Surface Science
Room 209 CDE W - Session SS-ThA

Late Breaking Discoveries from the Rising Stars in Surface Science

Moderator: Nan Jiang, University of Illinois - Chicago

2:15pm **SS-ThA-1 Molecular Nanosystems at Interfaces**, ***Johannes Barth***[1], TU Munich, Germany **INVITED**

The utilization and organization of molecular species is an important issue for advancing nanoscale science and underpins the development of novel functional materials. To this end we explore molecular bonding and assembly at well-defined homogenous surfaces, textured templates, nanoelectrodes and 2D-sheet layers. The developed bottom-up fabrication protocols employ tailored building blocks and exploit both supramolecular engineering and on-surface covalent synthesis. Structure formation, chemical conversions, electronic and other characteristics are addressed by a multitechnique experimental approach, whereby scanning probe microscopy provides molecular-level insights that are frequently rationalised with the help of computational modeling. We work toward a rationale for the control of single molecular units and the design of nanoarchitectures with distinct functional properties.

3:00pm **SS-ThA-4 On-Surface Reactions of Electronically Active Self-Assembled Monolayers for Electrode Work Function Tuning**, ***Shadi Fatayer***[2], KAUST, Saudi Arabia

Organic electronics enable the fabrication of devices with unique properties and low manufacturing costs. Self-assembled monolayers (SAMs) of electronically active materials placed between the conducting electrode and photoactive layer have a significant impact on device performance. They extract charge, passivate defects, and alter interfaces, ultimately increasing the efficiency of organic devices.

Experimental imaging techniques with sub-molecular resolution play a crucial role in studying the influence of SAMs on interfaces. These techniques surpass the limitations of traditional experimental methods, allowing for detailed examination of molecular properties and establishing correlations between device performance and molecular characteristics.

Here, we will discuss the contributions that can be achieved by employing scanning tunneling microscopy (STM) and non-contact atomic force microscopy (AFM) in the context of SAMs on conductive substrates. We will focus on key information, including molecular packing, adsorption orientation, and assembling properties. Additionally, we will demonstrate how these properties vary depending on the preparation conditions and its influence on devices performance.

3:15pm **SS-ThA-5 THz-Induced Metastability and Atomic-Scale Dynamics of Local Charge Order in 1T-TaS_2**, ***Melanie Müller***[3], Fritz Haber Institute of the Max Planck Society, Germany

Light-induced control of quantum materials has opened new frontiers in condensed matter physics, enabling the manipulation of electronic and structural phases on ultrafast timescales. While time-resolved pump–probe techniques provide insight into these dynamics, they typically lack the spatial resolution needed to probe atomic-scale variations arising from defects, heterogeneity, or domain boundaries.

Recent advances in ultrafast scanning tunneling microscopy (STM) have enabled real-space imaging of ultrafast dynamics with angstrom resolution. In particular, THz-lightwave-driven STM (THz-STM) has emerged as a powerful tool [1,2] for probing femtosecond carrier dynamics, molecular vibrations, and collective excitations at the sub-nanometer scale. However, applying THz-STM to quantum materials with easily perturbed ground states remains challenging, as it requires STM operation under intense localized THz fields that can strongly perturb the system. This is especially critical in layered materials such as 1T-TaS_2, where electron–phonon coupling, electron correlations, and stacking-dependent charge order render the system highly sensitive to external perturbations.

I will present THz-STM of the ultrafast dynamics of local charge order in the layered transition metal dichalcogenide 1T-TaS_2. At low temperatures, 1T-TaS_2 exhibits a commensurate charge density wave (CDW) phase with an insulating gap that arises from a complex interplay of electron correlations and interlayer orbital interactions. Starting from the C-CDW ground state, we demonstrate that THz excitation in the STM drives 1T-TaS_2 into a metastable state (MS) with a modified quasi-stationary insulating gap, which we assign to a THz-driven modification of the interlayer stacking order. On top, THz-lightwave-driven tunneling allows to probe the photoinduced dynamics of the collective charge order within the MS. In particular, coherent oscillations in the THz-driven tunnelling current reveal the 2.45 THz amplitude mode of the CDW, which persists in the MS. In addition, we find an unknown 1.36 THz mode that emerges near a local defect, which can be assigned to an interlayer shear mode which coherently modulates the interlayer orbital overlap and the low-energy states in 1T-TaS_2.

These results highlight the dual role of the tip-enhanced THz fields in THz-STM, both as a driver of metastability and for probing local ultrafast dynamics, and highlight the influence of defects on the dynamics of local charge order.

3:30pm **SS-ThA-6 Plasmonic Probes for Liquid-Phase Tip-Enhanced Raman Spectroscopy**, ***Naihao Chiang***[4], University of Houston

Tip-enhanced Raman spectroscopy (TERS) combines the chemical specificity of surface-enhanced Raman spectroscopy (SERS) with the unmatched spatial resolution of scanning probe microscopy (SPM). During the last few years, there has been an explosion of interest and activity in nanoscale vibrational spectroscopy. One of the key factors for successful TERS implementation is the quality of the plasmonic probes used. Electrochemically etched silver or gold tips are commonly used in scanning tunneling microscopy (STM) -based TERS, and sub-nanometer chemical mappings of single-molecule have been demonstrated under ultrahigh vacuum conditions.

We are developing plasmonic probes for scanning ion-conductance microscopy (SICM) and electrochemical STM (EC-STM) to extend TERS into the liquid phase. For SICM-TERS, quartz nanopipettes (<100 nm) were sputter-coated with silver or gold under high vacuum. SERS of small molecules directly tethered on the plasmonic nanopipettes were used to optimize the fabrication parameters. For EC-STM-TERS, electrochemically etched probes were coated with commercial ultraviolet (UV) cured polymers, aiming for a better chemical resistance and lower background signal compared to conventional nail-polish coatings. In the future, we expect these liquid-phase TERS probes to provide chemical information at interfaces relevant to the emerging catalysis, energy, and bioengineering applications.

3:45pm **SS-ThA-7 Surface Science Reception**,

[1] **Surface Science Keynote Lecture**
[2] **Rising Star in Surface Science**
[3] **Rising Star in Surface Science**
[4] **Rising Star in Surface Science**

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