O 77: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: HE 101

O 77.1 Thu 10:30 HE 101

Atomic-scale insights into frictional energy dissipation mechanisms during single-molecule manipulation — •Lukas Hörmann[1], Alfred J. Weymouth[2], and Reinhard J. Maurer[1] — [1]University of Warwick, Coventry, UK — [2]University of Regensburg, Regensburg, Germany

Friction causes significant energy loss in any moving mechanical device. As the miniaturisation of devices reaches the quantum limit, so do dynamical dissipation processes. Fundamentally quantum mechanical mechanisms govern friction at the nanoscale. We account for all relevant quantum mechanical effects, such as charge transfer, or van der Waals interactions, by employing density functional theory, and machine learning and use the probe particle model to simulate energy dissipation. Using this approach, we investigate dynamic friction at the natural limit of a singular atom moving a single chemical bond. This enables us to explore how the local bonding environment of the underlying sample surface affects the energy dissipation that a probe particle experiences. Focussing on the example of a CO-functionalised lateral force microscope that measures frictional energy dissipation above various organic adlayers on Cu(111), we find strong correlations between the local bonding environment and the energy dissipation. Our findings capture the qualitative trends found in experiment. Finally, we present a mechanistic interpretation of our findings that provides insights into the underlying physics of atomic/lateral force microscopy measurements.

O 77.2 Thu 11:00 HE 101

Analyzing structures of biomolecules at single molecule level by direct imaging on surface — •Kelvin Anggara — MPI for Solid State Research, Stuttgart

Diverse structures of biomolecules in living systems pose challenges for present analytical methods in analyzing their individual molecular structures. Ensemble-averaged measurement on molecules with extensive structural variation leads to loss of structural information for individual molecules. We herein bypass this problem by imaging and analyzing single biomolecules deposited intact on surfaces. Biomolecules were transferred to the gas-phase by electrospray, mass-selected, and soft-landed at a cold single-crystal metal surface, using the Electrospray Ion Beam Deposition (ESIBD) technique. The deposited molecules were subsequently imaged one-at-a-time by Scanning Tunneling Microscopy (STM) and interpreted by DFT calculations to reveal their individual structures on surface. We successfully applied our approach to glycans (1) as well as lipids and proteins densely decorated with glycans (2), whose analyses remain intractable by current analytical methods. Critical to our success is the choice of surfaces to deactivate diffusion and dissociation of biomolecules on surface, as well as the systematic molecular manipulation by the STM tip to unfold the intact biomolecule on surface. The ESIBD+STM+DFT approach opens a new avenue to access individual structures of any biomolecules that can be electrosprayed and deposited onto a surface. 1. Nature 582, 375-378 (2020). 2. Science 382, 219-223 (2023).

O 77.3 Thu 11:30 HE 101

Controlling the Yu-Shiba-Rusinov states of radical molecules on the superconductor Pb(111) — •Chao Li, Jung-Ching Liu, Outhmane Chahib, Thilo Glatzel, Remy Pawlak, and Ernst Meyer — Department of Physcis, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Radical molecules are considered to be a promising candidate for the future quantum computer. Here, we studied a radical molecule of 4,5,9,10-tetrabromo-1,3,6,8-tetraazapyrene (TBTAP) on a superconductor Pb(111). Low-temperature scanning tunneling microscope images reveal its rectangle shape on Pb(111). Moreover, scanning tunneling spectra show a Yu-Shiba-Rusinov (YSR) state inside the superconductor gaps on the molecules which was ascribed to one electron transferred from its environment. The evolution of YSR energy with tip-to-molecule distance shows a quantum phase transition between the singlet state and doublet state. Moreover, different constructions of the dimer and trimmer show typical coupling features among the molecules.

O 77.4 Thu 12:00 HE 101

Investigating many-body phenomena through molecular nanostructures — •Shantanu Mishra — IBM Research Europe - Zurich, 8803 Rüschlikon, Switzerland

This two-part contribution shows that individual organic molecules and molecular nanostructures on surfaces serve as an outstanding material platform to access many-body physics. In the first part, the tip-induced synthesis of an elusive organic molecule, namely indeno[1,2-a]fluorene, will be demonstrated on thin insulating NaCl films on (111) coinage metal surfaces [1]. The molecule exhibits ground state bistability, wherein it can be stabilized either in a (high-spin) open-shell state, or a (low-spin) closed-shell state, each of which shows characteristic experimental bond length alternation and frontier orbital densities that agrees with theory. Switching between open- and closed-shell states of an individual molecule is observed by changing its adsorption site on NaCl. In the second part, the on-surface synthesis of organic $S = 1$ antiferromagnetic quantum spin chains on Au(111) surface will be shown [2]. A systematic study of length-dependent magnetic excitations in both open-ended and cyclic spin chains reveal gapped spin excitations in the bulk, with the gap saturating for sufficiently long spin chains, and fractional $S = 1/2$ edge states at the chain termini, which manifest as Kondo resonances. It will be shown that these spectral features are direct evidence of emergent symmetry-protected topological order in the spin chains, ratifying Haldane's conjecture for integer-spin antiferromagnetic chains. [1] S. Mishra et al. arXiv:2303.04483 (2023). [2] S. Mishra et al. Nature 598, 287 (2021).

O 77.5 Thu 12:30 HE 101

Topology and chirality driven chemical reactions in multifold chiral semimetals — •Qun Yang and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany

The interplay between chirality and topology nurtures many exotic electronic properties. For instance, topological chiral semimetals display multifold band crossings with large Chern numbers in the bulk state and superlong topologically robust surface states without resistance and resistant to surface perturbations at the surface, which allows the entire crystal or surface to serve as catalytic active sites. These materials have the potential to revolutionize the design principle of high-performance catalysts for electrochemical energy conversion. In this talk, I will present our recent progress in developing highly efficient water-splitting electrocatalyst based on chiral multifold semimetals through theoretical and experimental studies. We found that these materials break the performance record of normal noble metal electrocatalysts. Through the theoretical band structure calculations incorporating the topological approach, we reveal the interaction mechanism between topological states and catalytic reactions. We found that the monopole-like orbital angular momentum texture driven by the chirality in the materials also offers great potential for exploring the asymmetric adsorption of chiral molecules, paving the way for understanding the asymmetric chemical reactions based on inorganic chiral materials.