2D Materials
Room 303 - Session 2D-ThA

2D Materials: From Materials Integration to Electronic Properties and Devices

Moderator: Rafik Addou, The University of Texas at Dallas

2:15pm **2D-ThA-1 All-van Der Waals Multiferroic Heterostructures***, **Cheng Gong***[1]*,* University of Maryland, College Park

Two-dimensional (2D) layered van der Waals (vdW) ferroics (e.g., ferromagnets [1,2] and ferroelectrics [3]) are atomic-thin crystalline flatlands with long-range ferroic order, underpinning a plethora of new physical phenomena and novel device functionalities enabled by the collective switching of spin and dipolar orders. However, ferroic orders in 2D systems are prone to destruction: in 2D systems, ferroelectric order [1] tends to be destructed by enhanced depolarization fields and magnetic order [2] tends to be suppressed by enhanced thermal fluctuations. Simultaneously attaining more than one ferroic order in a 2D platform thus appears even more challenging [4].

In this talk, I will present our updated work on the integration of long-range magnetic and ferroelectric orders into 2D vdW heterostructures by assembling ferroelectric and magnetic vdW layers. We unambiguously probe the inter-ferroic magnetoelectric coupling by demonstrating non-volatile electric control of 2D magnetism [5,6,7]. By systematic experiments on samples of various thicknesses, we reveal short-range interfacial interaction underlying the magnetoelectric coupling in vdW heterostructure multiferroics [6,7]. For the first time, we build all-vdW multiferroic tunnel junctions [8], consisting of two vdW magnetic layers separated by a vdW ferroelectric spacer with full tailorability on each constituent layer, and demonstrate four-state electrical resistance by toggling ferroelectric polarization and magnetization orientations, respectively. Finally, all the above demonstrations (multiferroic heterostructures or multiferroic tunnel junctions) have been recently achieved at room temperature [7,8]. The development of vdW multiferroic heterostructures and multiferroic tunnel junctions holds tantalizing possibilities for designer magnetoelectric quantum heterostructures and compact energy-efficient spintronic devices.

1. C. Gong et al. *Nature* 546, 265–269 (2017).
2. C. Gong, X. Zhang. *Science* 363, eaav4450 (2019).
3. Q. Wang, ..., C. Gong, *Matter* 5, 4425–4436 (2022).
4. C. Gong et al. *Nature Communications* 10, 2657 (2019).
5. S. Liang, ..., C. Gong, *Nature Electronics* 6, 199–205 (2023).
6. S. Liang, ..., C. Gong, *Nature Electronics* 9, 23–32 (2026).
7. Q. Wang, ..., C. Gong, *Science* (in press, 2026).
8. T. Xie, ..., C. Gong, *Nature Nanotechnology* 21, 366–373 (2026).

2:30pm **2D-ThA-2 Oxygen Plasma Assisted Nucleation of HfO2 ALD on MoS2 2-d Material for Gate Stack Applications***, **Robert Grubbs***,* IMEC Belgium*; Daire Cott, Benjamin Groven, Pierre Morin, Pawan Kumar, Kaustuv Banerjee, Cesar Javier Lockhart de la Rosa de la Rosa, Gouri Sankar Kar, Johan Swerts,* IMEC, Belgium*; Zsófia Baji,* HUN-REN Centre for Energy Research, Hungary

The demand for increased transistor density in logic circuits is forcing the transistor channel lengths to shorter dimensions which is forcing a proportional decrease in the channel height. Because of the conduction limitations of silicon in the small size limit, alternative materials are being considered to replace the silicon channel material. The most promising alternative materials for this application are the transition metal dichalcogenides (TMD). Most notable is the application of MoS_2 for the channel material. Unfortunately, TMDs come with their own set of challenges when integrating them as transistor channels. Three primary integration challenges include: growth of TMD or the material transfer, source-drain metallization of the TMD and high k dielectric gate formation on the TMD channel. Due to the inertness of the TMD surface, conventional dielectric ALD chemistries will only nucleate at defect sites, grain boundaries or at other vulnerable surface morphologies. This incomplete nucleation causes inhomogeneities in the field that controls the channel and can also produce gate leakage paths. The research presented in this talk uses a remote oxygen plasma to induce nucleation sites on the MoS_2 surface. The exposed surface can then conformally nucleate HfO_2 using tetrakisethylmethylamino hafnium (TEMAH) and water at 200C. Experiments were performed on mono and bilayer MoS_2 samples and characterized with AFM, XPS and electrical testing. It will be shown that there are differences in the surface chemistries between the mono and bilayer samples and that the electrical response indicates the underlying layer in the bilayer samples is electrically conducting.

2:45pm **2D-ThA-3 Highly Reactive Nature of HfSe2 Interface with Gold and Scandium Metal Contacts***, Joslin S. Prasanna,* The University of Texas at Dallas*; Christopher M. Sm,* Sandia National Laboratories*; Robert M. Wallace, **Rafik Addou**,* The University of Texas at Dallas

To continue building upon the major strides made in $HfSe_2$-based devices in recent years, it is essential to fundamentally understand the interfaces formed by gate oxides and metal contacts. While substantial effort has been directed toward improving the quality of the dielectric-$HfSe_2$ interface, this work provides detailed insight into the interface made with the metal contact, which remains a critical bottleneck for the integration of two-dimensional (2D) transition metal dichalcogenides into electronic devices. We utilize X-ray photoelectron spectroscopy (XPS) to study interfacial reactions between two metals with significantly different work functions, Au and Sc, when deposited on bulk $HfSe_2$ at different chamber pressures. Owing to the highly reactive nature of $HfSe_2$, interfacial reaction products formed for both metals, regardless of deposition pressure. Au, despite its well-known chemical inertness, forms an $AuSe_x$ compound at the interface, while Sc forms an intermetallic phase with $HfSe_2$. Band alignment measurements reveal possible Fermi-level pinning and deviations from predictions based on the Schottky-Mott principle.

This work was supported partially by the Jonsson School Research Initiative at the University of Texas at Dallas.

3:00pm **2D-ThA-4 Polarization-Driven Schottky-to-Ohmic Switching at the α-In2Se3/Fe5GeTe2 van der Waals Interface***, **Shashi Mishra**, Nicholas W. G. Smith, Sharadh Jois, Gregory M. Stephen,* Laboratory for Physical Sciences*; Sergiy Krylyuk, Albert V. Davydov,* National Institute for Science and Technology (NIST)*; Luis Balicas,* National High Magnetic Field Laboratory*; Aubrey T. Hanbicki, Adam L. Friedman, Pratibha Dev,* Laboratory for Physical Sciences

Stacking a two-dimensional ferroelectric semiconductor with a van der Waals ferromagnetic metal provides a promising route to electrically switchable, nonvolatile contacts. In α-In_2Se_3/Fe_5GeTe_2 heterostructures, our transport measurements reveal magnetic-field-assisted resistive switching. To uncover its microscopic origin, we performed first-principles calculations for the two opposite orientations of the α-In_2Se_3 ferroelectric polarization. Polarization reversal leaves the Fe_5GeTe_2 magnetism essentially unchanged: the Fe-d exchange splitting remains ≈0.35 eV and the average Fe moment ≈2.05 μ_B. In contrast, the interface electrostatics are strongly modified. Polarization-dependent charge transfer shifts the interfacial potential alignment by ≈0.8 eV, transforming the junction from a *p*-type Schottky contact with a calculated barrier of 0.36 eV, consistent with the measured 0.33–0.45 eV, to an n-type Ohmic contact when the polarization is reversed.

3:15pm **2D-ThA-5 Step-Edge–Induced Symmetry Breaking Enables Scalable Ferroelectric Multilayer h-BN***, **Cheng-Maw Cheng**,* National Synchrotron Radiation Research Center, Taiwan*; Sheng-Shong Wong,* Department of Physics, National Cheng Kung University, Taiwan*; Chia-Hao Chen,* National Synchrotron Radiation Research Center, Taiwan*; Ming-Hao Lee, Ming-Wen Chu,* Center for Condensed Matter Sciences and Center of Atomic Initiative for New Materials, National Taiwan University, Taiwan*; Kuang-I Lin,* Core Facility Center, National Cheng Kung University, Taiwan*; Tse-Ming Chen, Yi-Chun Chen,* Department of Physics, National Cheng Kung University, Taiwan*; Hung-Chung Hsueh,* Department of Physics, Tamkang University, Taiwan., Taiwan*; Chung-Lin Wu,* Department of Physics, National Cheng Kung University, Taiwan

Two-dimensional (2D) ferroelectrics that retain spontaneous polarization at atomic thicknesses are promising for next-generation nanoelectronics and nonvolatile information technologies beyond Moore's law. However, most van der Waals materials, including hexagonal boron nitride (h-BN), naturally favor centrosymmetric stacking configurations and therefore lack intrinsic ferroelectricity. Although symmetry breaking through artificial stacking has been demonstrated, achieving scalable and controllable growth of polarized multilayer structures remains a key challenge.In this work, multilayer h-BN films with controlled thickness were synthesized using nitrogen plasma–assisted molecular beam epitaxy (PA-MBE) on lattice-matched graphene grown on commercial 4H-SiC(0001) substrates with a 4° miscut. Under nitrogen-rich conditions, enhanced boron surface diffusion enables high-quality h-BN growth at relatively low temperatures. Microscopy and Raman spectroscopy reveal continuous, crystalline h-BN layers covering graphene terraces and extending across step edges. Preferential nucleation at graphene step edges promotes aligned island growth and seamless merging, resulting in uniform layer-by-layer epitaxial

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films.Angle-resolved photoemission spectroscopy (ARPES) measurements reveal clear layer-dependent band dispersions for mono-, bi-, and trilayer h-BN. The observed electronic structures agree well with layer- and stacking-dependent GW calculations, confirming polarized AB stacking for bilayer and ABA stacking for trilayer h-BN while excluding non-polar configurations. The spatial uniformity of the band structures further indicates homogeneous, millimeter-scale epitaxial growth.Density functional theory calculations and scanning transmission electron microscopy reveal that graphene step edges significantly lower the interfacial formation energy, acting as favorable nucleation sites that drive step-guided conformal epitaxy and mono-oriented polarized stacking. Ferroelectric behavior was confirmed by piezo-response force microscopy, showing clear polarization switching, butterfly-shaped amplitude loops, and coercive voltages of ~±1.5 V. Stable surface potential contrast and robust domain writing demonstrate nonvolatile polarization control.These results establish epitaxial multilayer h-BN as a scalable 2D ferroelectric platform and highlight step-edge–induced symmetry breaking as a viable route for engineering polarized van der Waals heterostructures.

[1]Sheng-Shong Wong et al., Advanced Materials 37, 2414442 (2025)

3:30pm **2D-ThA-6 Split-Gate Memtransistors for Energy-Efficient Adaptive Reinforcement Learning**, ***Zachary Trdinich***[1], *Mark Hersam, Vinod Sangwan,* Northwestern University

Real-time, on-chip learning has become increasingly important as edge-computing systems based on artificial intelligence (AI) and machine learning are deployed in dynamic environments. In particular, static pretrained models are insufficient for applications such as autonomous vehicles and robotics. To address this issue, analog in-memory computing hardware, such as gate-tunable MoS_2-based memtransistors, has been explored to alleviate energy and latency bottlenecks in edge computing applications. However, limited independent control of channel conductance and resistive switching has hindered reinforcement learning implementation in deployed AI agents. To overcome this bottleneck, we developed split-gate MoS_2 memtransistors in which small-grain (≈1 μm), monolayer MoS_2, grown via solid-state chemical vapor deposition (CVD) on sapphire, is transferred onto a prefabricated split-gate stack. Within this architecture, an ALD-grown Al_2O_3 gate dielectric (25 nm thick) enables local field-effect gating to be applied independently to the Schottky contact regions and the semiconducting channel, allowing the switching ratio and conductance state to be tuned through distinct, spatially separated mechanisms rather than a single global gate. This separation of control over device response function leverages the sensitivity of the transferred CVD-grown monolayer to gate-induced Schottky barrier modulation and gate-induced free charge carrier modulation, providing independent control over nonvolatile memristive switching and reconfigurable transistor-like gating within a single memtransistor. This device-level control enables efficient implementation of a novel multi-agent soft/hard reinforcement learning algorithm, benchmarked here on a cartpole balancing task, where nonvolatile synaptic weight updates combined with rapid parameter adjustments yield a 6-fold improvement in performance and a 5-fold reduction in programming steps.

3:45pm **2D-ThA-7 Charge Redistribution and Surface Electronic Structure in N-Doped Ti_3C_2 MXenes**, ***Cheolhwan Yoon***, *Jaeeun Park,* Ulsan National Institute of Science and Technology, Republic of Korea*; Dongkyu Lee,* Seoul National University, Republic of Korea*; Junseop Noh,* Ulsan National Institute of Science and Technology, Republic of Korea*; Gun-Do Lee,* Seoul National University, Republic of Korea*; Soon-Yong Kwon, Hyung-Joon Shin,* Ulsan National Institute of Science and Technology, Republic of Korea

MXenes are two-dimensional transition-metal carbides and nitrides with the general formula $M_{n+1}X_nT_x$, where X = C and/or N. During the etching process, MXene surfaces are terminated with functional groups such as –O, –F, and –OH, which play a crucial role in their electronic properties. The composition of these functional groups can be controlled to tailor the electronic properties of MXenes, while nitrogen doping provides another strategy for tuning their electronic properties through substitution at the X sites.

In this study, we investigated the local electronic structure of N-doped Ti_3C_2 MXenes using scanning tunneling microscopy (STM) with increasing concentration of N dopants. Atomic-resolution STM images of pristine MXene distinguish –O and –F termination sites, with –O exhibiting a higher local density of states (LDOS) than –F. Differential conductance map revealed dark regions that were not observed in the STM topography, indicating LDOS depletion at the MXene surface associated with buried N dopants. X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations quantitatively verified charge transfer from neighboring Ti atoms toward the N dopants. Our results verified the role of buried N dopant in modifying the local electronic structure of MXenes, suggesting a potential route for engineering their electronic properties.

4:00pm **2D-ThA-8 Assemblies of MXene and Metal-Organic Polyhedra with Post-Functionalized Re(I) Sites for Selective CO_2 Photoreduction**, ***Purna Kanta Boruah***, *Vitaly Ordomsky,* CNRS, France

MXenes are a family of 2D layered materials composed of transition metal carbides and nitrides, that revealed promising for applications in energy, sensing, catalysis, and environmental remediation due to their unique properties, including excellent electronic conductivity, rapid separation of photogenerated charge carriers, well-defined surface functionality with high density of groups for cation adsorption.However, like most other 2D materials, MXenes exhibit a strong tendency to self-stack, which results in a lack of intrinsic microporosity and photocatalytic activity and strongly diminishes performance. To overcome these limitations, MOFs and other metal/metal oxide nanoparticles have been used as spacers to prevent stacking and enhance porosity. Metal-organic polyhedra (MOPs) are created by self-assembling metal ions or clusters with organic linkers. Their diverse sizes, shapes, and customizable structures make them suitable as spacers for microporous composite materials. Taking advantage of the negative surface charge of the MXenes (which was further enhanced by surface functionalization), we prepared novel composite materials by self-assembly with positively charged tetrahedral ZrMOPs. A functional variant of ZrMOPs with ligands derived from 2,2'-bipyridine was used to prepare **ZrMOP-MXene** composites. This ligand offers readily accessible coordination sites, which was functionalized with Re(I)) (designated as **ZrMOP(Re)-MXene**) to enable selective photocatalytic reduction of CO_2. Since, the photocatalytic reduction of CO_2 to CO has emerged as a promising technique to initiate the chemical fixation of CO_2 and its conversion into useful products. **ZrMOP(Re)-MXene** showed good performance as a heterogeneous photocatalyst without the addition of an external photosensitizer, achieving a turnover number (TON) of 51 and an excellent selectivity of 93% for CO. The integration with MXene serves as an efficient electron transport mediator within the assembly, resulting TON is 4.5 and 7 times higher than those of the homogeneous controls of **ZrMOP(Re)** and $[Re(bpy)(CO)_3Cl]$, respectively.

References

Boruah, P.K. Nguyen, D. M., Dutta, R.; Das, M. R.; Ohtani, R.; Marinova, M.;Tomita, Y.; Ozawa, H.; Sakai, K.; Ordomsky*, V.; Le Ouay[a*], B.; Ohba[a*] M. Assemblies of MXene and Metal-Organic Polyhedra with Post-Functionalized Re(I) Sites for Selective CO_2 Photoreduction, *J Am. Chem. Soc.* **2026 (Accepted)**. doi.org/10.1021/jacs.6c09833

[1] **JVST Highlighted Talk**

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