# Wednesday Afternoon, November 8, 2023

## 2D Materials Technical Group
## Room C123 - Session 2D-WeA

### 2D-Materials: Electronic/Magnetic/Optical Properties

**Moderators: Zachary Krebs**, University of Wisconsin - Madison, **Xuedan Ma**, Argonne National Lab

2:20pm **2D-WeA-1 Josephson Diode Effect via Proximity Induced Superconductivity in 2D Materials**, ***Stuart Parkin***, Max Planck Institute for Microstructure Physics, Germany **INVITED**

Recently we have discovered a non-reciprocal Josephson diode effect in several Josephson junctions, both lateral and vertical, formed from conventional superconducting electrodes (Nb, $NbSe_2$) separated by several non-superconducting metals including the 2D van der Waals metals, $NiTe_2$ [1] and $WTe_2$[2], as well as sputtered layers of platinum that are magnetically proximitized via a magnetic insulator (YIG) [3]. Each of these materials becoming superconducting by proximity to the conventional superconducting electrodes. The superconductivity can be sustained over long distances of, in some cases, up to ~1 micron. The critical supercurrent densities for current flowing in opposite directions within the junction are distinct and can vary by up to 40% or more. For the van der Waals metals the non-reciprocity is only observed in the presence of a small magnetic field oriented perpendicular to the supercurrent, whereas for the Pt based junctions the diode effect is observed in zero field. For vertical Josephson junctions formed from $WTe_2$ we show that the non-reciprocity depends on the orientation of the magnetic field with respect to the crystal structure of the $WTe_2$, proving thereby the intrinsic origin of the Josephson diode effect. We also show how the magnitude of the asymmetry increases with the thickness of the $WTe_2$ barrier[2]. Finally, we discuss our recent work on spin-triplet supercurrent spin valves using 2D chiral Kagome antiferromagnets [4].

[1]B. Pal *et al.*, "Josephson diode effect from Cooper pair momentum in a topological semimetal," *Nat. Phys.,* vol. 18, pp. 1228-1233, 2022.

[2]J.-K. Kim *et al.*, "Intrinsic supercurrent non-reciprocity coupled to the crystal structure of a van der Waals Josephson barrier," *arXiv:2303.13049,* 2023.

[3]K.-R. Jeon *et al.*, "Zero-field polarity-reversible Josephson supercurrent diodes enabled by a proximity-magnetized Pt barrier," *Nat. Mater.,* vol. 21, pp. 1008-1013, 2022.

[4]K.-R. Jeon *et al.*, "Chiral antiferromagnetic Josephson junctions as spin-triplet supercurrent spin valves and d.c. SQUIDs," *Nat. Nanotechnol.,* 2023.

3:00pm **2D-WeA-3 Behavior of Excited States in 2H and 3R Bilayer $WSe_2$**, ***Kathleen McCreary***, *M. Phillips, H. Chuang, D. Wickramaratne, M. Rosenberger, C. Hellberg, B. Jonker,* Naval Research Laboratory

Transition metal dichalcogenide bilayers exhibit improved stability and higher carrier mobility compared to their monolayer counterparts, and may be attractive for a variety of applications. Both 2H and 3R bilayers are energetically stable and are expected to exhibit semiconducting behavior. However, 2H has received the bulk of attention due to its ready availability in the form of mechanically exfoliated flakes. Here, we detail the energies and temperature dependent behaviors of the ground and the first excited excitonic states in both 2H and 3R $WSe_2$ bilayers. Samples are obtained through chemical vapor deposition, encapsulated with hBN, and reflectance contrast (RC) is measured to identify 1s and 2s excitonic states. At cryogenic temperatures, a splitting of approximately 17 meV is experimentally observed in both the 1s and 2s states of 3R bilayers. This splitting is consistent with our DFT calculations and is due to lack of inversion symmetry, with the two peaks corresponding to distinct excitonic transitions in the upper and lower layers of the 3R $WSe_2$. As temperatures increases, excitonic states broaden and RC intensity decreases, preventing detection of 2s states above 100 K. The 1s state is evident at all temperatures between 4 K and 300 K, and splitting of the 1s state in 3R samples is detectable to approximately 250 K. This work provides much needed insight into bilayer systems and demonstrates that interlayer interactions are strong enough to significantly modify the optical properties in $WSe_2$ samples.

3:20pm **2D-WeA-4 2D $SnO/MoO_3$ van der Waals Heterojunction with Tunable Electronic Behaviors for Multi-functional Applications: DFT Calculations**, ***Junyu Lang***, ShanghaiTech University, China; *Y. Ma,* Shanghai Jiao Tong University, China; *Y. Yang,* ShanghaiTech University, China

Introduction

Following the advent of graphene in the late 1940s, two-dimensional (2D) materials, such as MXenes, transition-metal dichalcogenides (TMDs), black phosphorene, etc., have attracted extensive attention. Among various 2D materials, transition-metal oxides (TMOs) possess exceptional advantages, such as tunable redox property, high chemical stability, environmental friendliness and earth-abundant characteristic. Metal oxide van der Waals (vdW) heterostructures have attracted extensive attention in fundamental research and new-device design. The remarkable advantage of their tunable energy band structure makes it particularly important to develop versatile metal-oxide heterojunctions and to explore their mechanisms. Herein, 2D $SnO/MoO_3$ vdW heterojunction is successfully constructed by first-principles calculations.The electronic structure of the $SnO/MoO_3$ vdW heterojunction has been systematically investigated, and the underlying physical mechanism responsible for its band alignment has been further revealed. A Z-scheme charge transfer mechanism has been demonstrated in $SnO/MoO_3$ with remarkable photocatalytic $CO_2$ reduction capability. Most importantly, the band alignment can be efficiently tuned by varying the external electric field, indicating its multifunctional potential. Furthermore, the $CO_2$ reduction reaction pathway and product selectivity occurring at the surface of 2D $SnO/MoO_3$ vdW heterojunction can be optimized by adjusting the applied electric field.

Results and Discussion

The vdW heterojunction, $SnO/MoO_3$ has been designed by first-principles calculations. The formation of 2D $SnO/MoO_3$ vdW heterojunctions is not limited by the relative horizontal displacements between the different layers, which greatly facilitates fabrication processes and functional applications. In addition, a Z-scheme charge transfer mechanism has been demonstrated in $SnO/MoO_3$, exhibiting remarkable photocatalytic $CO_2$ reduction capability. Possible reduction reaction pathways for $CO_2$ on the surface of the $SnO/MoO_3$ vdW heterojunction were further explored and it was shown that $CH_4$ and $CH_3OH$ are the main products. Furthermore, we found that the electronic properties of 2D $SnO/MoO_3$ vdW heterojunction can be efficiently modulated by applying an external electric field, which is beneficial for optimizing the reaction path and improving the product selectivity of $CO_2$ reduction reactions. Most importantly, transitions between type-III and type-II band alignments are observed in the 2D $SnO/MoO_3$ vdW heterojunction at negative electric fields. These findings will provide a strong theoretical support for designing novel tunneling field-effect transistors and photocatalysts.

4:20pm **2D-WeA-7 2D Materials Explored Using nanoARPES**, *A. Bostwick, C. Jozwiak,* ***Eli Rotenberg***, Lawrence Berkeley Lab, USA **INVITED**

Angle-resolved photoemission is a premiere technique for measuring the electronic structure of materials, as represented by momentum-resolved electronic bands. Furthermore, with modern high-resolution instrumentation it is possible to access the single-particle spectral function $\boldsymbol{A}(k,\omega)$, which gives important information on the renormalization of excited state energies and lifetimes due to many-body interactions and defect scattering.

NanoARPES machines capable of spatially-resolving the ARPES spectrum on the mesoscopic scale are coming online at synchrotrons around the world, with spatial resolution in the range 100-1000nm. Combining these new small probes with arbitrary stacking orders of diverse materials assembled micromechanically, nanoARPES can obtain information on new materials far faster than in the past, when probe sizes limited us to wafer-scale, epitaxially grown heterostructures. Using small x-ray probes, nanoARPES can also study naturally or spontaneously-formed heterogenous materials. Most if not all nanoARPES machines are accessible through proposals to international user facilities, and the community specializing in these experiments is growing rapidly.

Most excitedly, nanoARPES offers the possibility to measure 2D materials and heterostructures at true device scales, and can thus enable for the characterization of materials under *in operando* conditions. In this talk I will review recent developments and pioneering experiments at the MAESTRO beamline at the Advanced Light Source in Berkeley, CA. These capabilities include the application of external fields (electrical, magnetic, and optical) and current. Prospects for the application of magnetic fields to create a new "MagnetoARPES" technique will be presented.

5:00pm **2D-WeA-9 Probing Many-body Effects in 2D Materials using nanoARPES**, ***Jyoti Katoch***, Carnegie Mellon University, United States Minor Outlying Islands (the)

Two-dimensional (2D) materials provide unprecedented opportunity to engineer their physical properties by modification to the electronic structure utilizing external perturbations- strain, gating, adsorbates,

defects, twist-angle, and interface engineering. This is expected to cause changes to the Hamiltonian describing the system and has resulted in exotic phenomena such as superconductivity, bound quasiparticles, topological states as well as magnetic phases, with implications for novel electronics and spin-device applications. In this talk, I will present our work on directly visualizing (without any assumption) the electronic structure of atomically thin systems utilizing *in-operando* angle-resolved photoemission spectroscopy with nanoscale spatial resolution (nanoARPES) on 2D heterostructures and their fully functional devices [1,2,3,4,5]. I will present the experiments which demonstrate on-demand tuning of the electronic band structure in atomically thin systems, such as transition metal dichalcogenides (TMDCs) and graphene, by varying the twist-angle between the atomic layers and external dopants. Specifically, I will discuss the electric field tuning of the electronic interactions that result in van Hove singularity and flat bands in twisted bilayer graphene and twisted double bilayer graphene heterostructures. In addition, I will show our recent results where we observe the formation of quasiparticle polarons due to many-body interactions in graphene/TMDC heterostructures.

**References:**

[1] Katoch et. al., Nature Physics 14, 355-359 (2018).

[2] Ulstrup [https://arxiv.org/search/?searchtype=author&query=Ulstrup%2C+S], et. al.,Science Advances, Vol. 6, no. 14, eaay6104, (2020).

[3] Jones, et. al., 2D Mater., 9 015032 (2022).

[4] Muzzio, et. al., Physical review B Rapid Communications 101, 201409(R) (2020).

[5] Jones, et. al., Adv. Mater., 32, 2001656 (2020).

5:20pm **2D-WeA-10 Electrical Transport of High-Quality CVD-Grown $MoSe_2$ Nanoribbons**, ***Y.-J. Leo Sun***, Laboratory for Physical Sciences*; O. Ambrozaite, Z. Zhang, T. Kempa,* Johns Hopkins University*; T. Murphy,* University of Maryland, College Park*; A. Friedman, A. Hanbicki,* Laboratory for Physical Sciences

Two-dimensional (2D) materials such as transition metal dichalcogenides are excellent candidates for creating novel nano-electronic and photonic devices. Previous research indicates that the edge states of $MoS_2$ could strongly influence its conductivity, and the 2D honeycomb structure enables different electronic performance along the zigzag and armchair edges. Understanding and controlling the conductivity is essential in devices like field effect transistors that use $MoS_2$ as the channel. To date, transport along edge states of $MoSe_2$ nanoribbons, which have substantially reduced dimensionality relative to 2D crystals, has not been explored. In this project, we used chemical vapor deposition (CVD) to synthesize $MoSe_2$ nanoribbons through a particle-seeded approach. This approach yields directed growth of monolayer $MoSe_2$ to form high aspect ratio (>7) nanoribbons. Tip-enhanced photoluminescence (TEPL) is used to probe the optical properties of the edge and surface of the $MoSe_2$ nanoribbons. To perform electronic transport measurements, we used e-beam lithography to pattern contacts on the nanoribbons in a Hall bar configuration with the side contacts at the edges and tips of the nanoribbons. The influence of edge states on the electrical performance of $MoSe_2$ nanoribbons was investigated by conductivity and Hall transport measurements. Current flow in the transverse and longitudinal directions of the nanoribbon was compared to analyze the importance of edge states on $MoSe_2$ nanoribbon conductivity.

5:40pm **2D-WeA-11 Strain-Exciton Coupling in Two-dimensional Semiconductors**, ***Jin Myung Kim***, *S. Nam,* University of California, Irvine, USA **INVITED**

In this talk, I will present our work on deterministic manipulation and confinement of excitons in two-dimensional (2D) semiconductors. I will discuss predictable and reconfigurable strain modulation in 2D transition metal dichalcogenides (TMDs) via wrinkle architectures. Strain exerted on wrinkled 2D TMDs was periodically modulated to tensile and compressive strain at peaks and valleys of the wrinkles, respectively. Furthermore, owing to the deformable nature of the wrinkle architecture, the applied strain can be tuned reconfigurably with the optical gap of TMDs dynamically modulated. We also observed exciton transport across apex and valley of strained TMDs as well as exciton localization at the apex due to strain gradient induced energy modulation of wrinkled TMDs. Finally, I will discuss an extension of our strain modulation approach to interlayer excitons in TMD vertical heterostructures where strain is used to tune both optical gap as well as interlayer coupling between the heterobilayers. I will share our perspectives on strain-exciton engineering toward quantum and optoelectronic devices.

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