Thursday Afternoon, November 9, 2023

2D Materials Technical Group
Room B110-112 - Session 2D2-ThA
2D-Materials: Surface and Interface Effects

Moderators: Huamin Li, University at Buffalo-SUNY, **Cristina Satriano**, University of Catania

2:20pm **2D2-ThA-1 Two-dimensional van der Waals Materials and Their Mixed Low-Dimensional Hybrids for Electrochemical Energy Applications***,* ***Fei Yao****,* University at Buffalo-SUNY

Compared with their 3D counterparts, two-dimensional (2D) van der Waals (vdW) materials exhibit quantum confinement where charge carriers are spatially confined at the physical boundaries. Particularly, when mixing 2D materials with other low-dimensional (LD) materials, they exhibit enormous potential in electrochemical energy applications due to the unique properties arising from reduced dimensionality and, more importantly, material integration synergy. In this work, 2D transition metal dichalcogenides and their mixed low-dimensional hybrids (MLDHs) are introduced with an emphasis on innovations covering 2D-based hybrid structure construction and electrochemical applications. Fundamental insight into the synergistic effect of the MLDHs integration for advancing the development of Li-ion batteries and electrocatalytic hydrogen evolution reaction will also be discussed. Leveraging the unique microreactor platform based on the 2D vdW platform, a mechanistic understanding of charge transport dynamics at the electrified interface will be highlighted. The knowledge gained on how mixed-dimensional physics and chemistry will shed light on the design principle of the electrode materials and deepen the understanding of the process-structural-property-performance (PSPP) relationship of the vdW-based hybrid structures.

2:40pm **2D2-ThA-2 Influences of Fe Vacancy and Te Vacancy on Magnetic Domains on Fe_3Gete_2 Surfaces***,* ***TeYu Chien****,* University of Wyoming*; D. Baral,* University of Arkansas*; Z. Fu, J. Tian,* University of Wyoming*; H. Chen,* Colorado State University

Fe_3GeTe_2 (FGT) is a van der Waals (vdW) ferromagnetic metallic material with Curie temperature around 230 K. Despite the central symmetric crystal structure, magnetic skyrmions and various magnetic domain textures have been reported in FGT. The magnetic domain textures can be widely tuned with thickness, temperature and magnetic field. Several ideas regarding the origin of the wild magnetic domain textures have been proposed, including oxidized layer induced DMI, Fe defect vacancy etc. Here, by utilizing spin polarized scanning tunneling microscopy (SPSTM), we revealed that, compared to Fe vacancies, the Te vacancies have stronger effects on altering the magnetic domains in the otherwise ferromagnetic system. A theoretical model will also be discussed to explain the difference between the Te vacancies and the Fe vacancies on the magnetic domain wall pinning.

3:00pm **2D2-ThA-3 Emergent Moiré Phonons Due to Zone Folding in WSe_2-WS_2 Van Der Waals Heterostructures***,* ***Hsun Jen Chuang****, B. Jonker,* Naval Research Laboratory

Bilayers of 2D materials offer opportunities for creating devices with tunable electronic, optical, and mechanical properties. In van der Waals heterostructures (vdWHs) where the constituent monolayers have different lattice constants, a moiré superlattice forms with a length scale larger than the lattice constant of either constituent material regardless of twist angle. Here, we report the appearance of moiré Raman modes from nearly aligned WSe_2-WS_2 vdWHs in the range of 240 cm^{-1} -260 cm^{-1}, which are absent in both monolayers and homobilayers of WSe_2 and WS_2 and in largely misaligned WSe_2-WS_2 vdWHs. Using first-principles calculations and geometric arguments we show that these moiré Raman modes are a consequence of the large moiré length scale which results in zone-folded phonon modes that are Raman active. These modes are sensitive to changes in twist angle, but notably, they occur at identical frequencies for a given small twist angle away from either the 0-degree or 60-degree aligned heterostructure.Our measurements also show a strong Raman intensity modulation in the frequency range of interest, with near 0 and near 60-degree vdWHs exhibiting a markedly different dependence on excitation energy. In near 0-degree aligned WSe_2-WS_2 vdWHs, a nearly complete suppression of both the moiré modes and the WSe_2 A_{1g} Raman mode (~250 cm^{-1}) is observed when exciting with 532 nm CW laser at room temperature. Temperature-dependent reflectance contrast measurements demonstrate the significant Raman intensity modulation arises from resonant Raman effects.

3:20pm **2D2-ThA-4 Stabilizing Metastable Constituent Structures via 2D Interlayer Interactions in Heterostructures***,* ***Fischer Harvel****, D. Johnson,* University of Oregon

The interactions between constituent layers in heterostructures provide an opportunity to stabilize 2D compounds not found in equilibrium phase diagrams. Utilizing 2D layers of 3D structures like rock-salt structured PbSe, commonly found in thermodynamically stable heterostructures known as misfit compounds, phenomena such as charge transfer to and surface stabilization can be used to stabilize new structures. In the iron-selenide system β-FeSe exhibits high-temperature superconductivity (T_c ~ 107 K) when grown in a monolayer on a $SrTiO_3$ substrate. This motivation sparked our interest in investigating possible Fe-Se phases when layers of controlled composition are spatially confined between adjacent layers of PbSe. Using a computational "island" approximation, potential candidate Fe-Se structures were placed between bilayers of PbSe and were relaxed in DFT calculations to assess stability of different structures. Of the trialed candidates, $(PbSe)_{1+\delta}(FeSe_2)$ with Fe in octahedral coordination (1T) maintained its structure when relaxed. Using the predicted densities of the relaxed model, precursors that mimic the nanoarchitecture of the heterostructure were prepared and annealed at low temperatures to prepare the heterostructures $(PbSe)_{1+\delta}(FeSe_2)_n$ where n = 1, 2, and 3. To probe the effect of different adjacent layers on the stability of the 1T $FeSe_2$ layers, we successfully stabilized 1T-$FeSe_2$ in $(PbSe)_{1+\delta}(NbSe_2)(PbSe)_{1+\delta}(FeSe_2)$. These systems provide insights into interfacial interactions between constituent layers in 2D heterostructures that can be used to prepare layers with structures not found in the phase diagrams of the constituent elements.

3:40pm **2D2-ThA-5 Comparative Study of How Growth Parameters Affect the Optoelectronic Properties of $MoSe_2$ and WS_2 on Sapphire Substrates Grown by Chemical Vapor Deposition (CVD)***,* ***Selena Coye****,* Department of Physics, Clark Atlanta University*; K. Johnson,* Morehouse College, Department of Dual Degree Engineering*; I. Matara Kankanamge, M. D. Williams,* Department of Physics, Clark Atlanta University

Two-dimensional molybdenum diselenide ($MoSe_2$) and tungsten disulfide (WS_2) exhibit remarkable properties that make them ideal for various applications in nanoelectronics, spintronics, valleytronics, and optoelectronics. The bandgap of these materials increases as their thickness decreases. Specifically, when reduced to a monolayer, the bandgap changes from indirect to direct. The bandgap of $MoSe_2$ is 1.1 eV for the bulk layer and 1.5 eV for the few layers. On the other hand, monolayer WS_2 has a direct bandgap of 2.15 eV, whereas bulk WS_2 has an indirect bandgap of 1.3 eV. These materials are grown on different substrates however, sapphire is an excellent substrate for growing these materials due to its remarkable mechanical and thermal properties and chemical stability. Consequently, it produces a mechanically robust and thermally stable film, making it indispensable for devices requiring durability and the ability to withstand high temperatures. By growing WS_2 on a sapphire substrate, it can achieve epitaxial growth by reducing the lattice mismatch between sapphire and WS_2. This leads to a high-quality WS_2 film with fewer defects, thus enhancing the material's overall structural quality. Chemical vapor deposition (CVD) is the widely used technique to grow these materials. However, the quality of the layers (including their crystallinity, crystallite size, and coverage area) grown by CVD depends on factors such as growth temperatures, growth time, precursors, flow rate, and substrate nature. Our research will study the effect of carrier gas flow rate and growth time on the bandgap, lattice structure, optical properties, and structural quality of MoSe2/sapphire andWS_2/Sapphire layers grown by CVD. We will analyze the properties of these films using Raman/PL, FTIR spectroscopy, and confocal microscopy.

4:00pm **2D2-ThA-6 Imaging Spin Filter for NanoESCA Based on Au/Ir or Oxide Passivated Fe***, M. Escher, N. Weber, T. Kuehn,* ***Marten Patt****,* FOCUS GmbH, Germany

The energy-filtered photoelectron microscope NanoESCA [1,2] is a powerful tool for various application including work-function mapping, imaging XPS and in the last years more prominently for momentum microscopy on 2D materials (e.g. see [3]).

This analyzer can be used with an efficient spin filter that enables to image a 2D-distribution of the electron spin polarization by scattering the electrons at a polarizing target. We will show results from the first commercial build Au/Ir Imaging Spin Filter. Sherman functions of +68% and -58% were found at a reflectivity of more than 1% (also see literature [4]).

Spin-filtered images of magnetic domains show that along the diameter of the field of view more than 100 separate image points can be resolved. This increases the effective 2D figure-of-merit of this analyzer by nearly four orders of magnitude compared to single-channel spin detectors. We also present proof of principal measurements of an Imaging Spin Filter with oxide passivated Fe as scattering target [5]. Oxide passivated Fe allows for an easy switch of the polarization detection direction, like it is known from FERRUM detectors [6] for ARPES.

References

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