

# Wednesday Morning, December 11, 2024

## Nano and 2D Materials

### Room Naupaka Salon 4 - Session NM1-WeM

#### Surface Engineering and Characterization

Moderator: Gregory S. Herman, Argonne National Laboratory

8:20am **NM1-WeM-2 Synthesis, Doping, and Encapsulation of 2D Transition Metal Dichalcogenides**, *Yu-Chuan Lin*, National Yang Ming Chiao Tung University (NYCU), Taiwan **INVITED**

Two-dimensional (2D) transition metal dichalcogenides (TMDC), such as  $\text{MoS}_2$  and  $\text{WSe}_2$ , exhibit useful material properties and versatile material chemistry for optoelectronic devices, quantum information, and energy missions. To realize these applications, we need to make them in large areas and be able to control their impurity concentrations. First, I will introduce our metalorganic chemical vapor deposition (MOCVD) process for deposition of TMDC epitaxial monolayers and the approach for growth of epitaxial TMDC multilayers on sapphire. Next, I will discuss how we introduced Re or V dopants into the cation sites of TMDC by MOCVD and their impact on the quality and properties of TMDC films.[3] In addition to cation substitutional doping, we can create Janus TMDC with an intrinsic dipole moment by replacing the elements at the anion sites (i.e., S and Se). I will present our result [4,5] of the conversion of 2D  $\text{WS}_2$  and  $\text{MoS}_2$  into 2D Janus  $\text{WSSe}$  and  $\text{MoSSe}$  by pulsed laser deposition and explain how we confirmed the presence of a dipole moment in 2D Janus TMDC optically. To improve the interface quality between TMDC and oxide dielectric materials for electronic applications, we developed thermal atomic layer deposition (ALD) of amorphous boron nitride (aBN) on both traditional and van der Waals surfaces. In the end, I will talk about nucleation and growth of aBN on  $\text{MoS}_2$  surface in our thermal ALD and aBN/ $\text{MoS}_2$  integration for improve field-effect transistor performance and quantum well fabrication.[6]

#### References

(1) Lin *et al.*, *ACS Nano* **2018**, *12*, 965–975. (2) Eichfeld *et al.*, *ACS Nano* **2015**, *9*, 2080–2087. (3) Torsi *et al.*, *ACS Nano* **2023**, *17*, 15629–15640. (4) Lin *et al.*, *ACS Nano* **2020**, *14*, 3896–3906. (5) Zheng *et al.*, *ACS Nano* **2022**, *16*, 4197–4205. (6) Chen *et al.*, *Nat. Comm.* **2024** *15*, 4016.

9:00am **NM1-WeM-4 Small Clusters of Molecular Anions: Locally Probing a Model Hubbard System**, *Sarah Burke*, University of British Columbia, Canada **INVITED**

Electronic correlations drive many important phenomena in materials that cannot be described by a single-electron picture. The Hubbard model captures a remarkable range of this behaviour by introducing an on-site interaction – the “Hubbard  $U$ ” – that competes with the kinetic energy of the electrons, or delocalization through wavefunction overlap – described by the hopping parameter  $t$ . While Hubbard models are not generically analytically or even exactly solvable, model systems such as clusters often are and can lend insights into more complex extended structures. The success of such models in describing correlated electron phenomena like Mott-insulator transitions, charge density waves, magnetically ordered states, and superconductivity<sup>1</sup>, is typically assessed by comparing to macroscopic quantities. However, as a model that captures the local character of electron-electron interactions, local tools provide a unique perspective. Noncontact atomic force microscopy (ncAFM) offers a particularly intriguing view through the ability to probe charge states and electrostatic interactions locally.

We used clusters of PTCDA molecules adsorbed on NaCl bilayer films on silver as an experimental prototype of a 4-site Hubbard model in a regime where  $U \gg t$ . PTCDA clusters have weak in-plane hybridization ( $t$  small), and isolated molecules have a Hubbard  $U$  in gas phase of  $\sim 3\text{eV}$ , reduced to  $\sim 1.4\text{eV}$  by screening of the nearby silver<sup>2</sup>. The large electron affinity of PTCDA leads to electron transfer from the silver substrate, so that isolated molecules carry a charge of  $-1$ . Thus, these clusters represent a half-filled Hubbard model where localization is expected, connected to a reservoir of charge. We used STM, STS, ncAFM and electrostatic force spectroscopy to probe the structures, charge states, and charging energies of two different geometries of 4-molecule clusters as well as isolated PTCDA- molecules. Equilibrium charge distributions of asymmetric clusters show charge segregation, while symmetric clusters show uniform charge. A 4-site extended Hubbard model was mapped onto the experimental results to identify the necessary interactions required to describe the ground state and charge excitations of the system. Once above a threshold where  $U/t$  drives localization, intersite energy differences and repulsion compete with hopping, driving the observed charge segregation and unexpected correlated behaviour.

1. M. Qin, *et al.*, *Annu. Rev. Condens. Matter Phys.* **13**, 1–28 (2021).

2. K. A. Cochrane, *et al.*, *Nat. Commun.* **6**, 8312 (2015)

9:40am **NM1-WeM-6 Tunable Areal Density and Defined Morphology Regimes of Langmuir Monolayers of PEGylated Gold Nanoparticles**, *H. Cameron, I. Curtis, R. Takai*, Mount Allison University, Canada; *M. Radford*, Simon Fraser University, Canada; *A. Williams*, Mount Allison University, Canada; *B. Gates*, Simon Fraser University, Canada; *M.-Vicki Meli*, Mount Allison University, Canada

The interfacial behaviour and control of nanoparticles has important consequences on their assembly into thin films, superstructures and subsequent materials suitable as metamaterials and nanophotonics applications. Our investigations into the interfacial self-assembly of nanoparticles coated with polyethylene glycol (PEG) and tetradecane thiols as a function of ligand shell and subphase composition will be presented. Methyl- and carboxylic acid-terminated PEG thiols are compared as a function of subphase pH. Film morphology is demonstrated as a function of ligand composition, transitioning from island-forming to isolated individual nanoparticles with controllable areal density. Transmission electron microscopy of the self-assembled films will be presented with corresponding surface pressure vs. area compression isotherms. Insights into NP film purity and (in)stability as it relates to the mentioned parameters will also be discussed. Compression-expansion isotherms with exceptionally large onset areas were measured. The effect of added tetradecanethiol into the ligand shell is shown to improve the stability and maintain the separation of the nanoparticles in the films.

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