O 8: Nanostructures at surfaces:1D, 2D, networks I

Time: Monday 10:30–12:30 Location: WILL/A317

O 8.1 Mon 10:30 WILL/A317

Quantum confinement of excited states in a two-dimension metal-organic coordinated network — •Lu Lyu[1], Martin Anstett[2], Wei Yao[3], Tobias Eul[1], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [3]Institute of Advanced Light Source Facilities, Shenzhen 518107, China

Quantum confinement effects of surface electrons in two-dimensional metal-organic coordinated networks (2D-MOCNs) provide a highly tunable platform for exploring the laws of quantum mechanics in condensed matter systems. Here, we focus on a porous network formed by coordinating pyridine-functionalized T4PT molecules with Co atoms on Au(111). One-photon photoemission (1PPE) experiments reveal a substantial energy shift of the Shockley surface state (SS) that is indicative of a hybridization with Co centers. This hybridization is responsible for a leaky channel for electrons between adjacent pores, which prevents the quantum confinement of SS electrons. In contrast, excited electrons into the unoccupied image potential states (IPS) reveal clear signatures of a substantial quantum confinement in a two-photon photoemission (2PPE) experiment. These contrasting observations of SS and IPS can be attributed to the 3D nature of the quantum well potential of the 2D-MOCNs and the distinct surface-perpendicular wave function distribution in the SS and the IPS.

O 8.2 Mon 10:45 WILL/A317

On-surface prepared 2D MOFs as models of single-atom catalysts: Fe-N$_3$ vs. Fe-N$_4$ — •Zdeněk Jakub[1], Jakub Planer[1], Dominik Hrůza[1], Ayesha Jabeen[1], Tadeáš Lesovský[1], and Jan Čechal[1,2] — [1]CEITEC, Brno University of Technology, Brno, Czechia — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czechia

What defines the reactivity of the so-called single-atom catalysts? Here, we utilize 2D Metal-Organic Frameworks (MOFs) synthesized on an inert graphene support to address this fundamental question. By temperature-dependent scanning tunneling microscopy and density functional theory, we quantify the CO adsorption strengths on threefold-coordinated (Fe-N$_3$) and fourfold-coordinated (Fe-N$_4$) iron sites embedded within Fe-DCA and Fe-TCNQ 2D MOFs. A significant 0.5 eV difference in CO binding strengths is found, despite the fact that the electronic parameters like Fe oxidation state, spin configuration, occupancy of the individual d-orbitals and their positions with respect to Fermi level are almost identical prior to CO adsorption. We trace the origin of the different reactivity to the higher structural flexibility of the Fe-N$_3$ sites compared to Fe-N$_4$. These results highlight the key role of local coordination and demonstrate that reactivity cannot be reliably predicted from electronic structure parameters alone.

Invited Talk O 8.3 Mon 11:00 WILL/A317

Controlling nanostructures on surfaces via intermolecular interactions — •Yunjun Cao — Physical Chemistry I, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Synthesizing sophisticated nanostructures on surfaces requires precise control over intermolecular interactions ranging from strong covalent bonds to weak van der Waals interactions. In the first part of the talk, I will present an irreversible, multi-step covalent coupling strategy for reactive molecules. By precisely controlling the reaction sequence, we synthesize highly branched nanostructures on a metal surface [1]. As a complementary approach, I will then introduce a reversible, multi-step self-assembly protocol for sterically crowded molecules, highlighting how intermolecular van der Waals interactions steer the formation of well-separated cyclic nanostructures with an unprecedented high yield [2]. Finally, I will turn to the single-molecule level and discuss how to control via van der Waals interactions the configuration of individual molecules [3] and the potential energy landscape of a dynamic chirality switch [4]. Our studies highlight how tunable intermolecular interaction strengths control the synthesis of tailored nanostructures on surfaces.

[1] Y. Cao et al., Nat. Commun. in press (2025). [2] Y. Cao et al., ACS Nano 19, 21942 (2025). [3] Y. Cao et al., Phys. Rev. B 111, 115426 (2025). [4] Y. Cao et al., Nat. Commun. 14, 4500 (2023).

O 8.4 Mon 11:30 WILL/A317

Autonomous Nanoworld: Building Nanostructure Without Human Intervention — •Bernhard Ramsauer[1], Qigang Zhong[2], Stefan Pranger[3], Bettina Könghofer[3], and Oliver T. Hofmann[1] — [1]nstitute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, 8010, Austria — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, 215006, China — [3]Institute of Applied Information Processing and Communications, Graz University of Technology, Graz, 8010, Austria

In this contribution, we present atomically precise molecular nanostructures fabricated without human intervention. We demonstrate that simultaneous control of molecular position and orientation is attainable - both are prerequisites for constructing covalently bonded nanostructures in the future. We employ deep reinforcement learning agents to learn the complex tip-molecule-surface interactions by determining the optimal manipulation parameters for moving and rotating molecules. Because exhaustive sampling of all possible manipulation parameters is impossible, we generate a simulation based on selected experiments. This simulation allows us to train robust agents that even generalize to unseen adsorption conditions and arbitrary nanostructures. With this strategy, we autonomously assemble molecular building blocks into arbitrary geometries, establishing a reliable platform for automated molecular assembly.

O 8.5 Mon 11:45 WILL/A317

The Tale of a Band Melting in a Low-Dimensional Nanostructure — •Lenart Dudy[1,2], Julian Aulbach[2], Joerg Schaefer[2], Ralph Claessen[2], Victor Rogalev[2,3], and Piotr Chudzinski[4,5] — [1]Synchrotron SOLEIL, France — [2]U Würzburg, Germany — [3]Diamond Light Source, UK — [4]Queen's U Belfast, UK — [5]Polish Academy of Sciences, Poland

We explore the unusual phenomenon of “band melting” in the quasi-one-dimensional nanostructure Si(553)-Au. Using angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STM), we observe a striking disappearance of a well-defined electronic band upon increasing temperature, while the atomic structure remains unchanged. Such dramatic temperature-driven changes are rare and typically associated with strongly correlated systems like Kondo or Mott phases.

Our findings point to electronic disorder and suppressed quantum coherence along one dimension. Supported by theoretical insights, we interpret this behavior within a phenomenological framework involving Luttinger-liquid physics and frustrated (pseudo-)spin interactions. This work sheds light on the interplay between dimensionality, correlations, and disorder in low-dimensional materials, opening new perspectives for understanding emergent electronic phases in nanostructures.

O 8.6 Mon 12:00 WILL/A317

Iron-porphyrin coordination network with surface-bound dysprosium adatoms: implications for long-range magnetic ordering — •Pierre Josse[1,2], Massine Kelai[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], and Fabio Donati[1,3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Ordering spins on surfaces offers significant promise for spintronic, magnetic, magnetoelectric, and magneto-optic technologies. One effective approach is to employ spin-active centers embedded within molecular frameworks capable of self-organizing on surfaces. Porphyrins, with their exceptional chemical versatility and tunability, stand out as particularly suitable candidates for this purpose. Various strategies can be used to achieve such spin ordering, including molecular self-assembly, metal-ligand coordination, and on-surface synthesis involving the formation of C-C bonds. In this work, we present the specific strategies we use to organize spins on surfaces and examine how these methods influence long-range magnetic ordering.

O 8.7 Mon 12:15 WILL/A317

On-Surface Synthesis on Oxide — •Sonja Bohl[1], Kassandra

Zoltner[1], Leonard Neuhaus[1], Stefan R. Kachel[1], Agustina Heredia[2], Cissie Slopianka[1], Sophie Schäfer[1], Lisa Arnold[1], Doris Grumelli[2], Sabine Wenzel[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Universität Marburg — [2]INIFTA, Universidad Nacional de La Plata

Oxide surfaces offer the advantage of weak molecule-substrate interactions, enabling a more direct and undistorted probing of the properties of adsorbed molecules compared to metal substrates. However, the reduced adsorption energies represent a central challenge for on-surface synthesis, requiring adjusted precursor strategies to prevent premature desorption from the oxide substrates. In this work, we explore approaches to enable on-surface reactions on thin-film oxides and well-defined bulk oxides. While various nano-carbon structures have previously been synthesized on metal surfaces, we investigate whether analogous processes can be realized on oxides. Furthermore, we examine how metal-organic nanostructures interact with bulk oxide surfaces and whether the substrate can induce changes in their coordination environment. Our methodology combines on-surface synthesis with scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and temperature-programmed desorption (TPD).