O 9: Organic molecules on inorganic substrates: electronic, optical and other properties I

Time: Monday 15:00–18:00 Location: HSZ/0201

O 9.1 Mon 15:00 HSZ/0201

Adsorption-induced chirality of an otherwise highly-symmetrical molecule — •Jannis Lessmeister[1], Chetana Badala Viswanatha[1], Andreas Windischbacher[2], Christian S. Kern[2], Lu Lyu[3], Vitaliy Feyer[4], Iulia Cojocariu[4], Daniel Baranowski[4], Martin Aeschlimann[1], Peter Puschnig[2], and Benjamin Stadtmüller[3] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Graz, 8010 Graz, Austria — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [4]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany

Chirality is a fundamental concept with far-reaching implications across chemistry, biology and materials science. In condensed matter, interest has grown around the chiral-induced spin selectivity (CISS) effect, which promises spin-dependent functionality in chiral molecules without magnetic or heavy-metal components. So far, however, the role of the interface for CISS remains unclear.

To illuminate the interactions at chiral metal-molecular interfaces, we explore how the highly-symmetrical molecule pentacene adsorbes on a naturally chiral copper surface. Employing momentum microscopy we identify changes of the emission pattern of the frontier molecular orbitals of pentacene adsorbed on chiral Cu(643) versus achiral Cu(110). In conjunction with density functional theory calculations, we can attribute these observations to a twisting of pentacene and thus to an adsorption-induced chirality of the otherwise symmetric molecule.

O 9.2 Mon 15:15 HSZ/0201

Explaining Principles of Tip-Enhanced Raman Images with Ab Initio Modeling — •Krystof Brezina[1], Yair Litman[2], and Mariana Rossi[1] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

Tip-enhanced Raman spectroscopy (TERS) is an emerging method for imaging vibrational motion and chemically characterizing surface-bound molecular adsorbates. Existing approaches to TERS simulation often build on strong approximations, including a simplification or neglect of the underlying metallic substrate, often leading to discrepancies with experiments. In this work, we present a new, *ab initio* finite-field formulation of a TERS simulation framework [1] that can efficiently address large-scale, realistic systems under periodic boundary conditions [2]. This treatment is essential as it eliminates known artifacts in simulated TERS images stemming from substrate approximations, as shown by our benchmarks on adsorbates and surface defects, and allows for simulations directly comparable to experiments. In this direction, our simulations of Mg(II)-porphine on Ag(100) correctly explain the spatial intensity variation of experimental TERS images and provide an insight into the fundamental principles that define substrate contribution to the scattering cross section in TERS. Our infrastructure is generally applicable to any solid substrate, is computationally efficient and available within the FHI-aims electronic structure code.

[1] Litman Y. et al. *J. Phys. Chem. Lett.*, 14, 6850–6859 (2023)

[2] Brezina K., Litman Y. and Rossi M. *arXiv:2509.13075* (2025)

O 9.3 Mon 15:30 HSZ/0201

Periodic Potential Engineering of 2D Superlattices for Enhanced Photocatalysis — •Qun Yang — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Atomically thin semiconductors hold great promise for photocatalytic solar energy conversion, yet often face key challenges such as rapid electron-hole recombination, inappropriate band gaps, and misaligned energy levels to redox potentials. We introduce a general design strategy based on symmetry-defined periodic potentials for 2D photocatalyst engineering. These long-range modulations reshape the band structure and induce robust electron-hole separation without altering the material lattice. Applied to a monolayer InSe photocatalyst, we show that experimentally achievable moiré patterns, such as those formed with twisted hBN, enable miniband formation and tunable spatial charge separation. Moreover, the periodic potential modulates local adsorption energetics, providing a new handle to enhance catalytic activity for both photocatalytic hydrogen and oxygen evolution reactions. Our results provide a path toward the realization of high-efficiency solar-to-chemical energy conversion in a broad range of 2D materials.

O 9.4 Mon 15:45 HSZ/0201

Supramolecular organisation of thermolabile $TbPc_2$ derivatives at surfaces — •Patrick Lawes[1], Joachim Reichert[1], Anthoula C. Papageorgiou[1,3], Joe Komeda[4], Svetlana Klyatskaya[4], Andreas Walz[1,2], Annette Huettig[1,2], Hartmut Schlichting[1,2], Rochio Sánchez-de-Armas[6], Nicolas Montenegro-Pohlhammer[6,7], Carmen J. Calzado[6], Jean-Pierre Bucher[5], Johannes V. Barth[1], and Mario Ruben[4,8] — [1]TU Münich, DE — [2]pureions GmbH, Gilching, DE — [3]National and Kapodistrian University of Athens, GR — [4]Karlsruhe Insitute of Technology, DE — [5]IPCMS Université de Strasbourg FR — [6]Universidad de Sevilla, ES — [7]DIC, CIBQA, Universidad Bernardo OHiggins, CL — [8]CESQ, ISIS, Université de Strasbourg, FR

Creation and study of novel materials towards the goal of quantum information processing, involves sophisticated chemistry integrated into useful architectures. The self-organization of single-molecule magnets, is widely studied and reported. Utilizing electrospray ion beam deposition permits the study of thermolabile, functionalised bis(phthalocyaninato) terbium complexes on surfaces. This work aims to tailor the lattices of spin centres. Complex ligand tuned structures were characterised by scanning tunneling microscopy allowing for potential study into quantum criticality and quantum technologies.

O 9.5 Mon 16:00 HSZ/0201

Orbitals of Artificial Atoms in a Gapped Two-Dimensional Vacuum — Mong-Wen Gu[1,2], Aizhan Sabitova[1,2], Taner Esat[1,2], Christian Wagner[1,2], F. Stefan Tautz[1,2,3], Aleksandr Rodin[4,5], and •Ruslan Temirov[1,2,6] — [1]PGI-3, Forschungszentrum Jülich, Germany — [2]JARA, Fundamentals of Future Information Technology, Germany — [3]RWTH Aachen, Germany — [4]NUS, Singapore — [5]Yale-NUS College, Singapore — [6]University of Cologne, Germany

Artificial atoms–engineered nanostructures that confine electronic states–offer a route toward atom-by-atom design of electronic functionality. In this work, we use low-temperature STM and STS to study single-molecule vacancies in a commensurate PTCDA/Ag(111) monolayer, which act as attractive potentials for the two-dimensional interface-state electrons.

Using feature-detection STS [1,2], we directly image the vacancy-induced bound states and identify artificial analogues of *s*- and *p*-orbitals that split from the parabolic band minimum and hybridise when two vacancies are brought into proximity. Beyond these conventional orbital analogues, the periodically corrugated interface-state band hosts partial band gaps that support additional quasi-localised states with no counterparts in natural atoms. Tight-binding simulations reproduce these high-energy states and reveal their origin in the gap regions of the 2D dispersion.

[1] A. Sabitova, et. al., PRB 98, 205429 (2018), [2] J. Martinez-Castro, Commun. Mater. 3, 57 (2022)

O 9.6 Mon 16:15 HSZ/0201

Thermal and photo-induced one-dimensional switching of azobenzene derivatives on a graphite surface — •Thiruvancheril Gopakumar[1], Hariom Birla[1], Showkat H. Mir[1], Khushboo Yadav[1], Thomas Halbritter[2], Alexander Heckel[2], and Jayant K. Singh[3] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt, Max-von-Laue-Str. 9, 60438 Frankfurt, Germany — [3]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India

In this presentation we demonstrate an unusual one-dimensional (1D) cascade effect in the thermal- and photo-induced switching of azobenzene derivatives deposited on graphite surface. Upon thermal- and photo-induction, molecules switch between their geometric states (trans and cis) along a selected lattice within the assembly up to several hundreds of nanometres. Generally, such directionality is observed only for a length scale of few nanometres. It is revealed that the strong intermolecular interaction along one of the lattices compared to the other is at the origin of the 1D cascading effect. Harnessing cooperative switching opens possibilities for engineering the responses of molecular film to external trigger and provides opportunities to control the directionality of switching/reactions, and novel nanostructures.

O 9.7 Mon 16:30 HSZ/0201

Accessing Energetically Restricted Optical Transitions in a Single Free-Base Porphyrin Molecule — •Eve Ammerman, Nils Krane, and Bruno Schuler — Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Charge transfer between a single molecule and the electrodes of an STM leads to a series of excitation and relaxation processes, including radiative relaxation from the molecule's optically active excited states. Utilizing the STM tunnel junction in electroluminescence experiments enables optical characterization on sub-molecular length-scales. However, the electroluminescence phenomenon is constrained by the alignment of ionization and optical state energies. Here, we show how positive ion resonance energy of a free-base tetrabenzoporphyrin (H2TBP) can be tuned relative to the optical emission energy through local gating by the STM tunnel junction or by work function engineering. The tuning of the energy level alignment allows us to produce optical emission from H2TBP on Ag(111), where electroluminescence is energetically restricted, or on Ag(110) where the molecule becomes bright.

O 9.8 Mon 16:45 HSZ/0201

Optical characterisation of single chlorophyll molecules at the sub-nanometre scale — Thiago G. L. Brito[1], •Daniel Arribas[1], Myriam Wadsack[1], Claudia Leticia Gómez Flores[1], Victor Feitosa[1], Klaus Kuhnke[1], Klaus Kern[1,2], Kelvin Anggara[1], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

As one of the main biomolecules harvesting light in photosynthetic organisms, chlorophyll plays a crucial role in biological systems, ultimately sustaining life on Earth. Therefore, the fundamental understanding of its optical properties has attracted widespread interest from the scientific community. However, traditional spectroscopic experiments, often probing complexes, only provide an averaged understanding of the rich photophysics of chlorophyll, where the effects of each possible molecular configuration and the local environment are smeared out. In this work, we address this by exploiting the sub-nm resolution of scanning tunnelling microscopy and the highly-localised plasmonic enhancement of the picocavity in the tunnelling junction. We characterise individual chlorophyll molecules, deposited by electrospray ion beam deposition on a Ag(111) surface with NaCl islands as decoupling layer. By analysing the fluorescence emission excited by the tunnelling electrons, we observe the structural dependency of the molecular opto-electronic properties. Our investigation opens new opportunities for the fundamental understanding of light-harvesting during photosynthesis with unprecedented sub-molecular resolution.

O 9.9 Mon 17:00 HSZ/0201

Polaronic transport through a molecular system with scanning probe microscopy — •Laëtitia Farinacci[1,2,3], Gaël Reecht[3], Christian Lotze[3], and Katharina Franke[3] — [1]University of Wuerzburg, Wuerzburg, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Stuttgart, Germany — [3]Freie Universitaet Berlin, Berlin, Germany

Polarons are quasi-particles in which electron excitations couple to distortions of the local ions network surrounding them. Typically, they are studied in metal oxides where they heavily influence charge transport and thereby often are key to understand and characterize the materials' properties. Here, we use scanning tunneling microscopy and atomic force microscopy to study the properties of Fe-porphine-chloride (FeP-Cl) molecules adsorbed on Pb(111). We observe distinct properties in the dI/dV signal that are indicative of polaronic transport.

More precisely, we find that the FeP molecules form islands in which Cl adatoms are trapped between the molecules. This leads to an effective gating of the molecules by local electric fields that stabilize either of two electronic configurations. Some FeP molecules display sharp peaks in their dI/dV reminiscent of vibrational modes. Importantly, the mapping of these peaks in dI/dV reveal the key role of the electric field and the necessity to account for charge transport through the island. These ingredients are the fundaments of polaron formation and will provide complementary understanding of the fundamental phenomena at the origin their formation in organic/inorganic interfaces.

O 9.10 Mon 17:15 HSZ/0201

Debromination and π-radical formation by single-electron injection on an insulator — •Ye Liu[1], Felix Giselbrecht[1], Lucía Gómez-Rodrigo[2], Manuel Vilas-Varela[2], Tzu-Chao Hung[1], Diego Peña[2], and Jascha Repp[1] — [1]University of Regensburg, Germany. — [2]Universidade de Santiago de Compostela, Spain.

The creation of π-radicals in nanostructures offers promising opportunities in spintronics and quantum technologies1,2, yet their controlled formation on an insulator remains challenging3. Here, we investigated the charge-induced reaction of 11-bromo-11H-benzo[b]fluorene on thick NaCl films ($>$ 20 monolayers) using non-contact atomic force microscopy. The injection of only one electron from the microscope's tip induces debromination, which yield an open-shell structure and a bromide anion. In contrast, removal of an electron from the precursor results in a cation without bond cleavage. The voltage threshold for debromination depends on the molecular adsorption geometry, specifically on whether the bromine atom points upward or downward, reflecting opposite orientations of the molecular dipole moment. We present a feasible tip-induced synthesis strategy for generating a π-radical in molecule on an insulator, offering a promising route toward constructing larger open-shell nanostructure with multiple π-radicals on such surfaces.

O 9.11 Mon 17:30 HSZ/0201

Intramolecular cyclization of helicenes towards non-benzenoid nanographenes via formation of radicals — •Daniel Rothhardt[1], Ming-Lun Pan[2], Christian Wäckerlin[3,4], Hans Josef Hug[1], Yao-Ting Wu[2], Karl-Heinz Ernst[1,5,6], and Miloš Baljozović[1] — [1]Empa, Dübendorf, Switzerland — [2]National Cheng Kung University, Tainan, Taiwan — [3]PSI, Villigen PSI, Switzerland — [4]EPFL, Lausanne, Switzerland — [5]The Czech Academy of Sciences, Prague, Czech Republic — [6]University of Zurich, Zurich, Switzerland

On-surface synthesis has recently become a leading tool for controllable C-C bond formation that would otherwise hardly be accessible by conventional solution chemistry. The advancement of on-surface synthesis gave rise to a novel class of magnetic materials, namely open-shell magnetic nanographenes. The magnetism here mostly stems from the formation of unpaired electrons (radicals) due to a sublattice imbalance, topological frustration or aromatic stabilization. Such carbon-based spin systems are often considered promising candidates for spintronics applications due to their weak spin-orbit coupling and hyperfine interaction, allowing for long spin-lifetime and spin diffusion lengths. Here we demonstrate that the radical formation within the non-planar hydrocarbons such as helicenes leads to intramolecular bond formation and reorganization on Au(111) substrate resulting in non-benzenoid nanographenes. The products are identified using ToF-SIMS, STM and nc-AFM, corroborating the proposed radical-induced cyclization mechanism.

O 9.12 Mon 17:45 HSZ/0201

A Molecule with Half-Möbius Topology — Igor Roncevic[1,2], Fabian Paschke[3], Yueze Gao[2], Leonard-Alexander Lieske[3], Lene A. Gödde[2], Jascha Repp[4], Florian Albrecht[3], Harry L. Anderson[2], and •Leo Gross[3] — [1]Department of Chemistry, The University of Manchester, Oxford Road, Manchester, United Kingdom — [2]Department of Chemistry, Oxford University, Chemistry Research Laboratory, Oxford, United Kingdom — [3]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [4]Institute of Experimental and Applied Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, Regensburg, Germany

Stereoisomers of $C_{13}Cl_2$ exhibiting helical orbitals around a ring of carbon atoms were synthesized by atom manipulation on bilayer NaCl on Au(111). We resolved the enantiomeric geometries of the closed-shell singlet states by atomic force microscopy and mapped their helical orbital densities by scanning tunnelling microscopy. A π-orbital basis of the helical, non-planar singlets that twists by 90° in one circulation is consistent with a half-Möbius topology. In such a topology, the π-orbital basis changes sign with respect to two circumnavigations and is periodic with respect to four circumnavigations. This is in contrast to a topologically trivial Hückel basis, which shows no twist, and a Möbius basis, which twist by 180° in one circulation. We demonstrate reversible switching of the topology, between the two singlets of oppositely threaded half-Möbius topology, and the planar, topologically trivial, triplet state.