

O 17: Poster Monday: Organic Molecules at Surfaces 1

Time: Monday 18:00–20:00

Location: P4

O 17.1 Mon 18:00 P4

Influence of a BlueP interlayer on the properties of P2O on Au(111) — ●FLORENTINE FRIEDRICH, MAXIMILIAN SCHAAL, FELIX OTTO, PHILIP GRIMM, MARCO GRUENEWALD, ROMAN FORKER, and TORSTEN FRITZ — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Two-dimensional (2D) materials have attracted much attention in solid state physics in recent years due to their unique properties. Amongst others, one novel representative is the phosphorus allotrope blue phosphorene (BlueP) with its high charge carrier mobility and suitable band gap, that is used here as an interlayer to obtain a decoupling of the functional organic molecule 6,13-pentacenequinone (P2O) from Au(111) surfaces. P2O is deposited in various film thicknesses (1 monolayer equivalent (MLE) up to 4-5 MLE) either on BlueP on Au(111) or directly on the metal substrate to investigate the influence of BlueP as an interlayer on the optical and structural properties of the P2O molecules. The film growth of P2O is monitored by in-situ differential reflectance spectroscopy (DRS), while the BlueP-Au substrate is kept at different temperatures. Further complementary experimental methods were low-electron energy diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and low-temperature scanning tunneling microscopy (LT-STM). It turns out that the BlueP interlayer influences the monolayer structure as well as the growth mode. In contrast to previous studies on C₆₀, the BlueP interlayer stays intact.

O 17.2 Mon 18:00 P4

Navigating the Polymorph-Jungle with Optimal Control techniques — ●SIMON HOLLWEGER, ANNA WERKOVITS, RICHARD K. BERGER, and OLIVER T. HOFMANN — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria

Properties of organic-inorganic interfaces are strongly dependent on the arrangement of the molecules on the surface. However, achieving a controlled growth of a polymorph with preferable physical properties is not straightforward at all - especially for metastable polymorphs.

In principle, starting from a thermodynamically easily accessible polymorph, kinetics can be utilized to stabilize a metastable polymorph. This can be done by promoting certain structural transitions by a-priori unknown sequentially changing growth conditions. Depending on the complexity of the transition network, often only a limited yield of the target polymorph can be reached during growth.

To computationally maximize the yield of the desired structure we use Optimal Control techniques. Therein, process parameters like temperature and pressure are varied to optimize parameter protocols. The transition network of our model system TCNE/Cu(111) is obtained via a combination of Transition State Theory and Density Functional Theory.

O 17.3 Mon 18:00 P4

Adsorption structure of mixed PTCDA derivatives on Ag(111) — ●AMIN KARIMI¹, JOSE M. GUEVARA¹, VERONIKA SCHMALZ², ULRICH KOERT², F. STEFAN TAUTZ¹, and CHRISTIAN WAGNER¹ — ¹Peter Grünberg Institut (PGI 3), Forschungszentrum Jülich, Jülich, Germany — ²Chemistry Department, Philipps Universität Marburg, Marburg, Germany

For molecular manipulation and SPM tip functionalization, the mode of anchoring molecules to the tip is decisive. We recently found that PTCDA binds to a Ag tip with two oxygen-metal bonds after it is retracted from the surface. While this is crucial for its stabilization in a vertical state, the two bonds reduce the degrees of freedom during manipulation in the tip-molecule-surface junction. To overcome this problem, we synthesized a PTCDA derivative (reduced PTCDA), in which one carboxylic oxygen is replaced by two H atoms. For molecular manipulation, this allows choosing between one or two tip-oxygen bonds. Here we present a study on the adsorption structures formed by a mixture of PTCDA and reduced PTCDA on the Ag(111) surface with the help of low-temperature NC-AFM/STM. We observe that despite the minimal modification of reduced PTCDA compare to PTCDA, the mixture of both molecules exhibits a strongly different behaviour compared to the regular island growth of pure PTCDA. Particularly striking is the coexistence of zero-, one-, and two-dimensional structures. A likely explanation for such diverse structures is the influence

of long-range electrostatic interactions related to the in-plane dipole moment of reduced PTCDA.

O 17.4 Mon 18:00 P4

Single-domain molecular layers on Ag (110) — ●RAVI PRIYA, WEISHAN WU, and PETER JAKOB — Department of Physics, Philipps-Universität Marburg, Germany

Single domain molecular layers have been explored on the non-hexagonal Ag(110) substrate. The absence of rotational domains for fcc (110) metal substrates allows for growing layers with uniform azimuthal orientation of deposited molecules. In our study we have investigated various molecules and configurations that may form single domain molecular layers (including mirror domains). Specifically, PTCDA, NTCDA, phthalocyanines (CuPc, SnPc, TiOPc) and regio-selectively substituted pentacene species (pentacene, pentacenequinone, pentacene-tetrone, quinacridone) were deposited and examined in terms of their structure using SPA-LEED, and their vibrational signature using IR - spectroscopy. Among them, PTCDA, NTCDA and pentacene have been found to form single domain structures. In the case of PTCDA two prominent phases, the brick-wall (BW) and the herringbone (HB) phases exist, and they are readily distinguished not only by their LEED patterns but also from their vibrational signatures. Another finding refers to the increased molecule - metal interaction on Ag (110) vs. Ag (111) that leads to an extra energy (down)shift of the LUMO, thereby having a significant impact on interfacial dynamic charge transfer (IDCT) of vibrational modes [1].

[1] P. Jakob, S. Thussing, Phys. Rev. Lett. 126 (2021) 116801, DOI:10.1103/PhysRevLett.126.116801

O 17.5 Mon 18:00 P4

Generation of synthetic chiral structured images for computer vision applications — ●JOHANNES TIM SEIFERT¹, PEER KASTEN¹, MANDY STRITZKE², BJÖRN MÖLLER³, TIMO DE WOLFF², TIM FINGSCHIEDT³, and UTA SCHLICKUM¹ — ¹Institut für Angewandte Physik, Technische Universität Braunschweig — ²Institut für Analysis und Algebra, Technische Universität Braunschweig — ³Institut für Nachrichtentechnik, Technische Universität Braunschweig

Scanning tunneling microscopy (STM) is a well-established tool to measure surface topographs with atomic precision. Since data generation is slow using STM, we present a tool to create synthetic images with realistic noise and defects, which provides labeled training data for neural networks. We compare two methods evaluating chiral structures in STM images using Deep Learning.

As one approach to classify structures, we are using semantic segmentation based on the U-Net architecture to create maps showing the distribution of both chiralities. Additionally, we use a faster R-CNN architecture for object detection to locate and classify each chiral structure individually.

Since the approaches serve different use cases, they also have separate label requirements. We show that models trained using only our synthetic images perform successfully for real STM Images.

O 17.6 Mon 18:00 P4

Ultrafast dynamics of quantum confined surface electrons in a T4PT-based metal-organic network on noble metals — ●NILS BELLENBAUM¹, LU LYU¹, EVA WALTHER¹, TOBIAS EUL¹, BENITO ARNOLDI¹, MARTIN AESCHLIMANN¹, and BENJAMIN STADTMÜLLER^{1,2} — ¹Technische Universität Kaiserslautern and Research Center OPTIMAS, Erwin-Schrödinger Straße 46, 67663 Kaiserslautern, Germany — ²Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany

Two-dimensional metal-organic networks have emerged as intriguing architectures to design and control quantum confinement of electrons at surfaces. In our work, we focus on the metal-organic network T4PT/Cu(111) comprised of triangular 2,4,6-tris(4-pyridine)1,3,5-triazine (T4PT) molecules adsorbed on a copper substrate. Using momentum-resolved photoemission, we demonstrate a spatial confinement of the free electron-like surface state of Cu(111) in the pores of the network structure. Similarly, the dispersion of the unoccupied image potential state (IPS) of Cu(111) is modulated by the network's periodic potential, leading to a severe increase of the effective band mass of the IPS. Finally, we discuss the influence of periodic modu-

lation of the IPS on its energy and momentum-dependent population time using timeresolved two photon momentum microscopy. Our findings provide a first glimpse onto tunability of the electron dynamics at surfaces by spatial confinement in nanoporous metal-organic network structures.

O 17.7 Mon 18:00 P4

Organic Molecules on the Cu(110)-(2x1)O Striped Phase — ●ILIAS GAZIZULLIN, CHRISTOPHE NACCI, and LEONHARD GRILL — Physical Chemistry Department, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

The deposition of molecules onto single-crystal surfaces allows their investigation at the single-molecule level by scanning tunneling microscopy (STM) and gives access to the controllable on-surface synthesis of 2D materials. Here, we have studied dibromo-p-terphenyl molecules on the Cu(110)-(2x1)O striped phase under ultra-high vacuum conditions with low-temperature STM. The Cu(110)-(2x1)O striped phase is of particular interest since it offers alternating stripes of (metallic) copper areas and of oxygen-covered areas where the adsorbed organic molecules are slightly decoupled from the metal substrate and hence have higher mobility.

Previously, the Cu(110)-(2x1)O striped phase was used as a template for the synthesis of organometallic structures having different sizes and shapes depending on the width of copper stripes [1]. The focus of our study is how annealing affects the molecular adsorption on the surface. It turns out that the molecules form organometallic chains on the copper areas, oriented in three surface directions. Increasing the sample temperature from 300 K to 450 K changes the orientation of the organometallic chains and the shape of the Cu-O areas. Possible interactions leading to such behaviour are discussed.

Reference: [1] Q. Fan, J. Dai, T. Wang, J. Kuttner, G. Hilt, J. M. Gottfried, and J. Zhu, *ACS Nano*, 3 (2016), 3747-3754

O 17.8 Mon 18:00 P4

Adsorption of phthalocyanine monolayers on Ag(110) — ●GAANA KAINIKKARA, RAVI PRIYA, and PETER JAKOB — Phillips University of Marburg

Vibrational properties and long range ordering of TiOPc, CuPc and SnPc molecular layers on the non-hexagonal Ag(110) surface have been investigated using IR-spectroscopy and SPA-LEED. Special emphasis is put on a comparison with the related Ag(111) substrate surface that is characterized by a somewhat weaker molecule - metal interaction strength. This hypothesis is supported by distinct differences in the vibrational line shapes of modes associated with interfacial dynamical charge transfer [1], the primary cause being an extra shift in the energetic position of the former LUMO with respect to the Fermi energy for the Ag(110) substrate. Another objective in our study was to identify structural changes in the (layered) structural arrangement, both during the growth process, as well as annealing of the layers. Due to their only slightly different footprint, the molecules display similar long range ordered phases. Our primary focus thus concerned the identification of possibly inclined arrangements in the coverage range of 1-2 monolayers [1] P. Jakob, Peter and S. Thussing. "Vibrational Frequency Used as Internal Clock Reference to Access Molecule-Metal Charge-Transfer Times." *Phys. Rev. Lett.* 126, 116801 (2021).

Part-O: Surface Science Division Type-Poster Presentation Topic-Organic Molecules on Inorganic Substrates: Adsorption and growth

O 17.9 Mon 18:00 P4

Growth of organic crystals on nanoparticle precovered surfaces studied by PEEM — ●KATHARINA ENGSTER¹, JÖRG HELLER¹, THORSTEN WAGNER², SYLVIA SPELLER¹, and INGO BARKE¹ — ¹University of Rostock, Institute of Physics, 18059 Rostock, Germany — ²Johannes Kepler University, Institute of Experimental Physics, 4040 Linz, Austria

Nanostructures can be used as plasmonic light sources [1] for local generation of excitons in organic semiconductors. This is a promising pathway to transfer energy in molecular aggregates from a defined starting point over longer distances via exciton propagation. In order to establish a suitable geometry of such a hybrid system, we are interested in the role of metallic clusters during subsequent molecular growth. Mass-selected silver nanoparticles are produced in a gas-phase cluster source and deposited onto a pristine HOPG surface. Afterwards, we use *in-situ* photoemission electron microscopy (PEEM) to monitor the physical vapour deposition of copper phthalocyanine (CuPc) molecules [2,3] on such surfaces. We observe a Stranski-Krastanov growth during deposition of CuPc and post-

deposition further morphology changes of the nanocrystallites.

[1] K. Oldenburg et al., *J. Phys. Chem. C* **123**, 1379 (2019).

[2] Y.-C. Chiu et al., *Cryst. Res. Technol.* **46**, 295 (2011).

[3] T. Wagner et al., *Ultramicroscopy* **233**, 113427 (2022).

O 17.10 Mon 18:00 P4

Visualizing self-assemblies of electro sprayed complex molecules on surface: a non-contact force microscopy study —

●GEMA NAVARRO¹, ANTOINE HINAUT¹, SEBASTIAN SCHERB¹, SHUYU HUANG¹, YIMING SONG¹, KLAUS MÜLLEN¹, THILO GLATZEL¹, AKIMITSU NARITA², and ERNST MEYER¹ — ¹Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland. — ²Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany.

Building up functional 2D supramolecular assemblies requires the unit blocks involved in their bottom up formation to be already complex. In the construction of the tailored nanostructures, different approaches can be adopted in order to circumvent the limitations of the traditional wet chemical methods [1,2]. Among them, specifically the Electro spray Deposition (EDS) technique emerges as suitable pathway to explore the adsorption of organic compounds with higher structural complexity [3].

In the present work, we report the adsorption of complex molecules on a noble metal surface. Our study focus on the influence of intermolecular and surface-molecule interactions in the observed assemblies. The deposition of the molecules is carried out by HV-EDS. Furthermore, visualization of the molecules is achieved by means a home-made Atomic Force Microscopy (AFM) set-up, in non-contact operation mode.

[1] Z. Qiu, A. Narita, and K. Müllen, *Faraday Discuss.* 227,8 (2021).

[2] S. Scherb et al., *Commun Mater* 1, 1 (2020).

[3] I. C.-Y. Hou, A. Hinaut, *Chem. Asian J.*, e202200220 (2022).

O 17.11 Mon 18:00 P4

C₆₀ - PEN Diels - Alder Cycloaddition Reaction on Ag(110) — ●MOHAMMED SUHAIL ANSARI, RAVI PRIYA, and PETER JAKOB — Department of Physics, Philipps - Universität Marburg, Germany

Ultrathin films of C₆₀ and pentacene (PEN) have been prepared on Ag(110) and their vibrational properties, as well as thermal evolution investigated by IR spectroscopy. Monolayer species are found to display distinctly different vibrational signatures as compared to higher layers, so the characterization of the grown hetero layers is straightforward. Moreover, the excellent spectral resolution and chemical selectivity allowed us to unambiguously identify the C₆₀ - PEN Diels-Alder adduct [1]. In our thermal evolution study, the formation and decomposition of the C₆₀ - PEN reaction product as well as the abundances of the C₆₀ and PEN compounds have been examined. Production of the adduct species requires a weak thermal activation (annealing to 350 K) and proceeds largely independent of the C₆₀ / PEN stacking sequence. We find that this reaction occurs exclusively at the (abrupt) interface of C₆₀ and PEN for layered arrangements and is fully reversible, meaning that further annealing to 450 K (and higher) produces again C₆₀ and PEN, with the latter desorbing thermally and thus depleting the initial concentration of reactants.

[1] F. Cataldo, D. A. García-Hernández and A. Manchado, On the C₆₀ Fullerene Adduct with Pentacene: Synthesis and Stability, *Fullerenes, Nanot. Carbon Nanostruct.* 23 (2015) 818-823.

O 17.12 Mon 18:00 P4

First Steps Towards Carbon-Based Heisenberg Chains on Au(111) — ●NILS KRANE¹, ELIA TURCO¹, ANNIKA BERNHARDT², MICHAL JURÍČEK², PASCAL RUFFIEUX¹, and ROMAN FASEL¹ — ¹nanotech@surfaces Laboratory, Empa - Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — ²Department of Chemistry, University of Zurich, Zurich, Switzerland

Carbon based π -magnetism has been a growing field of interest in the recent years. By tailoring nanographenes with atomically precise shape and size it is possible to tune their electronic properties and create magnetically non-trivial groundstates. A recent study has demonstrated the formation of triangulene-based Haldene chains, consisting of spin-1 building blocks and featuring gapped spin excitation in the bulk [1]. On the other hand, a Heisenberg chain consisting of coupled spin-1/2 units is predicted to be gapless, due to a continuum of spin excitations above the ground state.

Here we present the first steps towards synthesizing all-carbon spin-1/2 chains. Phenalenyl-based precursors are used for a bottom-up approach to form oligomers of different lengths and spin-excitation

gaps. The low activation barrier of hydrogen-passivated phenalenyl was found to be a potential inhibitor of the radical formation, which is required for the covalent coupling of the building blocks.

[1] S. Mishra et al., Nature **598**, 287-292 (2021).
<https://doi.org/10.1038/s41586-021-03842-3>