2D Materials Technical Group
Room 303 - Session 2D+EM-MoM

2D Materials: Electronic, Mechanical, and Optical Properties

Moderator: Sarah Haigh, University of Manchester, UK

8:20am **2D+EM-MoM-1 Scanning Tunneling Spectroscopy of 2d Electronic Materials – from Monolayers to Complex Heterostructures**, ***Chih-Kang (Ken) Shih***, Department of Physics, The University of Texas at Austin **INVITED**

Atomically thin, single-crystalline 2D electronic materials have recently emerged, offering a remarkably wide range of building blocks of nanostructures, ranging from metals (e.g. graphene), large gap insulators (BN), to semiconductors (transition metal dichalcogenides and black phosphorous). One key advantage of these van der Waals materials lies in the flexibility of stacking different types of materials to form heterostructures, providing a design platform for achieving novel device functionality.With the ability to probe electronic structures with atomic resolution, scanning tunneling microscopy/spectroscopy (STM/S) has played a crucial role in advancing our understanding of the electronic structures of 2D electronic materials and their heterostructures.

In this talk, I will present a comprehensive combination of different modes of scanning tunneling spectroscopy beyond the conventional constant height tunneling spectroscopy.I will use a few examples to show how such comprehensive investigations provide an in-depth understanding of the electronic structure evolutions from monolayer to complex heterostructures (including moire superlattices and beyond).

9:00am **2D+EM-MoM-3 Strain and Charge-Transfer at the Device Relevant Interface Between Single Layer MoS_2 and Gold: In-Situ Raman Study**, ***Stephanie Lough***, *J. Thompson,* University of Central Florida*; R. Rao,* Air Force Research Laboratory*; M. Ishigami,* University of Central Florida

Next-generation technology nodes will reach the sub-nanometer range via the introduction of ultra-thin and short-channel devices. Traditional semiconductors such as silicon (Si) suffer from device-degrading effects such as roughness-induced scattering or short-channel effects at this size scale. Two-dimensional transition metal dichalcogenides (2D TMDs) do not suffer from these effects. Therefore, they could be candidate materials for the next-generation nodes. Single-layer molybdenum disulfide (SL-MoS_2) devices exhibit carrier mobilities exceeding that of Si-based devices with similar thicknesses, but suffer from high contact resistance, reducing their utility in device technologies. Our previous results show that the physics at the interface between SL-MoS_2 and gold (Au) is complex and that thermal annealing (TA) under certain conditions could lead to lowered contact resistance by direct chemical hybridization and/or doping.

We performed detailed *in situ* Raman spectroscopy of exfoliated SL-MoS_2 on Au during and after annealing at temperatures ranging from room temperature (RT) to 300 °C in Ar. This revealed doping and mechanical strain induced in the SL-MoS_2 by the underlying Au layer. Using peak deconvolution, we identify the presence of two sub-peaks comprising each of the well-known MoS_2 fingerprint peaks (A_{1g} and E_{2g}), consistent with previous studies. The ratio of intensities and relative shifting of the sub-peaks indicates a strong interaction between the MoS_2 and the Au layer, which could be due to hybridization between the MoS_2/Au. The well-known Si peak at 520 cm^{-1} diminished as the temperature was increased. As such, we conclude that the MoS_2 delaminated from the Au layer at elevated temperatures. The coupling between the Au and MoS_2 was reestablished upon cooling to RT after annealing as indicated by the reappearance of the Si peak. Further, as the MoS_2 was annealed at progressively higher temperatures, it became increasingly electron-doped by the Au with the strain remaining constant at 1% in tension.

Our data shows that TA and cooling of the interface between SL-MoS_2 and Au produces stronger coupling, suggesting an increased level of hybridization between the MoS_2/Au. The hybridization results in a nearly charge-neutral MoS_2-Au heterostructure, indicating that TA could be a path toward achieving intrinsic contacts for device applications. Finally, the strain between these surfaces remains unchanged upon annealing, implying that annealing promotes stronger coupling between SL-MoS_2/Au, without increasing strain. Thus, annealing presents an ideal route towards generating charge-neutral MoS_2/Au contacts with minimal interfacial strain.

9:40am **2D+EM-MoM-5 Optical and Electrical Investigation into HfS_2 Oxidation Mechanisms**, *I. Chirca, A. Almutairi,* ***Stephan Hofmann***, University of Cambridge, UK

2D layered materials are emerging as potential candidates for energy-efficient conventional devices, as well as new memristive and neuromorphic device architectures. The focus to date has been on new semiconductor materials, particularly transition metal dichalcogenides (TMDs). Yet, feasible technology, especially in the optoelectronics field, relies on clean interfacing, particularly to a suitable dielectric. HfS_2 is one of the few materials that offer a native oxide conversion pathway, previously demonstrated in various experimental set-ups. Here we explore the oxide formation kinetics on HfS_2 layers and the achievable interface quality in HfS_2/HfO_x devices.

To accomplish this, we employ several HfS_2 oxidation methods, from thermal to plasma and pulsed water vapour exposure, and compare the electrical switching behaviour of MIM and MIS device structures while characterizing their dielectric properties via spectroscopic ellipsometry. The oxidative behaviour of HfS_2 and the buried HfS_2/HfO_x interface are observed optically using a combination of reflectance spectra and ellipsometric modelling. In order to determine the viability of such an approach for device fabrication, the natively grown HfOx is benchmarked against ALD grown hafnia.

Thus, our study is a step towards finer control of interface quality in HfS_2/HfO_2 devices through calibration of the native oxidation pathway.

10:40am **2D+EM-MoM-8 Electrical Characterization of β-In_2Se_3 Thin Films Synthesized via Molecular Beam Epitaxy**, ***Cooper Voigt***, Georgia Institute of Technology, USA*; B. Wagner,* Georgia Tech Research Institute*; E. Vogel,* Georgia Institute of Technology, USA

β-In_2Se_3 is a two-dimensional semiconductor that has long been believed to have a centrosymmetric crystal structure. α-In_2Se_3 is a closely related, two-dimensional, ferroelectric semiconductor [1,2] and has shown promise in low-power, neuromorphic electronic devices [3,4] and transistors [5]. Much work has been devoted to exploring the performance of α-In_2Se_3 in electronic devices due its unique combination of properties; however large-area thin-film synthesis of α-In_2Se_3 has not been established. Since 2018 there have been reports of polarization in a β'-In_2Se_3 phase arising from displacements of the center layer selenium atoms [6–8]; however, these studies have not included any fabrication and characterization of electronic devices. One study from 2018 claims deposition of large-area, ferroelectric In_2Se_3 thin-films via MBE; however, it is difficult to distinguish the α from β phase by the Raman spectra and TEM micrographs provided. Earlier this year, ferroelectric behavior was reported in transistors fabricated from metal-organic chemical vapor deposition (MOCVD) β-In_2Se_3 [9]. If β-In_2Se_3 does truly exhibit ferroelectric ordering, it would be a very promising material for low-power transistors and neuromorphic electronic devices.

In this study, we demonstrate molecular beam epitaxy (MBE) synthesis of β-In_2Se_3 thin-films and electrical characterization of β-In_2Se_3 transistors. We link processing parameters such as synthesis substrate temperature, and Se/ In flux ratio to resulting β-In_2Se_3 electrical properties and device performance.

[1]M. Küpers, et. al., Inorg. Chem. **57**, 11775 (2018).

[2]J. Xiao, et. al.,Phys. Rev. Lett. **120**, 227601 (2018).

[3]B. Tang, et. al., ACS Appl. Mater. Interfaces **12**, 24920 (2020).

[4]L. Wang, et. al., Adv. Funct. Mater. **29**, 1 (2019).

[5]M. Si, et. al., Nat. Electron. **2**, 580 (2019).

[6]S. Li, et. al., Sci. Adv. **4**, eaar7720 (2018).

[7]F. Zhang, et. al., ACS Nano **13**, 7, 8004–8011 (2019).

[8]Z. Zhang, et. al., Adv. Mater. **34**, (2022).

[9]S. Lee, et. al., 2D Mater. **9**, 025023 (2022).

[9]S. M. Poh, et. al., Nano Lett. **18**, 6340 (2018).

[10]S. Lee, et. al., 2D Mater. **9**, 025023 (2022).

11:00am **2D+EM-MoM-9 Mechanics of Pristine and Pyrolysed Carbon Nanomembranes (CNMs)***, **André Beyer**, F. Paneff, X. Zhang, A. Gölzhäuser,* Bielefeld University, Germany

The discovery of graphene has triggered a great interest in inorganic as well as molecular two-dimensional (2D) materials. Over the last years, a remarkable progress in the mechanical characterization of free-standing 2D materials was achieved [1]. In this contribution, we compare mechanical characterization of membranes by means of bulge tests and nanoindentation experiments. The bulge test was found to be a reliable method, which is suited for any kind of membrane. Nanoindentation was found to be suited for a number of membrane types while others entail a high risk of rupturing. With these two methods, a number of different pristine and pyrolysed carbon nanomembranes (CNMs) were examined. CNMs form by irradiation induced cross-linking of molecular layers e.g. self-assembled monolayers of terphenylthiol (TPT) molecules. Cross-linking between adjacent molecules was induced by low energy electron exposure. Pyrolysis of CNMs is known to yield nanocrystalline graphene, which is in agreement with the observed stiffening of the membranes. Part of this contribution will be devoted to a comparison of different approaches to analyse pressure-deflection measurement data of bulge tests. A sum of the limits approach is suggested as most precise method that employs an analytic pressure-deflection expression for determining the mechanical properties.

[1] X. Zhang and A. Beyer, Nanoscale 13, 1443 (2021).

11:20am **2D+EM-MoM-10 Interplay between Electronic, Magnetic and Mechanical Properties in 2D Crystals***, **Young-Woo Son**,* Korea Institute for Advanced Study, Republic of Korea **INVITED**

In this talk, I will discuss unique aspects of two-dimensional crystals that show intertwined nature between electronic, magnetic, optical properties and structural distortions. First, when a transition metal dichalcogenide (TMD) overlay another TMD forming moire superlattices, the softer one deforms itself to conform the mismatched lattices between them so that the unique whirlpool shaped lattice distortions occur [1]. I will show our recent theoretical and computational study shown that the pair of torsional distortions with the opposite chirality introduce characteristic fuzziness in Raman spectroscopy and interesting excitonic signatures irrespective twist angles. agreeing with experiments very well [1]. Second, a newly synthesized 2D carbon allotrope by linking biphenylene molecules is shown to host interesting type II Weyl fermions together with a possible magnetic orderings [2]. With external mechanical perturbations, our first-principles calculations including self-consistent extended Hubbard interactions reveal the anomalous Lifshitz transition of pair annihilations with merging onto zone-center saddle point.

[1] J. Kim, E. Ko *et al.*, *Nat. Mater.* (2022). https://doi.org/10.1038/s41563-022-01240-2

[2] Y.-W. Son *et al*., *Nano Lett.***22**, 3112 (2022).

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