O 69: Nanostructures at Surfaces II

Time: Wednesday 15:00–17:30 Location: H25

O 69.1 Wed 15:00 H25

Thermally-activated molecular rotors organised by porous networks on Au(111) — •Vishakya Jayalatharachchi[1], Roberto Robles[2], Milan Kivala[3], Nicolás Lorente[2,4], Meike Stöhr[1,5], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]Institute of Organic Chemistry, University of Heidelberg, Germany — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain — [5]University of Applied Sciences of the Grisons, Switzerland

Gaining insights into the precise control of molecular rotation on surfaces is crucial for making progress in nanoscale device innovation. In this study, we investigate the thermally triggered rotational motion of bromine-functionalized decacyclene (Br-DC) molecules, which are confined within a host-guest network of 4,4,'4"-nitrilotribenzoic acid (H3NTB) on Au(111). With scanning tunneling microscopy (STM) experiments at variable temperatures, we could determine both the onset of molecular rotation (around 110 K) and the barrier for rotation. Importantly, the Br-DC molecules do not possess a predefined intrinsic rotation axis. Instead, the rotational motion is facilitated by the attractive interactions between the Br-DC guests and the H3NTB host network. Computational simulations support our findings and provide further insights into the energetics. Our strategy provides greater flexibility and versatility compared to traditional confinement approaches based on precise size matching of rotor and host networks.

O 69.2 Wed 15:15 H25

Examination and Modification of Self-organized Nanostructures in the Ternary System Au/Co/Ge(001): Chain Growth and the Observation of a Zero-Bias Anomaly — •Nico Kubetschek, Till-Jakob Stehling, Ulrike Kürpick, Marcel Schlesag, Johann Tonhäuser, and René Matzdorf — Institute of Physics, University of Kassel, Heinrich-Plett-Str. 40, Kassel D-34132, Germany

The twofold symmetric reconstruction of the Ge(001) surface provides a template for the self-organized formation of various transition metal nanostructures [1]. We employed scanning tunnelling microscopy (STM) and spectroscopy (STS) at 77 K and 5 K to examine the nucleation, chain growth, and subsequent modification of hexagonal cobalt nanostructures embedded in Ge(001) [2] through the introduction of gold-induced defects [3]. Moreover, the introduction of additional amounts of Au resulted in the formation of previously unobserved nanorods [4]. The electronic properties of these rods were examined by STS, which revealed a zero-bias anomaly (ZBA) in the tunneling spectra. The formation of nanorods with high aspect ratios was subjected to a systematic statistical investigation.

[1] J. Schäfer et al. 2009, New J. Phys. 11 125011, [2] H. J.W. Zandvliet et al. 2011, Surface Science 605,1129, [3] J. Tonhäuser et al. 2022 Phys. Rev. B 106, 115404, [4] M. Schlesag et al. 2024 Phys. Rev. B 110, 195412

O 69.3 Wed 15:30 H25

Electrical Modulation of a Plasmonic Single Particle Resonance — Luka Zurak[1], Christian Wolff[2], Jessica Meier[1], René Kullock[1], •Asger Mortensen[2], Bert Hecht[1], and Thorsten Feichtner[1] — [1]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, 97074 Würzburg, Germany — [2]POLIMA Center for Polariton-driven Light-Matter Interactions, University of Southern Denmark, DK-5230 Odense M, Denmark

Acitive modulation of plasmonic resonances is a promising route towards optical switches smaller way that than the diffraction limit. However, due to the difficulties to directly electrically connect a single resonator most experiments in this direction have been performed on large scales and/or in electrochemical environments – hampering interpretation and application.

Here, we demonstrate fast modulation of the plasmonic resonance of a single electrically connected gold nano-rod [1]. We employ a lock-in amplifier to measure the relative change of scattering signal $\Delta S/S_0$ in the spectral range from 500 to 900 nm, while driving our structure with up to 50 kHz in frequency and up to 40 V in voltage amplitude. Results are of the expected order of magnitude according to existing theories. We discuss some of the theories in detail, like classical surface currents or the introduction of Feibelman parameters to account for non-classical electron spill-out at metal surfaces.

[1] Zurak, L., et al. (2024). Modulation of surface response in a single plasmonic nanoresonator. Science Advances, 10(36), eadn5227.

O 69.4 Wed 15:45 H25

On-surface induced fitting and mobility of conformationally flexible molecules inside nanometer-sized quantum confinements — Aisha Ahsan[1,2], •Aaron Oechsle[2,1], Luiza Buimaga-Iarinca[3], Lutz H. Gade[4], and Thomas A. Jung[2,1] — [1]Department of Physics, University of Basel, 4056 Basel, Switzerland — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5232 Villigen, Switzerland — [3]CETATEA, National Institute for Research and Development of Isotopic and Molecular Technologies, 400293 Cluj-Napoca, Romania — [4]Institute of Inorganic Chemistry, University of Heidelberg, 69120 Heidelberg, Germany

Host-guest architectures provide ideal systems to investigate site-specific physical and chemical effects. Condensation events in nanometer sized confinements are particularly interesting for the investigation of inter-molecular and molecule-surface interactions. They may be accompanied by conformational adjustments representing induced-fit packing patterns. Here, we report that the symmetry of small clusters of cycloalkane molecules, formed by condensation, their registry with the substrate, their structure as well as their adsorption height is characteristically modified by their packing in confinements. While cyclopentane and cycloheptane display cooperativity upon filling of the hosting pores, cyclooctane and to a lesser degree cyclohexane diffusively re-distribute to more favored adsorption sites. The site-specific modification of the interaction and behavior of adsorbates in confinements plays a crucial role in many applications of porous materials, e.g., as gas storage agents or catalysts and biocatalysts.

O 69.5 Wed 16:00 H25

Areas of lower local contact potential difference in the wetting layer in the system Pb/Si(111)-(7x7) — •Paul Philip Schmidt[1], Felix Hartmann[1], Ralf Metzler[1,2], Janet Anders[1,3], and Schmidt Hoffmann-Vogel[1] — [1]University of Potsdam, Institute of Physics and Astronomy, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang 37673, Republic of Korea — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

The description of the diffusion of Pb atoms on Si(111)-(7x7) is highly non-trivial. Previous studies show that although Pb grows in the Stranski-Krastanov mode, it exhibits explosive island growth and ultrafast mass transport [1,2]. The developing wetting layer plays a special role [3]. We have investigated this system using non-contact scanning force microscopy and Kelvin probe force microscopy. We have worked under ultrahigh vaccum conditions at variable temperatures between 120K and 300K. Our studies show inhomogeneities of the work function in the wetting layer. The areas with different work function seem to be related to the position of the islands and the step edges of the Si(111). We assume that the different work function values are caused by different Pb concentrations in the wetting layer, which are probably related to the preferred direction of growth of the islands, so that in certain areas Pb is extracted from the wetting layer with varying effectiveness. [1] M. Hupalo et. al. Phys. Rev. B, 23 (2007), [2] K. L. Man et al. Phys. Rev. Lett., 101 (2008), [3] M. T. Hershberger et al. Phys. Rev. Lett. 113 (2014)

O 69.6 Wed 16:15 H25

Pyridyl-functionalized tripod molecules on Au(111): Interplay between hydrogen bonding and metal coordination — •Sajjan Mohammad[1], Neeta Bisht[2], Anjana Kannan[1], Anne Brandmeier[2], Christian Neiss[2], Andreas Görling[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Department of Chemistry and Pharmacy, Chair of Theoretical Chemistry, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]University of Applied Sciences of the Grisons, Switzerland

Two-dimensional metal-organic coordination networks (MOCNs) offer rich opportunities for fabricating materials with potential applications in catalysis and molecular electronics. We investigated the self-assembly of pyridyl-functionalized triazine (T4PT) on Au(111) using low-temperature scanning tunneling microscopy (STM) complemented by density functional theory (DFT) calculations. T4PT forms a well-ordered, close-packed structure stabilized by hydrogen bonds upon adsorption at 300 K. Upon post-deposition annealing, the assemblies are additionally stabilized by metal-ligand bonding between the pyridyl ligands and native Au adatoms. Further post-deposition annealing to 473 K led to the breaking of the N-Au bonds, with the molecular assemblies transforming into a second close-packed hydrogen-bonded structure. Above 503 K, few covalently linked dimers formed, likely as a result of CH-bond activation. Our findings highlight the challenge of predicting and controlling 2D structure formation for porous MOCNs on metal surfaces due to competing interactions.

O 69.7 Wed 16:30 H25

Active manipulation of interface electronic structures by two-dimensional metal-organic coordination on metallic substrates — •Lu Lyu[1,2], Jonas Gödde[2], Martin Anstett[2], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, 86159 Augsburg, Germany — [2]Department of Physics, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Designing two-dimensional metal-organic coordination networks (2DMOCNs) on metallic substrates provides a unique approach for engineering interface electronic structures. To achieve this goal, we first investigate a protocol of pyridine-functionalized T4PT molecules with Co coordination (Co-T4PT) adsorbed on Au(111). In this system, the surface state electrons are bound to the Co metal centers, and charge transfer occurs between the Co and the substrate. By substituting the Co center with a Cu atom, the surface state electrons in the Cu-T4PT coordination exhibit weaker binding to the Cu centers and are partially confined within the pores surrounded by the molecular potentials. Additionally, replacing T4PT with cyano-functionalized DCA enhances the coordination between Co and DCA, resulting in altered charge transfer within the Co-DCA plane. Consequently, the orbital states of DCA undergo modifications in both energy and momentum space. Our study demonstrates that the manipulation of coordinated metals and functionalized molecules can actively tailor electronic structures at a 2DMOCN-metal interface.

O 69.8 Wed 16:45 H25

Unveiling hybrid electronic bands in 2D metal-organic frameworks: insights from density functional theory and photoemission spectroscopy — Dominik Brandstetter[1], Simone Mearini[2], Yan Yan Grisan Qiu[2], Daniel Baranowski[2], Andreas Windischbacher[1], Claus Michael Schneider[2,3], Vitaliy Feyer[2,3], and •Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-6, FZ-Jülich, Germany — [3]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

Two-dimensional metal-organic frameworks are atomically thin materials that combine properties of organic molecules with the characteristics of crystalline inorganic solids. The strong bonding between the organic linkers and transition metal centers may result in new electronic states with hybrid organic/inorganic character, from which two-dimensional, dispersing electronic bands emerge. However, until recently no experimental proof for such hybrid bands could be given and the requirements for efficient hybrid band formation remained unknown. Here, we combine density functional theory calculations with experimental angle-resolved photoemission spectroscopy to reveal the nature of the interaction between the transition metal atoms and the organic linker. On the example of the Ni-TCNQ network supported on Ag(100) and by employing photoemission orbital tomography, we observe how the molecular orbitals hybridize with the Ni d-states of appropriate symmetry. Our findings are not only based on electronic structure theory, but are also confirmed by the experimental photoemission fingerprints of the involved molecular orbitals.

O 69.9 Wed 17:00 H25

Atomic size effects in 1D metal-coordination polymers on silver — •Pengfei Zhao[1], Hongxiang Xu[1,3], Joachim Reichert[1], Anthoula C. Papageorgiou[1,2], and Johannes V. Barth[1] — [1]Technical University of Munich, Germany — [2]National and Kapodistrian University of Athens, Greece — [3]Peking University, China

Supramolecular coordination on solid surfaces provides a versatile approach to synthesize one-dimensional metal coordination polymers (1D-CPs), where the atomic size of metals plays a crucial role in determining the final structures and properties. Here, we systematically investigate 1H,1'H-2,2'-bibenzo[d]imidazole (H_2bbim) on silver substrates under ultra-high vacuum. Using scanning probe microscopy, we find that the shape of 1D-CPs can be steered by metal-coordination templating with different metal atom sizes. Specifically, H_2bbim molecules and cobalt atoms on Ag(100) allow the formation of micrometer-sized 1D-CPs with porphyrinoids formed by covalently fused H_2bbim dimers, which is distinct from its counterpart of holmium-coordinated chains of monomers. This suggests that size-tuned metal templating is a good strategy for tailoring the formation of 1D-CPs, demonstrating its potential for next-generation electronic devices.

O 69.10 Wed 17:15 H25

An insight into the thermally activated organometallic-to-covalent transition in novel Graphdiyne Molecular Wires Frameworks — •Alice Cartoceti[1], Simona Achilli[2], Paolo D'Agosta[1], Alessio Orbelli Biroli[3], Guido Fratesi[2], Valeria Russo[1], Andrea Li Bassi[1], and Carlo Spartaco Casari[1] — [1]Department of Energy, Politecnico di Milano, I-20133 Milano, Italy — [2]Department of Physics, Università degli Studi di Milano, I-20133 Milano, Italy — [3]Department of Chemistry, Università di Pavia, I-27100 Pavia, Italy

Graphdiynes (GDYs) are novel carbon allotropes with mixed sp-sp^2 hybridization, characterized by tunable optoelectronic properties. This study investigates the temperature-dependent atomic-scale structure and vibrational properties of 1,4-bBEB-based GDY molecular wires frameworks synthesized via Ullmann coupling on Au(100) and Au(111) surfaces. Scanning Tunnelling Microscopy revealed the transition from ordered frameworks of densely packed and oriented 1D organometallic wires (OMF) at room temperature, to progressively more disordered covalent frameworks (COF) at high temperatures. Density Functional Theory calculations and in situ Raman spectroscopy measurements tracked the OMF-to-COF transition, assigning specific Raman features to both phases. Raman spectroscopy also revealed that surface orientation influences the wires-gold interaction, resulting in a lower temperature for the OMF-to-COF transition on Au(100) than on Au(111).