

O 72: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00

Location: CHE 89

O 72.1 Thu 10:30 CHE 89

Imaging electrons in 1D: correlated states within MoS₂ mirror twin boundaries — ●WOUTER JOLIE — II. Physikalisches Institut, Universität zu Köln, Germany

Electrons are prone to strong correlations when confined into one-dimensional (1D) cavities. An ideal experimental testbed for the observation of correlated electronic behavior is found in mirror twin boundaries (MTBs) of the two-dimensional material MoS₂. These MTBs function as structurally perfect 1D cavities, are only weakly coupled to the environment and accessible to spatially resolved spectroscopic investigations using scanning tunneling microscopy.

In my talk I will show that the confined quasiparticles within finite MoS₂ MTBs transform into spin and charge modes as described by the Tomonaga Luttinger theory of strongly interacting 1D electrons [1]. In addition, a Kondo resonance, delocalized over the entire length of the MTB, emerges when the highest occupied mode is half filled [2]. The unique construction of our Kondo system enables us to directly measure the energies of both the Kondo resonance and the half filled confined level, as well as their correlated beating along the boundary. Lastly, I will outline how to alter the electronic system in MTBs through giant Fermi level shifts [3] and atomic manipulation.

[1] W. Jolie et al., *Phys. Rev. X* 9, 011055 (2019)

[2] C. van Efferen et al., arXiv:2210.09675 (2022)

[3] C. van Efferen et al., *2D Mater.* 9, 025026 (2022)

O 72.2 Thu 11:00 CHE 89

Interface-engineered quantum states in van der Waals heterostructures — ●FELIX LÜPKE — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany

The assembly of van der Waals (vdW) materials into heterostructures enables the engineering of exotic quantum states by interface effects such as moiré and proximity. Scanning tunneling microscopy (STM) has become an important tool to study the properties of such heterostructure, because it gives direct access to the resulting structural and electronic properties. While the possibilities to combine different vdW materials in Lego-like fashion are virtually infinite, the fabrication of samples with atomically clean surfaces, as required for STM, was typically limited to air-stable or epitaxially grown samples, which drastically diminishes the engineering capabilities. To address this problem, we have developed a novel dry-transfer flip fabrication technique, which allows the preparation and STM study of heterostructures with atomically clean surfaces and interfaces and without exposure to air. In my talk, I will summarize our developments in heterostructure fabrication and will show results of proximity-induced superconductivity in topological insulator WTe₂, interlayer interactions in twisted bilayer WTe₂, phonon gap supported tunneling and interfacial electric fields in Fe₃GeTe₂ heterostructures, and quantum dot lattices in NbSe₂ heterostructures.

O 72.3 Thu 11:30 CHE 89

Electronic States and Polarons on Polar Surfaces — ●MICHELE RETICCIOLI¹, FLORIAN ELLINGER¹, MARTIN SETVIN², and CESARE FRANCHINI^{1,3} — ¹University of Vienna (Austria) — ²Charles University, Prague (Czech Republic) — ³University of Bologna (Italy)

Polar surfaces of oxides exhibit an internal electric field and intrinsic excess charge that might be exploited for a wide range of applications, such as catalysis or electron-hole separation for solar light harvesting. However, there is very limited fundamental understanding of the processes induced by the surface polarity. In our study we attempt to

shed some light on the nature of the electric field and the interplay with surface charge. Our density functional theory calculations and scanning-probe microscopy measurements on KTaO₃(001) show spontaneous localization of the excess charge in the form of electron and hole polarons. In the absence of external perturbations, the internal electrostatic potential keeps the electron-hole polaron pairs spatially separated. We also show that the electronic properties of the surface can be tuned by adsorbing molecules and metal atoms. Finally, we apply these concepts to more debated cases, such as the SrTiO₃(001) surface, where the polarity is too weak to produce a large charge separation. We believe that our findings contribute to deepen the interpretation of polar surfaces of oxides and ionic compounds in general.

O 72.4 Thu 12:00 CHE 89

Submolecular-scale control of phototautomerization — ●ANNA ROSLAWSKA¹, KATHARINA KAISER¹, MICHELANGELO ROMEO¹, FABRICE SCHEURER¹, STÉPHANE BERCLAUD¹, TOMÁŠ NEUMAN², and GUILLAUME SCHULL¹ — ¹Université de Strasbourg, CNRS, IPCMS, UMR 7504, 67000 Strasbourg, France — ²Institut des Sciences Moléculaires d'Orsay (ISMO), UMR 8214, CNRS, Université Paris-Saclay, 91405 Orsay Cedex, France.

Photochemistry plays a central role in fundamental natural and artificial reactions such as photosynthesis, photocatalysis, or phototautomerization. Here, we demonstrate that using a tunable light source focused on a scanning tunneling microscope (STM) tip we drive and control the rate of a free-base phthalocyanine (H₂Pc) phototautomerization with sub-molecular precision, providing a path to pilot the intrinsic reactivity of the molecule with an external controllable stimulus. In addition, we probe the excited state of the molecule, which drives the tautomerization, by recording tip-enhanced photoluminescence (TEPL) spectra and maps where varying patterns for non-resonant and resonant excitation conditions are observed. These TEPL maps reflect different atomic-scale coupling between the localized plasmonic fields and the transition dipole moment of the molecule influenced by the hydrogen switching process.

O 72.5 Thu 12:30 CHE 89

Single-molecule synthesis by scanning probe manipulation of intra- and inter-molecular reactions — ●QIGANG ZHONG^{1,2}, ARTUR MARDYUKOV^{2,3}, EPHRATH SOLEL^{2,3}, ALEXANDER IHLE^{1,2}, DANIEL EBELING^{1,2}, PETER R. SCHREINER^{2,3}, and ANDRÉ SCHIRMEISEN^{1,2} — ¹Institute of Applied Physics, Justus Liebig University Giessen (JLU), Germany — ²Center for Materials Research, JLU, Germany — ³Institute of Organic Chemistry, JLU, Germany

Single-molecule synthesis by scanning probe manipulation has emerged as a powerful tool not only to visualize, but also to generate and couple highly reactive molecules, which often are not accessible by traditional synthetic methods. As an example of precise "intra-molecular surgery", we demonstrate the on-surface synthesis of the structurally elusive cyclotriphosphazene (P₃N₃) based on STM tip-induced sextuple dechlorination of a sub-nanometer P₃N₃C₁₆ precursor molecule on a Cu(111) surface [1]. Real-space atomic-level imaging of P₃N₃ reveals its planar D_{3h}-symmetric ring structure. This method is further expanded to the inter-molecular level to construct covalent organic nanostructures molecule-by-molecule [2]. We have achieved unprecedented control over the whole reaction process including activation, lateral transfer and inter-molecular coupling of halogenated precursors on an inert NaCl surface. Our work presents strategies for synthesizing elusive molecules as well as covalent nanoarchitectures, studying structural modifications and revealing pathways of on-surface reactions.

[1] Preprint [https://doi.org/10.21203/rs.3.rs-2169632/v1]

[2] *Nature Chemistry* 13, 1133-1139 (2021)