

2D Materials

Room 208 W - Session 2D+AQS+EM+NS+QS+TF-FrM

2D Materials: Devices and Applications

Moderator: Kai Xiao, Oak Ridge National Laboratory

8:15am 2D+AQS+EM+NS+QS+TF-FrM-1 Charge Transport in Printed Films of Two-Dimensional Materials for Printed and Wearable Electronics, *Felice Torrisi*, Imperial College London, UK

INVITED

Printed electronics has emerged as a pathway for large scale, flexible, and wearable devices[1], Internet-of-Things[2] and smart textiles[3]. Graphene and related two-dimensional (2D) materials offer an ideal platform of novel materials for high performance printed electronics [4,5]. Electronic inks from 2D materials with different electronic properties have been developed to print the different elements of a device: semiconducting or semimetallic inks in the active layer, insulating inks for dielectrics, and conducting inks for electrodes[6].

In this talk I will describe the charge transport mechanisms of surfactant- and solvent-free inkjet-printed thin-film devices of representative few-layer graphene (semi-metal), molybdenum disulphide (MoS₂, semiconductor) and titanium carbide MXene (Ti₃C₂, metal) by investigating the temperature, gate and magnetic field dependencies of their electrical conductivity.[7]

Charge transport in printed few-layer MXene and MoS₂ devices is dominated by the intrinsic transport mechanism of the constituent flakes. On the other hand, charge transport in printed few-layer graphene devices is dominated by the transport mechanism between different flakes.[7]

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8:45am 2D+AQS+EM+NS+QS+TF-FrM-3 Antimony as a Contact Material for Two-Dimensional Semiconductors: Interface Chemistry and Thermal Stability, *Fernando Quintero Borbon, Joy Roy, Robert Wallace, Rafik Addou*, University of Texas at Dallas

Antimony (Sb), a semimetal, has emerged as a promising contact material for two-dimensional (2D) semiconductors. Sb contacts have been shown to achieve ultra-low contact barriers. The formation of a Sb–Se bond has been demonstrated as an effective doping strategy in n- and p-FETs with a single WSe₂ channel through Sb–Pt contact modification. These findings underscore the necessity for further investigation into the interface chemistry and thermal stability of Sb on transition metal dichalcogenides (TMDs), to determine whether the interaction remains van der Waals or becomes chemically reactive upon thermal processing.

The present study offers a comprehensive study of the interface chemistry between Sb and TMDs, in particular MX₂ (M = Mo or W; X = S or Se), using X-ray photoelectron spectroscopy (XPS). Sb was deposited in ultra-high vacuum conditions (UHV) on bulk TMD surfaces, followed by annealing in UHV at 100°C, 200°C, and 300°C. The XPS measurements revealed an absence of chemical or interfacial reactions at room temperature, 100°C, and 200°C. However, upon annealing at 300°C, complete sublimation of the Sb layer was observed. These findings support the van der Waals nature of the interface, confirming that the interaction between Sb and the underlying TMDs remains non-reactive up to 200 °C. This thermal stability and inertness suggest that Sb could be a promising candidate for integration in 2D heterostructures and devices that require clean, weakly interacting interfaces.

[1] Y.-T. Lin et al. *Nano Lett.* (2024) 24, 8880–8886

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[3] T. Su et al. *J. Phys. D: Appl. Phys.* 56 (2023) 234001

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[5] Chou et al. *IEEE International Electron Devices Meeting (IEDM)*, San Francisco, CA, USA (2021) 7.2.1-7.2.4.

9:00am 2D+AQS+EM+NS+QS+TF-FrM-4 Metal-to-Semiconductor

Transition in Niobium Sulfoselenide Alloy and Niobium Sulfide Films by Compositional Control and Post Growth Sulfurization, *Tinsae Alem, Abir Hasan, Kory Burns, Nikhil Shukla, Stephen McDonnell*, University of Virginia

Transition metal dichalcogenides (TMD) have attracted increasing scientific interest due to their diverse properties including a tunable bandgap, optical anisotropy, low power consumption, and good elasticity. In this study, low-dimensional TMD films were grown with molecular beam epitaxy (MBE) to investigate the effects of varying chalcogen (sulfur and selenium) content in niobium sulfoselenide (NbS₂Se_{2-x}) alloys. Here, we focus on their electrical resistivity and electronic properties, including the transition from metallic to semiconducting behavior to have precise control over the material's electrical conductivity. Additionally, we analyzed the semiconductor-to-metal transition in NbS₂ films following post-growth sulfurization and the corresponding changes in resistivity. These MBE grown films were characterized using in-situ x-ray photoelectron spectroscopy (XPS) to analyze the chemical composition. Next, the electrical resistivity of films was calculated using their sheet resistance measured with a Jandel 4-point probe, and their thickness was estimated using x-ray reflectivity (XRR). We used transmission electron microscopy (TEM) to visualize these MBE-grown films at the atomic scale, enabling the correlation of atomic structure with electronic properties. Lastly, the temperature coefficient of resistance (TCR) measurements was performed to understand the resistivity of the films with temperature dependence and to determine their metallic and semiconducting behavior. Our results demonstrate that the transition from metal to semiconductor occurs with the addition of sulfur into the niobium selenide film. We also observed a trend of increasing resistivity as the sulfur content was increased in niobium selenide film. This work explores the potential of tuning the energy gap of TMD materials, making them ideal candidates for tunable nanoelectronics in various applications.

9:15am 2D+AQS+EM+NS+QS+TF-FrM-5 Evolution of the Electronic Gap of Directly Synthesized Versus Mechanically Transferred WS₂ Monolayer to Multilayer Films, *Xu He, Antoine Kahn*, Princeton University

Transition metal dichalcogenides (TMDs) have emerged as promising electronics and optoelectronics materials for their strong light-matter interaction, large exciton binding energies, and bandgap tunability through the control of composition and the number of layers. Among TMDs, WS₂ stands out for its strong photoluminescence and spin-orbit coupling, making it ideal for exploring charge transfer and interfacial phenomena. However, discrepancies in reported energy levels (electronic gap, ionization energy, electron affinity) remain due to variations in growth and measurement methods, impeding device design.

In this study, we directly compare the band structure of WS₂ films from monolayer to multilayer (up to four layers) prepared by two commonly used methods: direct growth via metal-organic chemical vapor deposition (MOCVD) and mechanical exfoliation with layer-by-layer transfer. We utilize a suite of characterization techniques, including Raman spectroscopy, photoluminescence (PL), UV–vis absorption, and X-ray photoelectron spectroscopy (XPS), to probe vibrational modes and optical transitions. A combination of ultraviolet photoelectron spectroscopy (UPS) and inverse photoemission spectroscopy (IPES) allows us to directly study the evolution of ionization energy and electron affinity, hence the electronic gap of the materials.

We find that the electronic gap (E_g) of WS₂ consistently decreases with increasing layer number, reaching bulk-like values by the trilayer for mechanically transferred layers. The exfoliated monolayer is found to have an E_g of 2.43 eV, which reduces to around 1.97 eV at the trilayer and stays at 1.98 eV for the tetralayer. This layer-dependent E_g reduction is driven firstly by an upshift of the valence band maximum (VBM) at the 1L-2L transition and then by a downshift of the conduction band minimum (CBM) at the 2L-3L transition.

Comparing differently processed layers, we find the MOCVD-grown monolayer WS₂ to exhibit an electronic gap of 2.56 eV, larger than 2.43 eV for the mechanically transferred one. The slightly larger E_g in MOCVD-grown monolayers also yields a higher exciton binding energy (~0.55 eV)

than in exfoliated monolayers (~0.43 eV). XPS analysis indicates that MOCVD samples contain more oxygen-related defect species, likely contributing to the subtle band gap differences and a small blue shift of their optical spectra relative to exfoliated layers.

Overall, this comparative study highlights the influence of the fabrication methods on the fundamental electronic structure of WS_2 . These findings provide important guidelines for tailoring band alignments for WS_2 -based heterostructures and optoelectronic devices.

9:30am **2D+AQS+EM+NS+QS+TF-FrM-6 2D Phase Diagram of Iron Sulfides on Au(111): From Hexagonal to Square Atomic Arrangement and Beyond, Andrea Berti**, University of Trieste, Italy; *Marco Bianchi, Paolo Lacovig, Silvana Lizzit*, Elettra-Sincrotrone Trieste, Italy; *Philip Hofmann*, Aarhus University, Denmark; *Alessandro Baraldi*, University of Trieste, Italy

Despite extensive research on two-dimensional (2D) materials, almost all experimentally synthesized 2D systems derive from van der Waals crystals (vdW). While the use of vdW crystals has been remarkably successful, it inherently restricts the 2D materials landscape to compounds that are already layered in their bulk form. Less than 5% of known inorganic materials possess a layered structure suitable for exfoliation, and the vast majority of functional compounds—such as oxides, sulfides, and nitrides—do not belong to this category. In recent years, increasing efforts have focused on the realization of truly two-dimensional monolayers from non-vdW compounds, which could unlock novel properties in fields such as high-temperature magnetism, catalysis, and strongly correlated electron phenomena. Beyond the class of vdW materials, only a limited number of compounds have so far been theoretically predicted to be stable in the 2D limit. In this context, iron-sulfur compounds have recently emerged as promising candidates. Density functional theory predicts that both hexagonal FeS_2 and tetragonal FeS phases can exist as stable monolayers, exhibiting strain-tunable magnetic properties. Although the Mermin-Wagner theorem precludes long-range magnetic order in ideal 2D isotropic systems, magnetic anisotropy can lift this constraint and allow stable ordering, enabling tunable magnetism at the atomic scale, which is essential for spintronics, as well as other emerging phenomena such as topological effects, multiferroicity, and proximity effects in heterostructures. However, compared to their bulk counterparts, Fe-S systems generally display a rich phase diagram, characterized by multiple stoichiometries and atomic arrangements. A similar complexity may also persist in the 2D limit, highlighting the need for a systematic experimental investigation into which 2D FeS_x phases can actually form. For this purpose, we systematically grow and characterize iron sulfide monolayers on Au(111) via in-situ co-deposition of Fe and S. Low-energy electron diffraction (LEED), scanning tunneling microscopy (STM), and X-ray photoelectron spectroscopy (XPS) reveal two primary phases: one with a hexagonal atomic arrangement consistent with FeS_2 (Fig. 1a), forming a moiré superstructure, and one with a square arrangement (Fig. 1b). By tuning sulfur exposure, we observe additional phases with varying stoichiometry and atomic arrangement, all belonging to the same 5×5 superstructure family (Fig. 1c). These results confirm the existence of a complex 2D phase diagram for FeS_x monolayers, establishing them as a versatile and tunable platform for exploring 2D magnetism in non-vdW systems.

9:45am **2D+AQS+EM+NS+QS+TF-FrM-7 The Electronic Band Structure and Conduction Band Formation of $HfSe_3$** , *Gauthami Viswan*¹, University of Nebraska-Lincoln, USA; *Alexey Lipatov*, South Dakota School of Mines and Technology; *Alexander Sinitskii*, University of Nebraska-Lincoln, USA; *Jose Avila*, Synchrotron SOLEIL and Université Paris-Saclay, France; *Takashi Komesu*, University of Nebraska-Lincoln, USA; *Maria C. Asensio*, Madrid Institute of Materials Science (ICMM), Spain; *Peter A. Dowben*, University of Nebraska-Lincoln, USA

Abstract: The anisotropic structure of Group 4 transition metal trichalcogenides (TMTCs) have gained significant interest due to their possible application in optoelectronics. In this work, the band structure of quasi one-dimensional $HfSe_3$ was investigated with nano-spot angle resolved photoemission spectroscopy (nanoARPES). $HfSe_3$ has a rectangular surface Brillouin zone where the effective hole mass along the chain direction is $-0.27 m_e$ which is smaller compared to the effective hole mass along the direction perpendicular to the chains, $-1.17 m_e$. The effective hole mass extracted from the band structure along different high symmetry directions is compared with that of TiS_3 and ZrS_3 from prior studies.¹ X-ray absorption spectroscopy (XAS) has been used to characterize the unoccupied states of $HfSe_3$ and will be compared to the XAS spectra of HfS_3

² and TiS_3 and ZrS_3 .³ The metal chalcogenide hybridization for Hf differs from the Ti and Zr trichalcogenides. This may be due to the increase in effective atomic number leading to strong spin-orbit interaction of Hf based TMTCs.

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10:30am **2D+AQS+EM+NS+QS+TF-FrM-10 Applications of Two-dimensional Materials in Energy, Water, and Healthcare, David Estrada**, Boise State University **INVITED**

The rapidly evolving field of 2-dimensional (2D) materials continues to open new frontiers in fundamental and applied research across water purification, healthcare, and energy applications. This talk will highlight our recent work in the synthesis of 2D and layered-materials-based inks, enabling energy innovations in microsupercapacitors, triboelectric nanogenerators, and electron devices [1-3]. In water applications, we introduce a flowing electrode capacitive deionization (FE-CDI) system utilizing $Ti_3C_2T_x$ MXene electrodes to efficiently remove and recover ammonia from synthetic wastewater and carbonates from simulated ocean water. This FE-CDI system demonstrates promising potential for managing nitrogen and carbon cycles while improving access to clean water [4]. In healthcare, the intersection of graphene and biology offers a powerful avenue for musculoskeletal tissue engineering, where graphene's exceptional physical properties contribute to fundamental biological insights [5-7]. Lastly, this talk will highlight recent insights into WS_2 nucleation and film growth on sapphire using tungsten hexacarbonyl and hydrogen sulfide precursors in an AIXTRON 2D Close Coupled Showerhead MOCVD 3×2 reactor, with in situ photoreflectometry monitoring. Together, these findings highlight the transformative role of 2D materials beyond graphene in addressing critical engineering challenges and advancing sustainable solutions across diverse fields.

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11:00am **2D+AQS+EM+NS+QS+TF-FrM-12 Electronic Structure Modulation in 2D Metal-Graphene-Metal Electrocatalysts for CO_2 Reduction and Hydrogen Evolution Reactions, Arturo Medina, Ines Saih, Vikas Muralidharan**, Georgia Institute of Technology; *Jinwon Cho*, NREL; *Faisal Alamgir*, Georgia Institute of Technology

Two-dimensional metal-graphene-metal (M/Gr/M) heterostructures provide a versatile platform for tuning electrocatalytic behavior through controlled interfacial strain and charge redistribution. In previous work, orbital-level descriptors were introduced to explain how pseudo-epitaxial strain alters the electronic structure of ultrathin metals, driving changes in

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catalytic activity for the CO₂ reduction reaction (CO₂RR). These concepts were grounded in density functional theory and validated experimentally by correlating spectroscopic strain signatures with shifts in catalytic onset potential.

Building on this framework, the present study expands the scope and range of electrocatalytic reactions studied in M/Gr/M systems. We integrate new measurements on the hydrogen evolution reaction (HER), exploring whether the same strain–electronic structure–reactivity relationships observed in CO₂RR extend to HER kinetics. This includes analysis of onset potentials, overpotentials, and durability across a diverse set of M/Gr/M configurations. Various metals from the 3d to 5d series were investigated as candidate electrocatalysts, deposited as atomically thin layers on single-layer graphene. The graphene is supported by both metal and metal oxide substrates, enabling systematic modulation of ligand effects and interfacial bonding.

To probe strain and charge transfer, we employ a suite of synchrotron-based and lab-scale techniques including carbon K-edge near-edge X-ray absorption fine structure (NEXAFS), extended X-ray absorption fine structure (EXAFS), ultraviolet photoelectron spectroscopy (UPS), X-ray photoelectron spectroscopy (XPS), and electron energy loss spectroscopy (EELS). We track strain-induced modifications in electronic structure through synchrotron-based spectroscopy, revealing systematic correlations between interfacial bonding, orbital structure, and catalytic performance. By comparing systems with and without graphene, we isolate the role of interfacial bonding in modulating both electronic structure and catalytic behavior.

This work experimentally explores theoretical predictions for HER in M/Gr/M systems and provides new insight into how strain-induced orbital modulation governs charge transfer and reactivity across multiple electrocatalytic reactions. Together, these results highlight M/Gr/M structures as a model system for disentangling the fundamental interactions between dimensionality, strain, and catalytic function.

11:15am 2D+AQ5+EM+NS+QS+TF-FrM-13 Large Area Nanostructuring of Van Der Waals Materials for Photon Harvesting in the Flat Optics Regime, Matteo Barelli¹, Francesco Buatier de Mongeot, Simone Di Marco, University of Genoa, Italy; Rajesh Chennuboina, University of Genoa, India; Giorgio Zambito, Giulio Ferrando, University of Genoa, Italy; Matteo Gardella, CNR-IMM, Italy; Maria Caterina Giordano, University of Genoa, Italy

2D-Transition Metal Dichalcogenides (2D-TMDs) are two-dimensional semiconductors featuring high optical absorption coefficient combined with good transport and mechanical properties. Although mechanically exfoliated TMDs flakes ensure the best optoelectronic properties, homogeneous large-area growth techniques are mandatory for real-world applications [1,2]. At the same time, in view of light conversion applications in the extreme thickness regime of 2D-TMDs, it is essential to develop effective photon harvesting flat optics strategies derived from nanophotonics.

Here we demonstrate that periodic modulation of few MoS₂ and WS₂ on large area nanostructured samples fabricated by laser interference lithography (either MoS₂ nanostripes arrays or conformal MoS₂ layers grown on top of nanogrooved silica templates). These nanopatterned layers can effectively steer light propagation via Rayleigh Anomalies in the flat optics regime, promoting strong in-plane electromagnetic confinement and broadband omnidirectional photon absorption enhancement, with strong impact in photoconversion. [3,4].

As a case study, we investigate the photocatalytic performance of periodically corrugated MoS₂ layers for photodissociation of Methylene Blue (MB), a widely used yet harmful textile dye. Under optimized angles coupling light to photonic anomalies, MB degradation is two times faster compared to planar MoS₂ films [5]. Additionally, periodic TMD nanostripes serve as directional scatterers, expanding possibilities for advanced light manipulation.

Another major challenge is the scalable fabrication of 2D van der Waals (vdW) heterostructures, often limited to micrometric flakes. Here, we demonstrate large-area (cm²-scale) nanoscale reshaping of vdW heterostructures. Specifically, we report a flat-optics platform using vertically stacked WS₂-MoS₂ heterostructures endowed with type-II band alignment, forming periodic nanogratings [6]. These engineered large-area

vdW heterostructures enable scalable applications in nanophotonics, photoconversion [7], and energy storage.

We recognize funding by the NEST - Network 4 Energy Sustainable Transition - PNRR partnership.

References

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11:30am 2D+AQ5+EM+NS+QS+TF-FrM-14 Exploring the Temperature Coefficient of Frequency (TC_f) in Graphene Trampoline Resonators, Yunong Wang, Nawara Tanzee Minim, S M Enamul Hoque Yousuf, Philip Feng, University of Florida

In this work, we report the first experimental investigation of the temperature coefficient of resonance frequency (TC_f) in graphene trampoline nanoelectromechanical system (NEMS) resonators. Trampoline resonators are widely used in photothermal sensing applications thanks to their superior thermal isolation, enabling high sensitivities. Leveraging the exceptional mechanical strength, thermal stability, and ultralow mass of two-dimensional (2D) materials, graphene trampoline resonators offer a compelling platform for ultrafast infrared (IR) detection. Characterizing the TC_f is essential for designing sensors with stable performance across a wide temperature range, enabling high-resolution IR detection, and developing robust NEMS for advanced light sensing applications.

We use focused ion beam (FIB) to make trampoline structure on our graphene drumhead resonator. The resonance characteristics of the device are measured by using a laser interferometry system. An intensity-modulated 405 nm blue laser is employed to drive the device photothermally, and a 633 nm He-Ne laser is used to read out device resonance motions. The reflected light is detected by a photodetector and converted to an electrical signal, which is analyzed by a network analyzer to obtain the resonance response. To measure the resonance frequency at different temperatures, we regulate the temperature of the device with a metal ceramic heater. The temperature of the chip is measured by a platinum resistance temperature sensor.

We measure the resonance response of the device at different temperatures and extract the resonance frequency and quality (Q) factor by fitting the measured spectrum to the damped simple harmonic resonator model. The drumhead resonator with 20 μm diameter shows a resonance frequency $f=3.44$ MHz and $Q=528$, while after FIB, the trampoline structure achieves a significantly higher $f=13.03$ MHz and $Q=5509$. As temperature increases, the negative thermal expansion of graphene causes an upward shift in resonance frequency. We observe a TC_f exceeding 30,100 ppm/°C from the drumhead structure, extracted from frequency shifts between 30 °C and 60 °C. After we FIB the drumhead structure into a trampoline, we found that the TC_f reduced to 588 ppm/°C.

A lower TC_f value from the stage heating-up method is desirable for stable operation across varying thermal conditions. Due to geometric isolation and reduced thermal coupling to the substrate, the trampoline is expected to exhibit a smaller TC_f than its drumhead counterpart. This makes the trampoline resonator a strong candidate for IR sensing applications that require stable performance over a broad range of temperatures.

¹ JVST Highlighted Talk

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