivity, bound quasiparticles, topological states as well as magnetic phases. In this talk, I will present our work on directly visualizing the electronic structure of graphene/WS₂/hBN heterostructure using micro-focused angle-resolved photoemission spectroscopy (microARPES). Upon electron doping via potassium deposition, we observe the formation of quasiparticle interlayer plasmon polarons in graphene/WS₂ heterostructure due to many-body interactions. I will discuss that such low-energy quasiparticle excitation is important to consider as they can have huge implications on the electronic and optical properties of heterostructures based on 2D transition metal dichalcogenides.

3:00pm **2D+LS+NS+SS-TuA-4 Harnessing the Synergy of X-ray Photoelectron Spectroscopy (XPS) and Argon Cluster Etching for Profound Analysis of MoS₂ and Graphene**, Jonathan Counsell, Kratos Analytical Limited, UK; C. Maffitt, D. Surman, Kratos Analytical Inc.; L. Soomary, K. Zahra, Kratos Analytical Limited, UK

Understanding the intricate properties of two-dimensional (2D) materials such as MoS₂ and graphene is pivotal for advancing their applications across diverse fields. However, achieving comprehensive characterization at the nanoscale requires advanced analytical techniques. This study explores the synergistic potential of X-ray Photoelectron Spectroscopy (XPS) coupled with Gas Cluster Ion Source (GCIS) etching and depth profiling to delve deeper into the structural and electronic intricacies of MoS₂ and graphene.

By integrating XPS with GCIS etching, we not only discern the elemental composition, chemical bonding, and electronic states of these materials with exceptional precision but also unravel their depth-dependent characteristics. The incorporation of GCIS etching facilitates controlled removal of surface layers, enabling depth profiling to uncover buried interfaces, defects, and contamination effects that influence spectral results.

The combined approach allows for the characterization of MoS₂-graphene heterostructures, providing insights into interfacial interactions and electronic coupling mechanisms. Through systematic analysis, we demonstrate the complementary advantages of XPS and GCIS etching in elucidating the structural and electronic complexities of 2D materials.

The integration of GCIS etching with XPS not only enhances the depth resolution and sensitivity of the analysis but also offers a deeper understanding of the nanoscale landscape of MoS₂, graphene, and their heterostructures. This multidimensional approach accelerates the

development of tailored devices and applications based on 2D materials, propelling advancements in nanotechnology and beyond.

3:15pm **2D+LS+NS+SS-TuA-5 Monark Quantum Foundry: Advancing 2D Quantum Materials Through Automated Pipelines**, Amirhossein Hasani, N. Borys, Montana State University, USA; H. Churchill, University of Arkansas

At the MonArk Quantum Foundry, located at Montana State University and the University of Arkansas, we are advancing the field of 2D quantum materials through the development of 2D Quantum Materials Pipelines (2D-QMaPs). These pipelines automate and streamline the critical stages of 2D quantum material sample preparation and device fabrication.

Robotic Exfoliation and Flake Hunting: Our process begins with an automated robotic exfoliator designed to produce up to 50 chips per hour, each measuring 1 cm by 1 cm. This machine carefully peels off thin layers from bulk materials, allowing precise control over factors such as temperature, pressure, and applied force, which is crucial for producing high-quality thin flakes, including single-layered crystals. After exfoliation, an automated optical cataloger identifies and catalogs the thin flakes. This system scans the entire chip, locates these flakes, and stores their information in a database. The cataloger uses advanced machine learning and AI algorithms for quick and accurate detection and features a motorized stage with photoluminescence and Raman spectroscopy capabilities, completing a full scan at 20x magnification in approximately 5 minutes.

Device Fabrication and Packaging: The identified flakes are then transferred to a specialized environment for device fabrication and packaging. This stage employs high-resolution thermal scanning probe lithography, laser writing systems, and electron beam evaporators to create devices. The entire process is conducted in an inert atmosphere (glove box), preserving the material's integrity by preventing exposure to air and moisture.

Characterization: The final stage integrates quantum device characterization tools, including photoluminescence (PL), Raman spectroscopy, magneto-optical probes, nano-optical spectroscopy, bulk and nanoscale cryogenic magnetometry, and magneto-transport measurements. These tools provide a comprehensive analysis of material and device properties, including mobilities, transition temperatures, photon autocorrelations, coherence times, and more.

Through the development of the 2D-QMaPs, the MonArk Quantum Foundry is revolutionizing the study of 2D quantum materials, paving the way for significant advancements in quantum computing, sensing, and other technologies.

4:00pm **2D+LS+NS+SS-TuA-8 Manipulation of Chiral Interface States in a Moiré Quantum Anomalous Hall Insulator**, Tiancong Zhu, Purdue University **INVITED**

Quantum anomalous Hall (QAH) effect reflects the interplay between magnetism and non-trivial topology characterized by integer Chern numbers, which is expressed by chiral edge states that carry dissipationless current along sample boundaries. The recent discovery of QAH effect in van der Waals moiré heterostructures provides new opportunities in studying this exotic two-dimensional state of matter. Specifically, magnetism in these moiré QAH systems is induced by orbital motion of electrons, which allows full electrical control of the magnetic and the corresponding topological state. In this talk, I will discuss our recent scanning tunneling microscopy and spectroscopy (STM/STS) measurements on twisted monolayer-bilayer graphene (tMBLG), where QAH effect with gate-switchable Chern numbers have been observed previously in transport measurement. First I will discuss local scanning tunneling spectroscopy measurements on the correlated insulating states at $\nu = 2$ and $\nu = 3$ electrons per moiré unit cell, where the $\nu = 3$ state shows a total Chern number of ± 2 . Under a small magnetic field, the sign of Chern number at the $\nu = 3$ states can be switched by changing the local carrier concentration with gating, which is a result of competition between bulk and edge orbital magnetization of the QAH state.¹ The observation of a gate-switchable Chern number provides us an opportunity to directly visualize the chiral edge state in a moiré QAH insulator for the first time, which I will show through gate-dependent STS measurement and dI/dV mappings.² I will also demonstrate the capability to manipulate the spatial location and chirality of the QAH edge state through controlling the local carrier concentration with the STM tip.

¹ C. Zhang, T. Zhu et al., Nature Communications, 14, 3595 (2023)

² C. Zhang, T. Zhu et al., Nature Physics (2024)

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4:30pm **2D+LS+NS+SS-TuA-10 Scanning Tunneling Microscopy and Spectroscopy of Single Layer NiTe₂ on Au**, *Stephanie Lough*, University of Central Florida; *M. Ishigami*, University of Central Florida

Previous angle-resolved photoemission studies [1, 2] have shown that NiTe₂ is a type II Dirac material that possesses a Dirac point very close to the Fermi level. In addition, the material has a topological surface state which can be valley spin-polarized. A recent study [3] has shown that this state can be exploited to develop Josephson diodes with potential applications as memory devices which can be coupled to qubits. There has been a significant interest [3-5] in studying properties of single layer NiTe₂ due to its strong interlayer coupling in bulk via Te pz orbitals.

In this talk, we will discuss the properties of single layer NiTe₂ on Au generated by gold-assisted exfoliation measured using low temperature scanning tunneling microscopy and spectroscopy. We find that this interface possesses rectangular lattice with periodicities that are different from bulk NiTe₂ or Au (111) by over 30%. Tunneling spectra reveals strong coupling between NiTe₂ and Au (111). We compare these results recent theoretical calculations [6] on strained NiTe₂ and its impact on topological surface states.

1. Ghosh, S., et al., *Observation of bulk states and spin-polarized topological surface states in transition metal dichalcogenide Dirac semimetal candidate NiTe₂*. Physical Review B, 2019. **100**.

2. Mukherjee, S., et al., *Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe*. Scientific Reports, 2020. **10**(1).

3. Pal, B., et al., *Josephson diode effect from Cooper pair momentum in a topological semimetal*. Nature Physics, 2022. **18**(10): p. 1228-+.

4. Zhao, B., et al., *Synthetic Control of Two-Dimensional NiTe Single Crystals with Highly Uniform Thickness Distributions*. Journal of the American Chemical Society, 2018. **140**(43): p. 14217-14223.

5. Zheng, F.P., et al., *Emergent superconductivity in two-dimensional NiTe crystals*. Physical Review B, 2020. **101**(10).

6. Ferreira, P.P., et al., *Strain engineering the topological type-II Dirac semimetal NiTe*. Physical Review B, 2021. **103**(12).

4:45pm **2D+LS+NS+SS-TuA-11 Nanoscale heterogeneities at Transition Metal Dichalcogenide-Au Interfaces**, *Taisuke Ohta*, *A. Boehm*, *A. Kim*, *C. Spataru*, *K. Thuermer*, *J. Sugar*, Sandia National Laboratories; *J. Fonseca Vega*, *J. Robinson*, Naval Research Laboratory

Two-dimensional geometry renders unique screening properties in transition metal dichalcogenides (TMDs). Consequently, the electronic properties of TMDs are susceptible to extrinsic factors (*e.g.*, substrate, strains, and charge transfer), and display spatial nonuniformities. Thus, material combinations (*i.e.*, TMD, dielectrics, and metals) and their nuanced interactions need to be considered when designing TMD-based devices. Of particular importance are the interfaces with metallic contacts. Uncovering the origin of heterogeneities at TMD-metal interfaces and establishing strategies to control TMD-metal interfaces could enable engineering pathways for future applications. We show that the electronic structures of exfoliated WS₂-Au interfaces exhibit pronounced heterogeneity arising from the microstructure of the supporting metal. These electronic structure variations indicate spatially nonuniform doping levels and Schottky barrier height across the junction. Through examination using photoelectron emission microscopy, we reveal key differences in the work function and occupied states. With *ab initio* calculation, electron backscatter diffraction, and scanning tunneling microscopy, our measurements show distinct variations in excess of 100meV due to the crystal facets of Au. Additionally, when multilayer WS₂ and Au(111) facets are azimuthally aligned, strong interactions induce mechanical slippage of the interfacing WS₂ layer, with respect to the rest of the WS₂ layers, resulting in local stacking variations with an occupied state energy shift of 20-50meV. Finally, we employed oxygen plasma treatment of Au to fabricate homogenous TMD-Au interfaces while also tuning the electronic properties of the TMDs. Our findings illustrate that the electronic properties of TMDs are greatly impacted by the interface interactions at energy and length scales pertinent to electronics and optoelectronics.

The work at Sandia National Laboratories (SNL) was supported by LDRD program and the US Department of Energy (DOE), Office of Basic Energy Sciences, Division of Materials Sciences and Engineering (BES 20-017574). The work at the US Naval Research Laboratory was funded by the Office of Naval Research. SNL is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly-owned subsidiary of Honeywell International, Inc., for the US DOE's National Nuclear Security Administration under contract DE-NA0003525.

This paper describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the US DOE or the US Government.

5:00pm **2D+LS+NS+SS-TuA-12 Xenon Trapping in Silica Nanocages Supported on Metal Powder**, *Laiba Bilal*, SBU; *A. Boscoboinik*, Brookhaven National Laboratory

Trapping of Xenon gas atoms in silica nanocages supported on metal powders (Ru and Co) is investigated by lab-based ambient pressure X-ray photoelectron spectroscopy (AP-XPS). Xenon, being a noble gas, has very low reactivity¹. This makes it useful for applications where chemical reactions are unwanted. The first use for Xenon was in flash lamps used in photography², and it is still used for this purpose today. It has wide applications, from its use in the cells of plasma television as a propellant in spacecraft that use ion propulsion³ to its various applications in the medical industry⁴.

Xenon occurs in slight traces within Earth, 1 part in 10 million by volume of dry air². Like several other noble gases, xenon is present in meteorites and manufactured on a small scale by the fractional distillation of liquid air. However, Xe's concentration in the earth's crust and the atmosphere are much lower than predicted, which is also known as the "missing Xenon paradox"⁵.

The Discovery of an effective way to trap and separate Xenon from other gases can have significant advantages. The presence of Xenon in nuclear fuel rods was partially responsible for the Chernobyl accident⁶. Consequently, the nuclear energy industry is also trying to imprint a way to control the release of Xe, produced during the nuclear fission of uranium. Characteristics of chemical interactions between Xe and metal surfaces have been observed and explained, also several low-energy electron diffraction studies at cryogenic temperatures have experimentally demonstrated an on-top site adsorption preference for Xe adatoms on metal surfaces⁷.

Prior studies on 2D silicate bilayers grown on metal supports at Brookhaven National Lab showed that these structures could irreversibly trap all noble gases larger than Ne⁸ at room temperature. The noble gas atoms were trapped within hexagonal prism-shaped silicate nanocages-like structures and could then be released by heating the materials to different temperatures, *i.e.*, Ar: 348 K, Kr: 498 K, Xe: 673 K, Rn: 775 K^{8,9}. Figure 1A illustrates the potential energy diagram for a noble gas atom getting trapped in a silica nanocage. It can be seen that the activated physisorption mechanism that traps noble gas atoms has a high desorption energy barrier (E_{des}).

Figure 1B shows a silicate bilayer structure (side and top views), while Figure 1C shows a hexagonal prism nanocage, the building block of the bilayer structure.⁸ Since synthesizing such silicate bilayers is very expensive and time-consuming¹⁰ for practical purposes, my project focuses on developing and testing scalable silicate nanocage⁹ materials to trap noble gases, with especial focus on Xenon.

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