

O 19: Poster Monday: Organic Molecules on Inorganic Surfaces

Time: Monday 17:45–20:00

Location: Poster F

O 19.1 Mon 17:45 Poster F

On the adsorption behavior of free base tetranaphthylporphyrin on Cu(111): mobility, intramolecular conformation and chirality — ●STEPHEN MASSICOT, JAN KULIGA, RAJAN ADHIKARI, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The controlled fabrication of molecular nanoarchitectures via bottom-up approach is an important objective within surface science. One of the most promising and extensively investigated class of adsorbates in that regard are porphyrins. In order to understand the adsorption behavior of porphyrins one has to closely study their adsorption geometry. In this study, we investigate the free-base tetranaphthylporphyrin (2HTNP) on Cu(111). Interestingly, 2HTNPs adsorb as individual molecules exhibiting an “inverted” conformation on the copper substrate, similar to the reports for the tetraphenylporphyrin. However, each naphthyl group of a single 2HTNP molecule has two different orientations parallel to the surface. As a result five atropisomeric and two enantiomeric conformations can be found. Furthermore, a specific dynamic behavior, i.e. a migration of the adsorbed 2HTNP molecules along the three high symmetry regions of the substrate is observed at room temperature. After annealing to 400 K only one conformation is present on the surface and the molecules are static. However, after further annealing to 450 K the molecules become mobile again and some molecules additionally change the substrate directions.

O 19.2 Mon 17:45 Poster F

Adsorption Geometry of 2-Iodotriphenylene on Ag(111) — ●ALEXANDER IHLE¹, DANIEL MARTIN-JIMENEZ¹, DANIEL EBELING¹, HERMANN WEGNER², TOBIAS SCHLÖDER³, DOREEN MOLLENHAUER³, and ANDRÉ SCHIRMEISEN¹ — ¹Institute of Applied Physics, Justus Liebig University Giessen, Germany — ²Institute of Organic Chemistry, Justus Liebig University Giessen, Germany — ³Institute of Physics and Chemistry, Justus Liebig University Giessen, Germany

On-surface chemistry is a powerful tool for building covalent molecular structures such as chains, networks, or graphene nanoribbons [1, 2]. In particular, the catalytic properties of the metal substrate as well as the 2D confinement facilitate the synthesis of new structures that are not accessible via solution chemistry. In order to control the bottom-up formation process precise knowledge about the adsorption geometry of the molecular precursors is needed since this will help to understand the reaction mechanisms in detail. Here we studied the adsorption geometry of 2-iodotriphenylene on Ag(111). By using low temperature atomic force microscopy with CO-functionalized tips we are able to identify the adsorption position and angles with high precision. Only two orientations are observed on the surface which is attributed to relatively strong molecule-substrate interactions.

[1] Cai, J. *et al. Nature* **466**, 470-473 (2010)[2] Grill, L. *et al. Nature Nanotechnology* **2**, 687-691 (2007)

O 19.3 Mon 17:45 Poster F

Scanning Tunneling Microscopy Study of Phthalocyanine Family Molecule with Reactive Moiety of Thiadiazole: Cobalt tetrakis (1,2,5-thiadiazole) porphyrines(CoTTDPz) adsorption on Au(111) — ●YU WANG^{1,3}, JIE HOU^{1,3}, KUNIO AWAGA², and TADAHIRO KOMEDA³ — ¹Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki-Aza-Aoba, Aoba-Ku, Sendai, Japan — ²Department of Chemistry & Research Center for Materials Science, Nagoya University, Chikusa-ku, Nagoya, Japan — ³Institute of Multidisciplinary Research for Advanced Materials (IMRAM, Tagen), Tohoku University, 2-1-1, Katahira, Aoba-Ku, Sendai, Japan

Metal-phthalocyanine(MPc) has been intensively studied in recent decades not only for its chemical and thermal stability but also due to tunable properties through using various center metal atoms. Here we report a LT-STM study of Pc family molecule: CoTTDPz, the terminal of ligand is S-N instead of carbon in Pc, indicating a strong lateral interaction between molecules. CoTTDPz is deposited on Au(111) substrate using thermal sublimation method, multiple molecule layers from 1st to 3rd can be distinguished from STM images. First layer molecules have two orientations which is different with previous works

for MPc, noted that first layer molecules had a unique orientation. In second layer, CoTTDPz shows two types of tilted configurations which can be judged from image and STS. Third layer molecules have two similar configurations absorbed on type1 and type2 of second layer, which has never been reported on Pc molecules.

O 19.4 Mon 17:45 Poster F

Investigation of Self-Assembled Caffeine Monolayer Formation on Au(111) — ●MALTE SCHULTE^{1,2}, ISMAIL BALTACI^{1,2}, PETER ROESE^{1,2}, and CARSTEN WESTPHAL^{1,2} — ¹Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4a, 44227 Dortmund, Germany — ²DELTA, TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany

In recent years the molecule caffeine gained particular interest due to its importance in pharmaceutical applications. The bioavailability of particular substances can be tuned by their structure. Furthermore, in bulk crystals caffeine shows a polymorph behavior with a stable β - and a metastable high-temperature α -phase. Moreover, an analysis of substrate induced caffeine crystalline growth on different substrates was done recently. Therefore an investigation of caffeine monolayer growth can reveal insides of the crystallite growth and gives details about different phases.

In order to study these aspects from a bottom-up approach we deposited caffeine molecules on an Au(111) surface under ultra-high vacuum conditions. To investigate the monolayer self-assembly of caffeine molecules on this surface we performed Scanning Tunneling Microscopy (STM), Low Energy Electron Diffraction (LEED) and X-ray Photoelectron Spectroscopy (XPS). Our results demonstrate successful caffeine monolayer formation, including an molecular alignment in two different directions the Au(111) surface.

O 19.5 Mon 17:45 Poster F

Heteromolecular interfaces on metals in the physisorptive regime — ●QI WANG¹, ANTONI FRANCO-CANELLAS¹, JIACHENG YANG², SAMUEL STRUZEK¹, MENGTING CHEN², STEFFEN DUHM², ALEXANDER GERLACH¹, and FRANK SCHREIBER¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — ²Institute of Functional Nano & Soft Materials (FUNSOM), Soochow University, Suzhou, China

Bilayers of pi-conjugated organic molecules, being considered as model systems for more complex thin film architectures, have been used to investigate the templating effect on metals. Because molecular exchange can hamper the controlled preparation of heteromolecular structures [1], a detailed characterization of different molecule-substrate combinations is required. We found that the organic-metal interaction strength is the decisive factor for the favorable sequential arrangement in organic heterostructures and molecular exchange is possible to occur for weakly interacting template layers [1]. To investigate the molecular arrangement in a physisorptive regime, we have studied the vertical arrangement and the chemical fingerprints of two bilayer systems deposited on Au(111) surfaces [2]. The adsorption properties of organic systems were investigated by X-ray standing waves (XSW), X-ray photoelectron spectroscopy (XPS), ultraviolet photoelectron spectroscopy (UPS).

[1] Q. Wang, *et al. J. Phys. Chem. C* **2018**, *122*, 9480-9490.[2] A. Franco-Canelas, *et al. Phys. Rev. Mater.* **2017**, *1*, 013001.

O 19.6 Mon 17:45 Poster F

Diels-Alder adduct formation of pentacene and C₆₀ on graphene/Ru(0001) and Cu/Ru(0001) — ●SEBASTIAN FLADE and PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The combination of pentacene and C₆₀ represents a prototypical donor-acceptor system that is ideal to study fundamental processes in organic photovoltaics. Very recently, an efficient Diels-Alder adduct formation at the heterolayer interface has been reported.¹ Using infrared-absorption spectroscopy we have unambiguously identified the reaction product and investigated the kinetics of this reaction. Specifically, the thermal evolution of the formation and decomposition of the C₆₀-PEN adduct has been examined. Another aspect concerned the dependence on layer thickness and stacking sequence which seem to play an only minor role for the described (reversible) interface reac-

tion. We demonstrate that the reaction likewise proceeds when one of the reaction partners is in direct contact with the substrate. This has been verified for inert substrates like graphene/Ru(0001), as well as the more reactive Cu/Ru(0001) template.

¹T. Breuer et al., *Adv. Mater. Interfaces* 3 (2016) 1500452.

O 19.7 Mon 17:45 Poster F

X-Ray Small Angle In-Situ Study of Porphyrin Adsorption on Stabilized Rutil Surfaces — ●KLAUS GÖTZ, ANNEMARIE PFNÜR, and TOBIAS UNRUH — Institute for Crystallography and Structural Physics, Erlangen, Germany

Dye sensitized solar cells (DSSCs) based on TiO₂ have been studied as an easy to produce, low-cost alternative to classical semiconductor solar cells with recent efficiencies of up to 13% for a long time [1][2]. We synthesized tunable titania nanoparticles with a diameter of 2-3 nm that are stabilized by oleic acid. Special emphasis of our work is focused on the exchange process of the oleic acid with porphyrins designed for a particular application.

This process is studied using a variation of different x-ray small angle scattering techniques. One method is the combination of small angle x-ray and neutron scattering (SAXS and SANS) experiments. These are well suited to study core/shell systems because of the different scattering lengths for x-rays and neutrons. On the other hand x-ray reflectivity measurements can be used to study layered systems on flat substrates. This offers the possibility to study the exchange of oleic acid with porphyrins on TiO₂ Wafers as a test system. The poster will give an overview over the different techniques and their usage in the characterization of the morphology of the produced particles and the ligand exchange from oleic acid to porphyrins.

[1] O'Regan & Grätzel; *Nature* 353, 737-740 (1991)

[2] Matthew S. et al.; *Nat. Chem.* 6; 242-247 (2014)

O 19.8 Mon 17:45 Poster F

Quantitative Determination of a Model Organic/Insulator/Metal Interface Structure — MARTIN SCHWARZ¹, DAVID A. DUNCAN², MANUELA GARNICA¹, JACOB DUCKE¹, ALEKSANDR BAKLANOV¹, PETER S. DEIMEL¹, JOHANNES KÜCHLE¹, PARDEEP K. THAKUR², TIEN-LIN LEE², FRANCESCO ALLEGRETTI¹, and ●WILLI AUWÄRTER¹ — ¹Technical University of Munich, Germany — ²Diamond Light Source, U.K.

Two-dimensional epitaxial materials including hexagonal boron nitride (hBN) are frequently employed as templates for self-assembled molecular films and nanostructures [1]. A quantitative structural characterization of the respective interfaces and adsorbate geometries however is largely missing. Here, we report on the geometric and electronic structure of a prototypical organic/insulator/metal interface, namely metallo-porphines (Co-P, Zn-P) on monolayer hBN on Cu(111), investigated by combining X-ray photoelectron spectroscopy, X-ray standing waves and scanning tunneling microscopy [2]. Specifically, we determine the adsorption height of the organic molecules and show that the original planar molecular conformation is preserved in contrast to the adsorption of Co-P on Cu(111) [3]. In addition, we highlight the electronic decoupling provided by the hBN spacer layer and find that the hBN-metal separation is not significantly modified by the molecu-

lar adsorption.

[1] W. Auwärter, *Surf. Sci. Rep.*, doi:10.1016/j.surfrep.2018.10.001

[2] M. Schwarz, et al., *Nanoscale* 10, 21971 (2018)

[3] M. Schwarz, et al., *J. Phys. Chem. C* 122, 5452 (2018)

O 19.9 Mon 17:45 Poster F

On-Surface Synthesis and Characterization of Lanthanide and Actinide Tetrapyrrole Complexes — ●ERIK RHEINFRANK, MATHIAS PÖRTNER, CARMEN N. BEYERLE, PETER FEULNER, PETER S. DEIMEL, FELIX HAAS, FRANCESCO ALLEGRETTI, JOHANNES V. BARTH, and WILLI AUWÄRTER — Technical University of Munich, Germany

Metal-organic complexes and coordination architectures on metal surfaces have attracted considerable interest. Specifically, lanthanide-based structures provide distinct structural, electronic, and magnetic properties [1], whereas actinides are rarely explored to date. Lanthanides and actinides can be sandwiched between macrocyclic ligands, resulting in 3D complexes, such as tetrapyrrole double- and multideckers [1]. Here, we report on the in-situ synthesis of Th-TPP complexes on a Ag(111) surface under ultra-high vacuum conditions by exposing a tetraphenylporphyrin (TPP) multilayer to an atomic beam of Th followed by a temperature-programmed reaction and desorption of surplus material. The nature of the interaction between Th and the TPP molecules, as well as the electronic properties of this metal-organic compound were investigated using X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). The findings will be discussed in relation to Ce-based complexes, such as Ce-phthalocyanine sandwich compounds.

[1] D. Eciija et al., *Acc. Chem. Res.* 51, 365 (2018)

O 19.10 Mon 17:45 Poster F

Adsorption of organic molecules with high dipole moment on the Au(111) surface — ●TOBIAS MÜLLER¹, PHILIPP RIETSCH², SIEGFRIED EIGLER², and BERND MEYER¹ — ¹Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — ²Institute for Chemistry and Biochemistry, FU Berlin

Molecules with high dipole moment exhibit promising electronic properties for possible single-molecule electronic devices [1]. Of particular interest is how they couple to conducting substrates and how this coupling changes electronic states and intramolecular charge distribution.

To obtain first insights into the behavior of such high dipole molecules on a metallic substrate we have studied the adsorption of N₂-Ethan-Tetracyanoquinodimethan and N₂-Benz-Tetracyanoquinodimethan on a Au(111) surface using density functional theory (DFT). We have identified the preferred adsorption sites and molecular orientations on the surface and we determined possible periodic arrangements for dipolar stripes. Calculated scanning tunneling microscopy (STM) and local contact potential difference (LCPD) images will be presented and changes in the electronic structure of the molecules within the dipolar stripes will be discussed.

[1] P. Rietsch, F. Witte, S. Sobottka, B. Sarkar, B. Paulus, U. Resch-Genger, S. Eigler, *Diaminodicyanoquinone: A Novel Class of Fluorescent Electron Acceptor Dyes with High Dipole Moments*, submitted