O 50: Poster Organic Molecules on Inorganic Substrates: Adsorption and Growth

Time: Tuesday 18:00–20:00 Location: P2

O 50.1 Tue 18:00 P2

Polymorphism of Naphthalene on Ag(111) in and out of thermodynamic equilibrium — •Lorenz Brill[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich-Schiller-Universität, Jena, Germany — [2]Technische Universität, Graz, Austria

Even with a seemingly simple molecule like naphthalene, a rich polymorphism has been observed on Cu(111). Additionally, calculated phase diagrams predict multiple different structures of naphthalene on Ag(111), depending on the pressure and temperature during naphthalene deposition. In this poster, we present first experimental results of naphthalene structures formed in thermodynamic equilibrium obtained in our custom chamber specially designed to enable molecular growth in thermodynamic equilibrium. We compare our results to naphthalene structures grown using a conventional setup.

O 50.2 Tue 18:00 P2

Coverage-dependent assembly of functionalized helicenes — •Elise Fürch[1], Jonas Brandhoff[1], Fumi Nishino[2,3], Keisuke Fukutani[2,3], Marco Gruenewald[1], Maximilian Schaal[1], Felix Otto[1], Roman Forker[1], Takashi Hirose[4], Satoshi Kera[2,3], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Okazaki, Japan — [3]The Graduate University of Advanced Studies, Hayama-cho, 240-193 Kanagawa, Japan — [4]Institute of Chemical Research, Kyoto University, Uji, Kyoto 611-0011, Japan

Recently, the interest in chiral molecules has spiked. The chirality-induced spin selectivity (CISS) promises a high spin-polarizability for electrons traversing a chiral molecule. However, the CISS effect is yet not fully understood. To be able to probe the CISS effect with area averaging methods like photoelectron spectroscopy a well-defined chiral thin film, consisting of helical molecules, is needed. In this study the chiral molecule thiadiazole[9]helicene (TD[9]H) is investigated on Au(111) and Ag(111) surfaces. To understand how chirality from one single molecule evolves into a fully chiral overlayer, a coverage dependent study, showing different structural motifs of TD[9]H, was performed. This structural evolution was investigated using scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). In combination, these methods reveal a chiral lattice, and the role of the different molecule-molecule and molecule-substrate interactions will be discussed.

O 50.3 Tue 18:00 P2

Determining the Epitaxial Relations of Lead Phthalocyanine on Graphitic Surfaces — •Marco Gruenewald, Roman Forker, Matthias Spoddeck, and Torsten Fritz — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

The epitaxial relations between lead phthalocyanine (PbPc) layers and single-crystal graphite (SCG) as well as few-layer graphene/SiC(0001) are determined. Compared to previous reports, we obtain a clearly improved precision by combining the following concepts: [i] the use of distortion-corrected, calibrated low-energy electron diffraction (LEED), [ii] the complementary use of large-scale scanning tunneling microscopy (STM) with high resolution, [iii] the evaluation of multiple scattering features in LEED and Moiré spots in Fourier-transformed STM images, [iv] the simulation of those reciprocal-space patterns with an objective numerical fitting to the experimentally discernible spots, and [v] the analysis of the STM Moiré patterns in real space. Our independently determined LEED and STM results mutually confirm each other due to the remarkably similar structural parameters obtained. For all systems investigated we find noncommensurate, point-on-line coincident registries, and the epitaxial relations of PbPc layers on SCG and on graphene/SiC(0001) are found to be nearly identical despite the different compositions of those substrates. https://doi.org/10.1021/acs.cgd.4c01055

O 50.4 Tue 18:00 P2

Solvent-Free Fabrication of Supported Lipid Bilayers Incorporating Carbon Quantum Dots and Gramicidin A for Biosensing Applications — •Daniel A. Saavedra[1], Benjamín Ruz[1], Nicolás Moraga[1], Nancy Gomez-Vierling[1], Marcelo A. Cisternas[2], Susana D. Rojas[2], and Ulrich G. Volkmann[1] — [1]Instituto de Física, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]Escuela de Ingeniería Industrial, Univ. de Valparaíso, Chile

This study employed two phospholipids for the formation of supported lipid bilayers (SLBs): DPPG, with a net negative charge for enhanced adsorption to surfaces and biomolecules, and DPPC, which is neutral. SLBs were fabricated using a solvent-free, dry, ultra-high vacuum (UHV) approach [1], designed for protein insertion and nanoscale biosensor development for Forster energy transfer (FRET) detection mechanism.

Gramicidin A, a stable ion-channel protein, was incorporated into SLBs via physical vapor deposition monitored by high-resolution ellipsometry, followed by thermal treatment to enhance stability. Carbon quantum dots (CQDs), synthesized through hydrothermal carbonization of chitosan, were added via spin-coating. CQDs were selected for their photostability, low toxicity, and tunable fluorescence [2].

Acknowledgements: ANID Ph.D. Fellowships (DAS, NM, NGV), PUENTE-UC 2024-25. References: [1] Cisternas, M.A. et al., IJMS, 21, 6819 (2020). DOI: 10.3390/ijms21186819 [2] Wu, Q., et al., Nano Research, 16, 1835-1845 (2023). DOI: 10.1007/s12274-022-5189-2

O 50.5 Tue 18:00 P2

Long range ordering of molecular layers on Ag(110) — •Ravi Priya, Weishan Wu, and Peter Jakob — Department of Physics, Philipps University of Marburg, Germany

Single domain molecular layers have been explored on the non-hexagonal Ag(110) substrate in terms of their long-range ordering using SPA-LEED and vibrational signature using high-resolution FT-IRAS. The absence of rotational domains for fcc(110) metal substrates allows for growing layers with uniform azimuthal orientation of deposited molecules. We have investigated various molecules and configurations that may form single domain molecular layers (including mirror domains). Specifically, monolayers of PTCDA, NTCDA, and regio-selectively substituted pentacene species (pentacene (PEN), pentacene-quinone (P2O), pentacene-tetrone (P4O), quinacridone (QA)) were deposited on Ag(110) and examined in terms of their structure using SPA-LEED, and their vibrational signature using IR - spectroscopy. Among them, PTCDA, NTCDA, PEN, and QA have been found to form parallel-oriented, single domain structures. For QA two novel heterochiral phases are found after annealing, in addition to the single-domain homochiral phase present $T < 500$K. For P2O and P4O, steric hindrance and hydrogen bonding lead to the formation of 1D islands and 2D islands, respectively, at sub-monolayer coverages. 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.

O 50.6 Tue 18:00 P2

Structural and vibrational properties of mixed (CuPc + P4O) molecular layers on Ag(111) — •Yeondu Kim, Ravi Priya, and Peter Jakob — Department of Physics, Philipps University Marburg, Germany

Structural properties of mixed layers comprising CuPc and P4O on Ag(111) and their thermal evolution have been investigated by means of Fourier-transform infrared absorption (FT-IRAS) and electron diffraction (SPA-LEED). For this material combination several long-range ordered phases at different relative ratios are found. Their formation and thermal stability have been analyzed in the temperature range 80 - 500 K, limited by thermal desorption and/or dissociation of the CuPc and P4O compounds at high temperature. Lateral interactions between CuPc and P4O within the mixed layers lead to characteristic frequency shifts of out-of-plane modes. In parallel, the intensities of in-plane vibrational modes of CuPc and P4O are strongly attenuated when adsorbed at nearby locations, indicating a major change in the associated interfacial dynamical charge transfer (IDCT). Specifically, IDCT that is quite prominent for the pure CuPc/Ag(111) and P4O/Ag(111) monolayers, is substantially attenuated for the mixed layers. This is ascribed to a through-metal charge transfer from CuPc to P4O that is associated with an upshift of the CuPc former LUMO and the correlated downshift of the P4O former LUMO. These correlated shifts lead to substantially lower density of states at the fermi level for both molecular species and thereby a weakening of IDCT induced bands.

O 50.7 Tue 18:00 P2

Structure and thermal Stability of (C60+P2O) and (C60+P4O) Heterolayers on Ag(111)

— •Mohammed Suhail Ansari, Ravi Priya, Keda Jin, and Peter Jakob — Department of Physics, Philipps-Universität Marburg, Germany

This study investigates the interactions between C_{60} fullerene and two organic semiconductors, 6,13-pentacenequinone (P2O) and 5,7,12,14-pentacenetetrone (P4O), on Ag(111) substrates using IRAS, SPA-LEED, and TDS. The aim is to elucidate the structural properties and transformation processes of C_{60} and P2O/P4O under varying preparation conditions and thermal processing. Our findings reveal three different vertical arrangement scenarios of the heterostructures based on the deposition sequence and thermal treatments: (a) Formation of a well-defined bilayer on a pre-deposited monolayer corresponding to the deposition sequence, (b) a complete interlayer exchange of molecules, and (c) a partial interlayer exchange leading to mixed layers. Scenario (a) is observed with a P2O bilayer deposited on a well-defined C_{60} monolayer. Interestingly, P2O adsorbs in an inclined orientation on the C_{60}/Ag(111) monolayer. Scenario (b) is observed with deposition of a monolayer of P2O followed by a bilayer of C_{60} at room temperature that results in P2O migration to the second layer, emphasizing the weaker interaction of P2O with the substrate Scenario (c) is found for the combination of C_{60} and P4O and it involves migration of P4O to the second layer if it was deposited in the first layer, and vice-versa. We will discuss in detail the evolution of the grown heterolayers in terms of molecular orientations, interlayer exchange, and intermixing.

O 50.8 Tue 18:00 P2

Molecular self-assembly of BDA on $CsPbBr_3$(100)

— •Hannah Loh, Andreas Raabgrund, 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. By choosing perticular anchoring groups of organic molecules (here the carboxylic COOH-group) the interaction with the perovskite material may be tuned.

In this contribution we investigate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial $CsPbBr_3$ on Au(100) [2] by STM. For submonolayer coverage of BDA on $CsPbBr_3$ we find that upon deposition at 305 K molecules grow epitaxially in compact islands. The islands consist of chains with a V-structure inside the chains similar to the way BDA self-assembles on Cu(111) [3].

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Schmitt T. et al., J. Phys. Chem. C, **120(2)**, 1043-1048, (2016)

O 50.9 Tue 18:00 P2

Structure and charge carrier dynamics of an organic donor/acceptor heterostructure: a LEEM/PEEM study

— •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — IEPT, TU Clausthal, Germany

We combine low-energy electron microscopy (LEEM) and two-photon photoemission electron microscopy (2P-PEEM) to study the relation between structure and charge carrier dynamics in well-ordered organic donor/acceptor (D/A) heterostructures of para-sexiphenyl (*p*-6P) and copper-hexadecaphthalocyanine (F_{16}CuPc). While *p*-6P monolayers deposited on SiO_2 exhibit structural order only on a nanometer scale, *p*-6P islands in the second layer comprise micrometer sized single-crystalline domains. Using microspot low-energy electron diffraction (μLEED) and dark-field LEEM, on many islands we observe two mirror domains which we attribute to different tilt angles of the *p*-6P molecules in the second layer. Using μLEED we confirm epitaxial growth of monolayer F_{16}CuPc on SiO_2/*p*-6P which results in a structurally well-defined organic D/A interface. Especially on *p*-6P bilayer regions, large single-crystalline F_{16}CuPc domains are observed. With 2P-PEEM we observe increased photoemission from SiO_2/F_{16}CuPc after optical pumping at 810 nm. In contrast, for SiO_2/*p*-6P/F_{16}CuPc the photoemission signal decreases. Also, the reflectivity for low-energy electrons changes upon optical pumping. We relate these long-lived pump-induced effects to intermolecular charge transfer which is more pronounced for bilayer-*p*-6P/F_{16}CuPc than for monolayer-*p*-6P/F_{16}CuPc.