O 31: Poster: Organic Molecules on Inorganic Substrates

Time: Tuesday 18:00–20:00 Location: Poster C

O 31.1 Tue 18:00 Poster C

Probing Borazine on Au(111): from single molecules to clusters — •Matthias Zeilerbauer, Marco Thaler, and Laerte Patera — Department of Physical Chemistry, University Innsbruck, Austria

Borazine is the isoelectronic and isostructural inorganic analogue of benzene. However, due to the large difference in electron negativity between N and B most of the charge is drawn by the nitrogen atom, which is expected to lead to polarized B-N bonds. Here, we demonstrate borazine dosing on Au(111) exploiting a cold trap, which removes borane impurities from the gas phase [1]. Upon deposition on Au(111) at 25 K, we observed monomers as well as self-assembled clusters in various sizes, exhibiting a preferential orientation with respect to the substrate. In scanning tunneling microscopy images borazine molecules present a three-fold appearance, being attributed to the different radii of B and N. Despite the high polarity of borazine favoring dipole-dipole mediated intermolecular interactions, the molecules in the clusters are typically surrounded by hydrogen molecules. Spatially resolved tunneling spectroscopy provides maps of the inelastic electron tunneling probability, allowing for the identification of the hydrogen structures. [1] Marc G. Cuxart et al. Sci. Adv.7 2021

O 31.2 Tue 18:00 Poster C

Electrospray Deposition of Large Ring-Molecules — •Ken Kolar[1], Grant Simpson[1], Caroline Storey[2], David Leigh[2], and Leonhard Grill[1] — [1]Dept. of Physical Chemistry, University of Graz, Austria — [2]Dept. of Chemistry, University of Manchester, UK

Study of large molecules on the individual scale is of importance in biological contexts; however, their intact deposition onto a surface poses many challenges due to their large size. In this study, we present the room temperature deposition of large ring-molecules with a mass of 1124 u on an Au(100) surface within a high vacuum environment, using an optimized electrospray deposition (ESD) apparatus. The simple setup consists only of an electrospray stage [1,2] and does not contain any mass separation unit as used in more sophisticated setups [3]. Sample characterization was done by low-temperature scanning tunneling microscopy after sample transfer with a vacuum suitcase between different ultrahigh vacuum machines. The results show the successful deposition of intact molecules with very little surface contamination and thus confirm the potential of this simple technique for studying larger molecules under clean conditions at surfaces [4-6].

[1] https://www.molecularspray.co.uk/, (29.11.2023)
[2] F. Paschke, M. Fonin et. al, Q. M. R., 1:e200002, (2020)
[3] X. Wu, M. Delbianco, K. Anggara et al., Nature 582, 375 (2020)
[4] R. Pawlak, J.G. Vilhena, A Hinaut et al., N. C. 10, 685 (2019)
[5] J. Holec et al., Angew. Chem. Int. Ed. 60, 7752 (2021)
[6] S. Scherb, A. Hinaut, R. Pawlak et al., C. M. 1, 8(2020)

O 31.3 Tue 18:00 Poster C

Orientational transition of dimolybdenum tetraacetate on Au/Cu(111) — •Alexei Nefedov[1], Thomas Strunskus[2], Maria Brzhezinskaya[3], Martin Anstett[4], Benjamin Stadtmüller[4], Martin Aeschlimann[4], and Angelika Kuehnle[5] — [1]Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany — [2]University of Kiel, Kiel, Germany — [3]Helmholtz-Zentrum Berlin fuer Materialen und Energie, Berlin, Germany — [4]University of Kaiserslautern, Kaiserslautern, Germany — [5]University of Bielefeld, Bielefeld, Germany

Dimolybdenum tetraacetate (MoMo) adsorbed on metal single crystal surfaces shows a partial transition from an ordered close-packed upright standing configuration (chain phase) to a low-packed phase upon cooling (mesh phase). On the base of DFT calculations it is supposed that this phase consists from flat lying molecules. In order to confirm upright/flat orientation of the MoMo molecules in different phases NEXAFS spectroscopy was applied. The MoMo layer of different (0.1-1 ML) coverages were evaporated on the Au/Cu(111) substrate both at room and low temperatures. XPS/NEXAFS measurements were carried out at deposition temperature as well after cooling or/and warming the sample. After NEXAFS experiments it was found that a molecule coverage also plays very important for the transition. Moreover, it was established that, in addition to thermodynamics, kinetic processes may play a crucial role in this process as well.

O 31.4 Tue 18:00 Poster C

Functionalization of AsP monolayer via Amino acids adsorption — Pinar Kaya[1], Okay Tercan[1], Çağil Kaderoğlu[1], Ethem Aktürk[2], and •Handan Arkin[1] — [1]Ankara University, Faculty of Engineering, Department of Physics Engineering — [2]Aydin Adnan Menderes University, Department of Physics

2D materials attract great attention from the scientific world because of their distinct chemical and physical characteristics. Nevertheless, a few shortcomings of these materials restrict their use [1]. Biomolecules and 2D materials can be combined to address these drawbacks [2]. In this study, the single-layer honeycomb structure of the AsP, which is promising in technological applications and has a wide band gap [3,4], was used as a starting point of the hybrid system and adsorption of amino acids Glycine, Serine, which have great potential for use in industry and biomedicine [5] were investigated. Various geometric models of these amino acids on AsP single-layer pristine and vacancy were developed and their structural and electrical characteristics were examined. References [1] Zhang, Hua, et al., Bioactive Materials, 2020, 5, 1071-1086. [2] Mallineni, Sai Sunil Kumar, et al., ACS Applied Materials & Interfaces, 2016, 8,26, 16604-16611. [3] Benam, Z. H.; Arkin, H.; Aktürk, E., Comput. Mat. Sci., 2017, 140, 290-298. [4] Ozdemir, I., et al., Mat. Research Express, 2019, 6,6, 065032. [5] Gioacchinogi, Michael, et al., J. of Molecular Liquids, 2020, 301, 112407.

O 31.5 Tue 18:00 Poster C

A Detailed Look at the Self-Assembly of 1,4-Benzoquinone on Ag(111) — Hendrik Tamm[1], •Lorenz Brill[1], Christoph Wachter[2], Oliver T. Hofmann[2], Roman Forker[1], and Torsten Fritz[1] — [1]Friedrich Schiller University Jena, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany. — [2]Graz University of Technology, Institute of Solid State Physics, NAWI Graz, Petersgasse 16/II, 8010 Graz, Austria.

Since many material properties are closely linked to its structure, understanding the structure formation is imperative when trying to engineer new materials. However, many competing effects impact the final structure formation, complicating accurate predictions. Here, we investigate 1,4-benzoquinone on Ag(111) and use CO-functionalized scanning probe microscopy in conjunction with density functional theory calculations to reveal the non-intuitive, tilted adsorption of the molecules. While the self-assembly of 1,4-benzoquinone on Ag(111) has been studied previously, our study provides additional clarification and insights into its structure that were inaccessible at that time.

O 31.6 Tue 18:00 Poster C

LEEM/PEEM study of F_{16}CuPc/*p*-6P organic thin films on SiO$_2$ — •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

Systematic investigations of the influence of molecular order on the charge-carrier dynamics in organic semiconductors require well-defined and controllable model systems. While single-crystalline metal surfaces are suitable substrates for the epitaxial growth of long-range ordered organic layers, strong molecule-metal interaction also modifies the carrier dynamics in the layer. In contrast, organic thin films on weakly interacting substrates such as SiO$_2$ exhibit only poor structural order in general.

Here, we present a low-energy electron microscopy (LEEM) study of the structure of thin copper-hexadecafluorophthalocyanine (F_{16}CuPc) films, which were deposited on the native oxide of Si(100) substrates after precovering of the surface with a monolayer of para-sexyphenyl (*p*-6p) molecules. The in vacuo thermally evaporated *p*-6P layer comprises crystalline domains of upright standing molecules. F_{16}CuPc films deposited on *p*-6p precovered substrates exhibit μm-sized, well-ordered domains. In contrast, only nm-sized domains are formed if F_{16}CuPc is deposited directly on the native oxide. Structural investigations with μLEED and AFM are combined with polarization-dependent two-photon photoemission electron microscopy (2P-PEEM) to reveal the influence of molecular order on optical excitations in the F_{16}CuPc film.

O 31.7 Tue 18:00 Poster C

N-Heterocyclic carbenes and olefins on silicon — •Robert Zielinski[1,5], Sandhya Chandola[3], Maximilian Koy[4], Hazem Aldahhak[2], Mowpriya Das[4], Matthias Freitag[4], Uwe Gerstmann[2], Mike T. Nehring[1], Denise Liebig[1], Adrian K. Hoffmann[1], Canan Kosbab[1], Max Rosin[1], Simone Brozzesi[7], Ankita Das[4], Viktoria Balfanz[1], Juls Brühne[1], Wolf Gero Schmidt[2], Conor Hogan[6,7], Mario Dähne[1], Frank Glorius[4], Norbert Esser[1,5], and Martin Franz[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [4]Organisch-Chemisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [5]Leibniz-Institut für Analytische Wissenschaften - ISAS e.V., Berlin, Germany — [6]Istituto di Struttura della Materia-CNR (ISM-CNR), Rome, Italy — [7]Department of Physics, Università di Roma "Tor Vergata", Italy

N-Heterocyclic carbenes and olefins are known to be excellent modifiers and anchors for the functionalization of surfaces. Here their adsorption behavior on Si(111) is investigated using scanning tunneling microscopy, X-ray photoelectron spectroscopy, and density functional theory. Covalently bound monolayers with high thermal stability and large work function reductions are found. The adsorption geometry and ordering behavior depend on the specific molecule and the domains size correlates with the defect density of the substrate.

O 31.8 Tue 18:00 Poster C

Measuring and Mapping Molecular Elongation by NC-AFM: The Case of Nonahelicene and Coronene on Ag(110) — •Max Halbauer[1], Takashi Kumagai[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institute for Molecular Science, 38 NishigoNaka, Myodaiji, Okazaki 444-8585, Japan

Non-contact atomic force microscopy (NC-AFM) has become a standard tool for the investigation of individual atoms and molecules on surfaces. However, the measurement of elasticity in single molecules and its submolecular resolution have remained as a largely open question. To address this issue, a spring molecule - nonahelicene ([9]H) - was investigated and compared with its flat counterpart - coronene (cor). The molecules were imaged first by high-resolution scanning tunneling microscopy (STM) and NC-AFM on a Ag(110)-surface at cryogenic temperatures (4.8 K), ultrahigh vacuum (UHV) conditions and CO-tips. Interactions of metallic tips with [9]H and cor and the associated elongations were studied then by frequency shift- distance measurements. A novel model for the description of the NC-AFM signals considering an elastic response in the molecular spring was utilized subsequently to rationalize the behavior of both molecules. The spring constant of [9]H was thereby successfully determined to be 5.6 N/m. A position dependent systematic study of the response above the [9]H molecule was performed then to resolve the elastic component with submolecular resolution. The results demonstrate NC-AFM as a powerful tool for the detection of deformation on the atomic scale.

O 31.9 Tue 18:00 Poster C

Electronic Properties of N-Heterotriangulene Derivatives Adsorbed on Au(111) Investigated with Two-Photon Photoemission Spectroscopy — •Jakob Steidel[1], Ina Michalsky[2], Milan Kivala[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Germany — [2]Organisch-Chemisches Institut, Universität Heidelberg, Germany

In many organic opto-electronic devices donor-acceptor systems (D-A systems) play a crucial role, for example as the emitting layer in organic light emitting diodes or to enhance charge separation in organic photovoltaics. Triphenylamine derivatives like the planar N-Heterotriangulene-550 (N-HTA-550) are promising electron donors. The introduction of an etheno bridge closes a seven membered ring in N-HTA-557 and strongly modifies the electronic structure of the molecule while retaining its steric demands. By oxidation of the etheno bridge and subsequent condensation with quinoxaline-2,3-diamine N-HTA-557-P, an intramolecular D-A system, is synthesized. In the present contribution we investigate the electronic structure of N-HTA-550, N-HTA-557 and N-HTA-557-P adsorbed on Au(111) with two-photon photoemission spectroscopy (2PPE). In agreement with the results of UV/Vis-absorption spectroscopy we found the optical gap of N-HTA-550 and N-HTA-557-P to be 3.7 eV and 2.6 eV respectively. For N-HTA-557 the electron affinity level and occupied molecular states were determined, yielding a fundamental gap of 2.9 eV. By means of femtosecond time-resolved 2PPE two coverage dependent exciton decay pathways in thin films of N-HTA-557-P were identified.

O 31.10 Tue 18:00 Poster C

Enhanced conductance of molecular states at interstitial sites — Jan Homberg[1], Manuel Gruber[2], Alexander Weismann[1], and •Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel — [2]Fakultät für Physik, Universität Duisburg-Essen

Arrays of phthalocyanine molecules on Pb(100) are investigated with scanning tunneling microscopy. Maps of the differential conductance exhibit drastic changes as the sample voltage is being varied. Maximal conductances are observed at positions between the molecules mimicking bonding states. However, the maxima are shown to result from a superposition of non-interacting states. We expect that this effect may be observed from many other molecules.

O 31.11 Tue 18:00 Poster C

functionalized platform molecules on Au and Ag (111) studied with scanning tunneling microscopy — •Behzad Mortezapour[1], Alexander Weismann[1], Sebastian Hamer[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Otto-Diels-Institut fur Organische Chemie, Christian-Albrechts-Universität zu Kiel, Germany

To prepare well-ordered molecular architectures on solid surfaces we use the triangular molecular platform trioxatriangulenium. Its central carbon atom enables vertical attachment of various ligands. We present low-temperature scanning tunneling microscopy results for platforms with the ligands phenyl, 3-pyridyl and sec-butyl. The molecules were sublimated onto Au (111) and Ag (111) surfaces at ambient temperature with 99 % of the molecules remaining intact. On the reconstructed Au substrate, the molecules arrange into hexagonal and honeycomb arrays, preferentially in fcc areas. On Ag, the molecules solely adopt closed-packed hexagonal patterns. Single molecules were manipulated with the scanning tunneling microscope tip. We show first spectroscopic results and present current-distance measurements that cover the transition from tunneling to a single molecule contact.

O 31.12 Tue 18:00 Poster C

Charge transfer at organic-metal interfaces mediated by strong external electric fields — •Nina Kainbacher[1,2] and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]Institute of Solid State Physics, Graz University of Technology, Austria

Charge transfer at organic-metal interfaces plays a key role in the charge injection properties of organic-based devices. In this work, we investigate how external electric fields affect the interfacial charge transfer. This offers a new window into deepening our fundamental understanding of charge transfer processes at hybrid interfaces. To investigate this with low computational effort, we perform a theoretical study on prototypical systems using ground-state density functional theory under static external fields applied perpendicular to the substrate plane. The chosen systems comprise the π-conjugated molecules, p-sexiphenyl, PTCDA and pentacenetetrone on three kinds of metal surfaces, Cu(110), Ag(110) and Ag(111), respectively. This choice enables us to compare molecules with different electron affinities as well as substrates with varying interaction strength. Charge transfer at the interface is induced by the vibration of the molecule perpendicular to the substrate plane and by the polarization in response to the electric field. For the former effect, we analyze the density of states as well as the bond lengths as a function of the adsorption distance. Finally, we show how the electric fields affect charge transfer at the interface by studying charge density differences and projections of the density of states.

O 31.13 Tue 18:00 Poster C

Benchmarking theoretical electronic structure methods in a wide binding energy range with photoemission orbital tomography — •Anja Haags[1,2,3], Xiaosheng Yang[1,2,3], Larissa Egger[4], Dominik Brandstetter[4], Hans Kirschner[5], Alexander Gottwald[5], Mathias Richter[5], Georg Koller[4], Michael G. Ramsey[4], François C. Bocquet[1], Serguei Soubatch[1], F. Stefan Tautz[1], and Peter Puschnig[4] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Fundamentals of Future Information Technology, 52425 Jülich, Germany — [3]Experimental Physics IV A, RWTH Aachen University, 52074 Aachen, Germany — [4]Institute of Physics,

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Photoemission orbital tomography (POT) has become a powerful tool to investigate the electronic structure of organic molecules on surfaces. In this combined experimental and theoretical technique, the measured photoemission intensity distributions at particular binding energies can be understood using calculated momentum-space signatures of molecular orbitals. For bisanthene adsorbed on Cu(110), we apply POT in a wide binding energy range to obtain an experimentally-derived molecular orbital projected density of states. We not only identify 13 π and 22 σ orbitals, but also access the respective binding energies of each orbital. This allows us to benchmark the performance of density functional theory calculations in order to account for a precise orbital energy alignment at the molecule/metal interface.

O 31.14 Tue 18:00 Poster C

Quantum transport across single-molecule junctions bridging adlayer-modified electrodes

— •Mong-Wen Gu[1,3], Chi-Ta Lai[1], I-Chih Ni[2], Chih-I Wu[2], and Chun-hsien Chen[1] — [1]Department of Chemistry, National Taiwan University, Taipei, Taiwan — [2]Graduate Institute of Photonics and Optoelectronics, National Taiwan University, Taipei, Taiwan — [3]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany

To explore the complexity of quantum transport across single-molecule junctions, it is essential to develop new types of electrode materials beyond gold electrodes which are overwhelmingly popular due to their reliability and inertness in the fabrication of molecule junctions. Herein, two electrochemical techniques, underpotential deposition and surface-limited redox replacement, were used to prepare gold electrodes which were modified by an atomic layer of platinum and palladium. The single-molecule conductance of α,ω-hexanes (X-(CH$_2$)$_n$-X, X = -SCH$_3$ and -CN, n = 4,6,8) on the bimetallic electrodes was found to be 2*30 times higher than that on bare gold electrodes. This enhanced conductance is ascribed to the partially filled d-shells on the bimetallic electrodes. Such a feature leads to a significantly increased SDOS at the Fermi energy and thus to an improved efficiency of interfacial transport. This work demonstrates a rational strategy for engineering the molecule-metal surface to develop emergent single-molecule testbeds.

O 31.15 Tue 18:00 Poster C

LT-STM investigation of 9-Anthrol on Au (111)

— •Franz Plate[1], Suchetana Sarkar[1], Diego Peña[2], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Centro de Investigación en Química Biolóxica e Materiais Moleculares (CiQUS), Universidade de Santiago de Compostela, Santiago de Compostela 15782, Spain

We present a low temperature scanning tunneling microscope (STM) investigation of 9-Anthrol adsorbed on the Au (111) surface. This chemically unstable tautomer of Anthrone, is studied at the single molecule level, showing its structural and electronic properties. Anthrone was deposited on Au(111) by direct contact deposition followed by annealing at 200°C. High resolution STM images in constant height mode using a CO functionalized tip are presented, as well as scanning tunneling spectroscopy spectra and differential conductance maps of the single molecules.

O 31.16 Tue 18:00 Poster C

Towards k-space imaging molecular orbitals on ferromagnetic surfaces

— •Martin Anstett, Gregor Zinke, Lu Lyu, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany.

Interfaces between organic molecules and ferromagnets are the key functional units of all molecular spintronic applications. The device functionalities are determined by the details of the strong chemical interactions at the interfaces, which typically lead to strong distortions of the wave functions of the molecular orbitals on the ferromagnetic surfaces.

In this contribution, we present our recent progress in imaging the orbitals of molecules on ferromagnetic surfaces at room temperature by combining spin- and momentum-resolved photoemission spectroscopy and photoemission orbital tomography. The main challenge in this endeavour is the lack of ordered or even aligned molecular films on magnetic surfaces. Using ultrathin cobalt films on Au(111) as a ferromagnetic substrate, we are able to realise long-range self-assembled molecules on this surface. These films show distinct emission patterns for the different molecular orbitals. We will discuss signatures of the strong molecule-surface interaction in the molecular orbital emission pattern.

O 31.17 Tue 18:00 Poster C

Collective States in 2D Molecular Monolayers

— •Sabrina Juergensen[1], Moritz Kessens[1], Charlotte Berrezueta-Palacios[1], Nikolai Severin[2], Sumaya Ifland[2], Jürgen P. Rabe[2], Niclas S. Mueller[3], and Stephanie Reich[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany — [3]NanoPhotonics Centre - University of Cambridge, Cambridge, UK

Organic monolayer crystals have emerged as a new material to replace conventional semiconductors like silicon or TMDs and have become a wide research area in recent years. Mostly these 2D materials are grown out of dye molecules that tend to form J-aggregates leading to outstanding optical properties. In J-aggregates the dipole moments of the molecules are aligned resulting in a strong coupling of the molecules, forming a collective state. The photonic excitation of the collective states to higher electronic levels will result in a very narrow and strong emission also known as superradiance.

To study the collective state in an 2D material in dependency of the dielectric environment, we grew monolayers of a perylene derivative on two different van der Waals materials with different electronic properties, providing a perfect platform to study the fundamental mechanism of the collective state. High resolution AFM was used to determine the packing density of the molecules in a monolayer. Different optical methods were used to characterize the collective state of the molecular monolayer. The experimental data were further compared to real space simulations.