Surface Science
Room 305 - Session SS-ThM

Reduced Dimensional Systems

Moderators: Rachael Farber, University of Kansas, **Nan Jiang**, University of Illinois - Chicago

8:00am **SS-ThM-1 Large Moiré Potential in a Weakly Interacting Organic/2D Material Heterostructure**, ***Oliver Monti***, University of Arizona **INVITED**

Layered materials provide an exceptional platform for manipulating electronic states and spin properties, with examples ranging from the emergence of strongly correlated phases to exciton condensates and the appearance of multiferroicity. Key to these advances in creating a sandbox for materials "synthesis" is the concept of proximitization of two materials. Conventionally, this is achieved by few-layer heterostructures of 2D materials to create moiré potentials by lattice mismatch and twist angle. The depth of this potential is often restricted to some tens of meV. Achieving deeper moiré potential would enable the control of correlated phenomena to significantly higher temperatures, expanding the utility of moiré heterostructures and potentially revealing new phenomena. In this presentation, I will discuss how this can be achieved in a hybrid organic/van der Waals layered material heterostructure, with the case of C_{60}/T_d-WTe_2. We employ angle-resolved photoemission spectroscopy and scanning tunneling microscopy to reveal that the interface forms a quasi-periodic moiré potential owing to a lattice mismatch between C_{60} and T_d-WTe_2. The C_{60} rotational orientation on the surface establishes a quasi-periodic superlattice locked to the moiré pattern, which in turn modulates the molecular bandgap. This manifests as a moiré potential with an unusually deep modulation depth of 130(20) meV.

This discovery reveals a new path for creating highly tunable moiré heterostructures that lend themselves for creating flatband systems that may enable the study of correlated physics at elevated temperatures. The wide space of available organic molecules in combination with the growing library of 2D materials makes this a promising new avenue to pursue, with the potential to afford larger wavelength moiré structures with fewer defects than conventional 2D/2D heterostructures fabricated by exfoliation and transfer can provide.

8:30am **SS-ThM-3 Epitaxial Moiré-Graphene for Resonance Excitonic Energy Transfer in Moiré -Graphene-TMDC Heterostructures**, ***Abdullah Al-Mahboob***[1], *Asish Kundu, Dario Stacchiola, Jerzy T. Sadowski,* Brookhaven National Laboratory

Two-dimensional (2D) quantum materials, specifically, Moiré-Graphene (MGr) and Van der Waals heterostructures (HSs) of quantum materials have attracted great interest because of their exotic quantum properties and having promises in novel optoelectronic and photonic applications. HSs made of stacking atomically thin layers of transition-metal dichalcogenides (TMDCs) allow us to manipulate the optical and spintronic properties. In TMDC HSs of monolayers having the resonance between dark excitonic states, recently, we observed unconventional energy transfer (ET) process massively enhancing photoluminescence (PL) and valley polarization (VP) [1]. In-order to elucidate underlying mechanism, we synthesized scalable epitaxial MGr (EMGR) in ultra-high vacuum system and fabricated HSs of WSe_2-hBN-EMGr in Ar-atmosphere. We employed in-situ, low-energy electron microscopy and X-ray photoemission electron microscopy (LEEM/XPEEM) for in-situ growth study and electronic/structural characterization of both EMGR and HSs, high-resolution ARPES for obtaining band-structure of EMGR and series of optical, microscopy and spectroscopy techniques for the study of the resonant excitonic exchange in HSs. The electronic band structure of EMGR revealed that the energy of optical transition between Moiré Dirac-cone to Van Hove Singularity states across M-point in EMGr has matching with resonance excitation energies in WSe_2. The observed optical data could be understood via vvacuum-fluctuation-mediated phonon-bypass mechanism suppressing non-radiative recombination of exciton and valley depolarization in Van der Waals HSs.

Research was carried out at the Center for Functional Nanomaterials and the National Synchrotron Light Source II at Brookhaven National Laboratory under Contract No. DE-SC0012704.

[1] Arka Karmakar, Abdullah Al-Mahboob, Natalia Zawadzka, Mateusz Raczyński, Weiguang Yang, Mehdi Arfaoui, Gayatri, Julia Kucharek, Jerzy T. Sadowski, Hyeon Suk Shin, Adam Babiński, Wojciech Pacuski, Tomasz Kazimierczuk, Maciej R Molas, Twisted MoSe2 Homobilayer Behaving as a Heterobilayer, Nano Lett. 24, 31, 9459–9467 (2024).

8:45am **SS-ThM-4 Can the Binding Energy of H_2O Admolecules on the Ice Ih(0001) Surface Exceed the Bulk Cohesive Energy?**, ***Jörg Meyer***, Leiden University, Netherlands

The adsorption of water molecules on ice surfaces is of significant importance in many respects, in particular for gaining a deeper understanding of ice crystal growth. There is a wide distribution in the binding energy of the admolecule on the ice Ih surface due to the proton disorder, and previous theoretical calculations have indicated that it can even exceed the cohesive energy of the crystal at certain sites [1]. While the accuracy of those calculations has been contested [2] and direct measurement of these binding energy remains elusive, such strong binding sites have been tentatively brought up to rationalize experimental observations [3].Here, we study the adsorption of a water molecule on the ice Ih(0001) surface using recently developed polarizable many-body interaction potential functions [4,5], which provide high accuracy for a number of ice properties. We show that sites with binding energy larger than the cohesive energy are found on surfaces with a wide range of proton ordering. Although the binding energy is dominated by electrostatics, it is also significantly influenced by dispersion interactions. Furthermore, we show how the local environment at the binding site affects the binding energy, and propose a descriptor that serves as a predictor of the binding energy at a given site.[1] E. R. Batista and H. Jónsson, Comp. Mater. Sci. 20, 325 (2001).[2] C. Thierfelder, A. Hermann, P. Schwerdtfeger, and W. G. Schmidt, Phys. Rev. B 74, 045422 (2006).[3] M. Mehlhorn and K. Morgenstern, Phys. Rev. Lett. 99, 246101 (2007).[4] E. Ö. Jónsson, S. Rasti, M. Galynska, J. Meyer, and H. Jónsson, J. Chem. Theory Comput. 18, 7528 (2022).[5] G. R. Medders, V. Babin and F. Paesani, J. Chem. Theory Comput. 9, 1103 (2013); V. Babin, C. Leforestier and F. Paesani, ibid. 9, 5395 (2013); V. Babin, G. R. Medders, and F. Paesani, ibid. 10, 1599 (2014).

9:00am **SS-ThM-5 Templated Growth and Intercalation Pathways of Nickel Nanoclusters on Graphene/Ir(111)**, ***Shilpa Choyal***[2], *Nan Jiang, Michael Trenary,* University of Illinois Chicago

Two-dimensional graphene moiré superlattices on transition-metal substrates provide periodic templates for organizing metal adatoms into size- and shape-controlled nanostructures with tailored catalytic and magnetic properties. Despite extensive studies of other transition metals, the growth and thermal evolution of nickel on graphene/Ir(111) have remained largely unexplored. Here, we report a comprehensive scanning tunneling microscopy (STM) investigation of Ni nanocluster nucleation, growth, and intercalation on the Gr/Ir(111) moiré superlattice under ultra-high vacuum.

At room temperature, Ni deposition produces well-defined triangular nanoclusters with edges aligned along the ⟨110⟩ direction of Ir(111), reflecting the templating effect of the moiré. Site-resolved STM analysis reveals strong selectivity: 77% of clusters nucleate at fcc regions, 23% at atop sites, and none at hcp sites — a preference attributed to local rehybridization of graphene toward sp^3-like bonding upon Ni adsorption. By comparing stepwise and continuous deposition, we identify two distinct growth regimes: continuous deposition produces uniform triangular islands with narrow size distributions, whereas stepwise growth yields broader, irregular morphologies governed by uphill diffusion, Ostwald ripening, and Ehrlich–Schwoebel barriers.

Annealing to ~900 K drives complete intercalation of Ni beneath graphene. STM reveals two distinct inverted moiré contrasts "round" and "clover-like" corresponding to site-selective Ni occupation within the supercell. The intercalated Ni grows pseudomorphically, adopting the Ir(111) in-plane lattice and preserving the original (10×10)/(9×9) moiré periodicity. The random spatial distribution of intercalated islands beneath an intact graphene monolayer, combined with Ni's strong C-binding affinity, supports an exchange-intercalation mechanism in which transient Ni–C bonding enables atom-by-atom penetration followed by graphene self-healing. Stepwise annealing up to 1500 K shows partial Ni desorption while the moiré remains intact.

These findings elucidate registry-controlled growth and demonstrate a viable route for fabricating low-roughness graphene-based

[1] **JVST Highlighted Talk**

[2] **AVS Graduate Research Awardee**

heterostructures, with implications for spintronics, heterogeneous catalysis, and graphene-based device engineering.

9:15am **SS-ThM-6 Probing local structural variations in metal–organic framework thin films using nano-FTIR***, **Tomoko Shimizu,** Yukihiro Matsumoto, Kento Takenaka,* Keio University, Japan*; Hiromasa Sato,* Institute for Molecular Science, Japan*; Yuto Fujita,* Keio University, Japan*; Toshiki Sugimoto,* Institute for Molecular Science, Japan

Precise control over coordination structures and orientation is crucial for integrating metal–organic framework (MOF) thin films into functional devices.Structural defects, such as missing metal ions or unbound functional groups leading to incomplete coordination, can markedly impact the pore architecture and alter material properties. Therefore, techniques capable of probing local bonding states and defect distributions are essential for understanding and ultimately controlling structural irregularities in MOF films.

In this study, we employed infrared scattering-type scanning near-field optical microscopy (IR s-SNOM), which combines atomic force microscopy (AFM) with nano-Fourier transform IR spectroscopy (nano-FTIR), to definitively characterize local coordination bonding in a representative MOF thin film, NAFS-1, fabricated at the air/liquid interface and transferred to Si substrates[1].

Variations in structural features and nano-FTIR spectra revealed inhomogeneities in coordination bonding and orientation. In NAFS-1 prepared by the conventional method, which incorporated a water-rinsing step after each film transfer cycle, peaks attributed to uncoordinated carboxyl groups (COOH) were found to be distributed throughout the film,indicating incomplete coordination. In contrast, certain sparse features, such as particle-like aggregates and large, elevated features, exhibited enhanced coordination, as evidenced by the increased intensity of the carboxylate (COO^-) vibrational peaks. Notably, while omitting the post-transfer water-rinsing step increased structural inhomogeneities at the nanoscale, macroscopic spectroscopies, such as the transmission-mode FTIR and UV-Vis absorption spectroscopy, suggested more effective coordination and expanded conjugation.

Our findings emphasize the necessity of integrating nanoscale imaging with spatially resolved spectroscopy to identify the local crystallinity and orientation of MOF thin films. This approach provides a crucial framework for evaluating and optimizing the structural integrity of this class of materials, preventing misinterpretation of macroscopic data that would otherwise obscure irregularities due to averaging effects.

[1] Matsumoto *et al.*, Langmuir, Accepted.

9:30am **SS-ThM-7 Spatially Resolved Understanding of Electronic-Metal Support Interactions on Pristine and Defected Cu/TiO_2(110)***, **Lindsey Penland*** [1] *,* The University of Kansas*; Hirushan Arachchige, Nadith Dissanayake,* The University of Kansas, Sri Lanka*; Rachael Farber,* The University of Kansas

Oxide-supported metal nanoparticle catalysts are commonly used in heterogeneously catalyzed chemical transformations due to their high selectivity, efficiency, and stability. There is a unique interplay between the metal nanoparticles and oxide support which results in strong metal support interactions (MSI). These MSI lead to observed changes in catalytic activity. Electronic metal-support interactions (EMSI), a subcategory of MSI characterized by electronic perturbations attributed to charge transfer across a metal/support interface, have a direct influence on the physicochemical properties of oxide supported metal nanoparticles. There are, however, several coexisting factors that can influence the degree of EMSI in a system such as the identity, size, and morphology of the nanoparticles and the Lewis acidity and oxygen defect density of the oxide support. Consequently, the coexisting nature of these factors makes it difficult to distinguish their respective effect on EMSI. As such, there is a need to develop a thorough understanding of the material properties leading to EMSI in a controlled and isolated way. In this work, insight into how the electronic landscape of a Cu/TiO2(110) model catalyst evolves as a function of EMSI was obtained through the use of low-temperature scanning tunneling microscopy (LT-STM) and spectroscopy (STS). It was found that the local density of states (LDOS) of clean rutile TiO2(110) has subtle variations in the valance region depending on the exact surface reconstruction of the TiO2(110) substrate. STM characterization post sub-monolayer Cu deposition highlighted variations in Cu morphology induced by thermal aggregation. LDOS measurements taken atop, near, and away from Cu particles show that electronic perturbations occur not only at the immediate metal/support interface but also extend into the near-interfacial region surrounding the Cu particles. Distinct variations in the LDOS perturbation radius and intensity suggest the degree of EMSI is correlated to nanoparticle size and morphology. These findings not only highlight how the presence and morphology of metal nanoparticles have direct influence on the electronic structure of the support but also opens the door to determining how electronic heterogeneity may play a role in heterogeneously catalyzed transformations. Ongoing and future work is focused on expanding these findings to structurally heterogeneous surfaces to understand how the inherent electronic heterogeneity of defected TiO2(110) influences the EMSI between Cu and TiO2(110).

11:00am **SS-ThM-13 Structure and Electronic Properties of Two-Dimensional Iron-Based Oxides on Silver***, **Lindsay R. Merte,*** Malmö University, Sweden **INVITED**

Reduced dimensionality can stabilize oxide structures, coordination environments, and electronic states that differ substantially from those of bulk materials. Two-dimensional iron oxides grown on silver surfaces exemplify this, forming structures distinct from both bulk iron oxides and from strongly bound wetting layers observed on more reactive substrates such as platinum. In particular, a 2D-Fe_3O_4 phase forms with mixed Fe^{2+}/Fe^{3+} valence and both tetrahedral and octahedral coordination, analogous to bulk magnetite but composed exclusively of close-packed layers. Incorporation of cobalt or nickel is expected to modify the electronic structure and catalytic behavior of these oxides, making them attractive model systems for energy-conversion materials. Here we present structural and electronic characterization of pure and mixed Fe–Co and Fe–Ni two-dimensional oxide phases prepared by co-evaporation on Ag surfaces using STM, synchrotron XPS and NEXAFS, surface X-ray diffraction, and anomalous diffraction techniques. Complementary DFT calculations are used to explore the atomic structure and electronic properties of the observed phases. We further demonstrate anomalous surface X-ray diffraction measurements under ambient-pressure conditions, enabling element-selective structural characterization of these complex multicomponent 2D oxide phases during exposure to reactive environments.

11:30am **SS-ThM-15 A Multiscale Framework for Oxygen Adsorption, Surface Reconstruction, and Reactivity on Ag(111)***, **Bright Daniel,*** University of Tennessee Knoxville*; Braden Penuel,* University of Tennessee, Knoxville*; Carson Mize,* Leiden University, Netherlands*; Lonnie Crosby, Sharani Roy,* University of Tennessee Knoxville

Understanding oxygen behavior on Ag(111) is central to improving silver-based catalysts for ethylene epoxidation, yet capturing this behavior across realistic length and time scales remains a fundamental challenge. While density functional theory (DFT) provides atomic-level insight, its limited system size restricts direct exploration of coverage effects, subsurface oxygen formation, and surface reconstruction under catalytic conditions.

In this work, a multiscale framework was developed to bridge this gap by integrating DFT, lattice-gas modeling, and Monte Carlo (MC) simulations. First, DFT calculations were used to systematically study oxygen adsorption on Ag(111), including adsorption energetics, coverage-dependent surface saturation, subsurface oxygen formation, and pairwise interaction energies. The computed trends were consistent with experimental observations and prior theoretical studies, providing a reliable foundation for model development.

These DFT-derived interactions were then used to construct a lattice-gas model, enabling efficient exploration of large surface models beyond DFT-accessible scales. Monte Carlo simulations in both canonical (NVT) and grand canonical (μVT) ensembles were employed to probe oxygen adsorption behavior as a function of temperature and chemical potential. This approach captures coverage-dependent ordering, subsurface incorporation, and thermodynamic stability of oxygen populations. Building on this framework, the model was extended to investigate surface reconstruction by incorporating Ag–Ag and Ag–O interactions. Co-adsorption of oxygen and silver adatoms reveals emergent restructuring phenomena driven by oxygen coverage and local coordination environments, providing insight into dynamic surface evolution under reaction-relevant conditions. Finally, configurations derived from these studies were used to examine ethylene epoxidation pathways with and without chlorine promotion, linking surface structure directly to catalytic performance.

Overall, this work establishes a unified, physics-based framework that connects atomistic energetics to mesoscale surface behavior, offering a

[1] **SSD Morton S. Traum Award Finalist**

pathway to rationally design and control catalytic surfaces under realistic conditions.

11:45am **SS-ThM-16 Atomic-Scale Study of Boron Nanostructure Growth on Platinum***, **Nozomi Shirato**,* Argonne National Laboratory

Low-dimensional boron nanostructures have attracted significant attention due to their intricate structural polymorphism, unique electronic states, and catalytic relevance. Despite growing interest, the growth mechanisms governing boron nanostructure formation on metal substrates remain poorly understood. Here, we investigate the growth of boron on an Pt(111) single crystal surface, aiming to understand the complex interplay between surface geometry, boron-boron interactions, and boron-platinum binding that collectively drives polymorph selection and structural evolution. Low-temperature scanning tunneling microscopy (LT-STM) is employed to characterize the intricate surface structures at atomic resolution, revealing the detailed morphology of the resulting nanostructures. X-ray photoelectron spectroscopy (XPS) measurements provide insight into the chemical states of boron and its bonding conditions with the substrate. Combined, the techniques reveal structural and chemical states of boron growth on Pt(111) and lay the groundwork for tailoring boron nanostructures for catalytic applications.

12:00pm **SS-ThM-17 Differentiable Multivariate Curve Resolution for X-Ray Absorption Spectroscopy***, **Changhae Kim**, Jennifer Bjorklund, Brian Lee,* Brookhaven National Laboratory*; Esteban Fornero,* Instituto de Desarrollo Tecnológico para la Industria Química, Argentina*; Dario Stacchiola, Xiaohui Qu, Sara E. Mason,* Brookhaven National Laboratory

Time-resolved *in situ* X-ray absorption spectroscopy (XAS) is a premier technique for probing atomic structure and reaction dynamics. Deconvolving spectral sequences into invariant components and relative concentrations can draw direct connections between spectroscopic data and chemical kinetics. However, chemically meaningful deconvolution remains challenging. Multivariate curve resolution (MCR) is widely used for this purpose, but conventional implementations offer limited flexibility for incorporating prior knowledge. Here, we present a differentiable optimization framework inspired by machine learning fields that enables simultaneous regression of spectra and concentration profiles, with flexible, chemically informed constraints. We demonstrate this approach on XAS measurements of redox reactions at the $CuGaO_2$ (011) surface. The method can isolate small surface signals from the dominant bulk contributions and can distinguish catalytically active species by leveraging coupled multi-species kinetics, capabilities which are challenging to achieve with conventional approaches. In addition, preprocessing with a blind-spot denoising network can improve robustness. These results highlight the potential of differentiable MCR for analyzing complex, multi-dimensional spectroscopic data.

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