O 45: Organic molecules on inorganic substrates: Adsorption and growth – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 45.1 Tue 14:00 P2

Domain mixing of coronene and nonahelicene with CuO$_x$ species on Cu(110) — •Max Halbauer, Martin Wolf, and Akitoshi Shiotari — Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany

Various surfaces are known to reconstruct as a result of surface energy minimization (e.g. Pt(110)-(2×1), Si(111)-(7×7)). For certain systems, the surface reconstruction is induced by the adsorption of molecules or atoms (e.g. C$_{60}$/Cu(111) [1]). In this work, we show how the organic molecules, coronene and nonahelicene, interrupt the growth of copper oxide rows of the typical Cu(110)-p(2×1)O reconstruction and mediate the formation of mixed domains instead. The resulting adlayer domains on Cu(110) were imaged by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) under ultrahigh vacuum and cryogenic conditions. Models for the adsorption structures of the molecules and CuO$_x$ species are discussed and confirmed with simulated images. A mechanism for the mixed domain growth is proposed, whereby surface diffusion and favourable lateral interactions between the molecules and oxide species drive the formation of the observed coordination framework. The finding opens prospects for controlling the lateral chemical and electronic interactions between adsorbed molecules by partial oxidation of the Cu(110) surface.

[1] L. Forcieri, S. P. Jarvis, *et.al.*, *Phys. Rev. B* **2021**, *104*, 205428.

O 45.2 Tue 14:00 P2

Importance of Electrostatic Effects for Interpretation of X-ray Photoemission Spectra of Self-Assembled Monolayers — •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

The subject of this contribution is electrostatic effects in X-ray photoemission (XP) from self-assembled monolayers (SAMs), which are application-relevant ultrathin molecular films, coupled to the substrate by a suitable anchoring group. Whereas, in most cases, the standard concept of chemical shift is fully sufficient to describe XP spectra of these systems, consideration of electrostatic effects is frequently necessary for their proper interpretation. Due to the insulating character of the SAM matrix, decoupled electronically from the substrate, the introduction of a dipolar "sheet" at the SAM-substrate interface or within this matrix creates a potential discontinuity, shifting the energy levels above the "sheet" with respect to those below it. This shift is reflected then in the matrix-related spectra, resulting in shifts and splitting of the characteristic photoemission peaks. Representative examples in this context underline the importance of electrostatic effects in photoemission and suggest that they should be considered on equal footing with the chemical shift.

O 45.3 Tue 14:00 P2

Self-assembled quasi-one-dimensional metal-organic framework — Jonas Brandhoff, Jule S. Hölzer, Felix Otto, Torsten Fritz, and •Roman Forker — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We compare condensed monolayers of 4,5,9,10-pyrenetetrone (Py4O) on Cu(111) in two fundamentally different configurations, namely with and without adatoms. To this end, we employ density-functional theory (DFT) calculations to understand the structural configurations as well as the electronic properties. We uncover the coupling between the organic molecule, surface, and possible adatoms. Furthermore, we demonstrate how a quasi-one-dimensional arrangement including a Cu adatom is thermodynamically stable. This interpretation is substantiated by means of scanning-tunneling microscopy (STM) experiments, along with low-energy electron diffraction (LEED) patterns. Additionally, we use photoelectron spectroscopy to assess the electronic structure. Finally, we elucidate the bond formation between the d-orbitals of the Cu adatom and the p-orbitals of the molecular oxygen.

O 45.4 Tue 14:00 P2

Landing-Energy-Controlled Surface Conformation of Electrosprayed Foldamer Molecules on Au(111) — •Jue Wang[1], Dennis Meier[1,2], Shengming Zhang[1], Patrick Lawes[1], Pengfei Zhao[1], Jinhua Wang[3], Victor Maurizot[3], Andreas Walz[1,4], Annette Huettig[1,4], Hartmut Schlichting[1,4], Anthoula C. Papageorgiou[1,5], Joachim Reichert[1], Ivan Huc[6,7], and Johannes V. Barth[1,7] — [1]TU Munich, DE — [2]Tufts University, US — [3]CNRS, Univ. Bordeaux, FR — [4]pureions GmbH, Gilching, DE — [5]National and Kapodistrian University of Athens, GR — [6]LMU Munich, DE — [7]Cluster of Excellence e-conversion, DE

Preserving the structural integrity of biomimetic foldamers upon surface deposition is essential for their integration into functional molecular architectures. In this study, we investigate the electrospray ion beam deposition of foldamer molecules in ultra-high vacuum and examine how their conformation depends on the mean landing energy during deposition. With a low mean landing energy of about 0.6 eV, intact foldamers are observed on the surface. Higher landing energies predominantly result in unfolded molecules. The unfolded conformation are further accessible by annealing of the adsorbed folded molecules. These results highlight the importance of soft-landing conditions to maintain hydrogen bond-stabilized architectures on surfaces, offering a model platform for studying the structure-function relationship of surface-supported thermolabile biomolecules

O 45.5 Tue 14:00 P2

Adsorption, Dissociation and Chain Formation of 2NHC-azo-iPrl on Au(111) — Ebru Cihan[1], Natasha Khera[1], Franz Plate[1], Ningwei Sun[2], Soyoung Park[2,3], Franziska Lissel[2,3], and •Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — [2]Institute of Macromolecular Chemistry Leibniz Institute of Polymer Research, Hohe Strasse 6, Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, Hamburg, Germany

In this study, we investigated 2NHC-azo-iPrl molecules on the Au(111) surface. While the central azobenzene core is clearly visible in STM images, in most cases, only two isopropyl groups are present per molecule. Our results indicate the possibility of a reaction between I- counterions and the isopropyl (iPr) side groups, which may lead to the dissociation of iPrI upon heating. Furthermore, experiments using STM lateral manipulation, which facilitate the separation of chain structures on azobenzene bridges, suggest that the chains are likely connected to each other by weak van der Waals or hydrogen bonds. Additionally, to further investigate the azobenzene core of the molecule, voltage pulses were applied to the molecule using the STM tip. This investigation reveals the potential for cis-trans isomerization in the azobenzene core.

O 45.6 Tue 14:00 P2

Tuning molecular self-assembly of BDA on CsPbBr$_3$(100) — •Hannah Loh, Milan Möller, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

CsPbBr$_3$ is a promising alternative to organic-inorganic perovskites in solar cells and light emitting diodes [1]. In these devices, organic layers are often used as charge transport layers and hence interface properties are of particular interest. Depending on the termination of the CsPbBr$_3$ substrate [2] the adsorption properties can be tuned [3].

In this contribution we invesitgate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial CsPbBr$_3$ thin films on Au(100). Independent of surface termination the BDA molecules lie flat and form compact islands. On the CsBr-terminated surface, molecules follow a head to tail hydrogen-bridge stabilized arrangement. The interaction with the PbBr terminated surface is stronger causing partially a slight tilt of the molecules to adapt to the substrate unit cell and deprotonation.

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Loh H. et al., ACS Nano, **19**, 10199-10206 (2025)

O 45.7 Tue 14:00 P2

Force mapping of a pyridyl-functionalized platform molecule by noncontact atomic force microscopy — •Hyeji Choi[1], Behzad Mortezapour[2], Martin Wolf[1], Richard Berndt[2], and Akitoshi Shitotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Institut für Experimentelle und Angewandte

Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Platform molecules based on trioxatriangulenium (TOTA) form triangular adsorption motifs on metal surfaces with a functional group protruding to the vacuum [1]. However, probing the atomic-scale structure of such steric molecules remains challenging. Here, we study pyridyl-TOTA on Ag(111) and perform single-molecule force mapping, using noncontact atomic force microscopy (NC-AFM) at 6 K. We obtained force and potential maps of the pyridyl group interacting with a metal tip by measuring frequency shift as a function of tip height and location. These maps reveal anisotropy depending on the direction relative to the pyridyl ring plane. Simulations using Lennard-Jones potential reproduce the map appearances, enabling estimation of the preferred ring orientation and directional stiffness. We thus demonstrate the high potential of single-molecule force mapping for the structural characterization of steric adsorbate.

[1] Mortezapour, B., et al., ACS Nano 19, 38773-38780 (2025)

O 45.8 Tue 14:00 P2

Decoupling of Organic Monolayers from Cu(111) Using Blue Phosphorene — •Felix Otto, Wiebke Makowski, Jonas Brandhoff, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Two-dimensional (2D) materials are promising for future electronics due to their tunable properties. Since graphene's discovery in 2004, materials like MoS_2, h-BN, and Blue Phosphorene (BlueP) have been synthesized, offering high charge mobility and adjustable band gaps. BlueP can be grown on substrates such as Cu(111), making it suitable for decoupling organic layers. This study investigates whether BlueP can effectively decouple PTCDA monolayers from Cu(111). Two BlueP phases – hexagonal and chiral – were prepared and characterized, revealing structures with hexagonal unit cells but significantly stretched lattices compared to free-standing BlueP. Despite structural differences, both phases exhibited similar chemical and electronic properties. PTCDA was deposited on both phases, forming ordered herringbone structures. On the chiral phase, a single structural model sufficed, while two were necessary for the hexagonal phase. Spectroscopic analyses indicated weak interactions and evidence of integer charge transfer, supporting the idea that BlueP acts as an effective decoupling layer. These findings contribute to understanding how 2D-materials can be used to electronically isolate organic monolayers, advancing their application in nanoelectronics.

O 45.9 Tue 14:00 P2

Density functional study of the geometric and electronic properties of a tetracene-adduct molecule on Ag(110) — •Fabian Dixer[1], Eric Fackelman[2], Veronika Schmalz[3], Monja Stettner[2], François C. Bocquet[2], Andrei C. Matetskii[2], Serguei Soubatch[2], Ulrich Koert[3], Frank Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-3, FZ Jülich and RWTH Aachen University, Germany — [3]Department of Chemistry, Philipps-Universität Marburg, Germany

We present a density-functional theory (DFT) investigation of the adsorption behavior of the tetracene-maleic anhydride Diels-Alder adduct (4A-MAD) on Ag(110). This molecule serves as a model system for studying light induced retro 4+2 cycloadditions on surfaces. Using a repeated-slab approach with a van-der-Waals corrected GGA functional, we explore the adsorption energy landscape by sampling multiple initial configurations and performing local relaxations. The most favorable geometries are examined in terms of work-function changes, charge-density-difference distributions, and projected densities of states. We further simulate photoemission momentum maps of the frontier molecular orbitals within photoemission orbital tomography and compare them with angle-resolved and angle-integrated photoemission data from our experimental collaborators. This combined analysis provides a comprehensive picture of the molecule-substrate interaction and lays the groundwork for future studies of on-surface photochemical cleavage of the Diels-Alder adduct.

O 45.10 Tue 14:00 P2

Theoretical Investigation of Halogenated Polycyclic Aromatic Hydrocarbons on Clean and Coated Metal Surfaces — •Florian Pfeiffer[1], André Schirmeisen[2], Daniel Ebeling[2], and Simone Sanna[1] — [1]Institute for Theoretical Physics, JLU Giessen, Germany — [2]Institute for Applied Physics, JLU Giessen, Germany

Halogenated organic precursors are the building blocks for the on-surface synthesis of complex structures with precisely tuned properties. While chemical synthesis is typically performed on clean metallic surfaces, a NaCl bilayer might be employed to electronically decouple substrate and adsorbates, increasing mobility and thus simplifying manipulation.

To improve our understanding of the fundamental interactions of halogenated precursors on (isolated) surfaces, we examined charge redistribution as well as the adsorption geometry, distance, and energetics for several substrate-adsorbate systems, e.g. Dibromopyrene and Iodotriphenylene on NaCl/Cu and halo-tetracenes on coinage metals.

The Vienna Ab initio Simulation Package [1] implementation of density functional theory was used to calculate potential energy surfaces and nudged elastic bands for modelling adsorption behaviour and diffusion pathways, respectively. Comparability with experimental results [2] was achieved by simulation of atomic force microscopy using the Probe-Particle Model [3].

[1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993)

[2] Q. Zhong et al., Nat. Chem. 13, 1133 (2021)

[3] P. Hapala et al., Phys. Rev. B 90, 085421 (2014)

O 45.11 Tue 14:00 P2

Formation and Electronic Interaction of Donor–Acceptor Heterostructures — •Philipp Janzen, Jonas Brandhoff, Felix Otto, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Combining donating and accepting molecules lies at the heart of many electronic devices. These molecular heterostructures allow for a delicate tailoring of charge-transfer interfaces. In this work, we investigate such heterostructures formed by the adsorption and structural organization of 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) and 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) on Au(111). Owing to their shared symmetry, HHTP and HATCN form a well-matched co-assembly on the surface. Employing scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), we are able to resolve the structural properties of the individual systems, as well as the combined heterostructure. Additionally, X-ray photoelectron spectroscopy (XPS) and photoemission orbital tomography (POT) provide insights into charge-transfer processes and the electronic structure at the interface.