

O 55: Poster Wednesday: Organic Molecules at Surfaces 2

Time: Wednesday 18:00–20:00

Location: P4

O 55.1 Wed 18:00 P4

Self-assembly and debromination of a functionalized borazine on Ag(111) — ●BIRCE SENA TÖMEKCE¹, MARC G. CUXART¹, MARTINA CROSTA², MARCO FRANCESCHINI², DANIELE POLETTI², DAVIDE BONIFAZI², and WILLI AUWÄRTER¹ — ¹Physics Department E20, Technical University of Munich, Germany — ²Institute of Organic Chemistry, University of Vienna, Austria

On-surface synthesis is a promising route towards the generation of doped graphene nanoarchitectures with tunable electronic properties [1]. To fabricate atomically precise hybrid BNC materials, distinct precursors incorporating BN units can be used [2]. In this study, we employed a precursor with a borazine core and Br and OH functionalization. We report on a low-temperature scanning tunneling microscopy/spectroscopy and X-ray photoelectron spectroscopy characterization of well-ordered phases of this precursor on Ag(111). At low temperatures, the molecules adsorb intact. At moderate temperatures, debromination is activated and the self-assembly of a chiral kagomé lattice coexisting with a hexagonal packing is observed. At elevated temperatures, completion of cyclodehydrogenation leads to full planarization of the molecules, followed by covalent intermolecular coupling, thereby forming random BNC-based networks. We further investigated the electronic structure of the kagomé lattice on the single molecule level. Our findings constitute a step towards exploiting the structural and electronic properties of BNC architectures.

[1] R. Pawlak et al., *Angew. Chem. Int. Ed.* 2021, 60, 8370-8375

[2] C. Sánchez-Sánchez et al., *ACS Nano*. 2015, 9, 9228-9235

O 55.2 Wed 18:00 P4

The investigation of self-assembly molecule on metal substrate — ●YONG-HE PAN and GERMAR HOFFMANN — Department of Physics, National Tsing Hua University

Field-effect transistors (FETs) made out of organic materials are lighter, mechanically more flexible, have lower costs and have higher field-effect mobility. For picene-(C₁₄H₂₉)₂ the highest field-effect mobility in all FETs was recorded. Here, phenacene-(C₁₄H₂₉)₂ is deposited on Au(111) by thermal evaporation and is investigated by STM and Scanning Tunneling Spectroscopy (STS) at 70 K under UHV conditions. The self-assembly molecule forms a rhombohedral unit cell with a two molecular basis, and the alkyl chain, flexible up to 15 degrees, is nearly parallel with the nearby molecules. Scanning close to the bandgap region of the phenacene-(C₁₄H₂₉)₂ leads to imaging of the LUMO-state, which also shows the pronounced electronic state on the phenacene core and energetically broad state on the alkyl chain.

O 55.3 Wed 18:00 P4

adsorption structure and mechanical properties of single nonahelicene molecules on Ag(110) — ●MAX HALBAUER^{1,2}, AKITOSHI SHIOTARI¹, TAKASHI KUMAGAI³, KYOKO NOZAKI², and MARTIN WOLFF¹ — ¹Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany — ²Department of Chemistry and Biotechnology, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, 113-8656 Tokyo, Japan — ³Center for Mesoscopic Sciences, Institute for Molecular Science, 38 Nishigo-Naka, Myodaiji, 444-8585 Okazaki, Japan

Helicenes are a class of compounds that has received great attention due to their chiroptical properties, while the single-molecule mechanical behavior has often been overlooked. Scanning tunneling microscopy (STM) and atomic force microscopy (AFM) measurements of nonahelicene ([9]H) molecules on Ag(110) were performed in order to address this issue. The adsorption structure of isolated and aggregated [9]H molecules on the surface is revealed by high-resolution imaging. Interactions of the molecule with a probe tip are quantified by force curve measurements and a comparison with co-adsorbed coronene gives insights into the impact of the helical backbone on the mechanical properties.

O 55.4 Wed 18:00 P4

Changes in the coupling of a single-molecule magnetic moment to a Cooper pair condensate by the sequential removal of molecular moieties — ●STEFAN SCHULTE¹, NICOLAS NÉEL¹, KRISZTIAN PALOTAS², and JÖRG KRÖGER¹ — ¹Institut für Physik, Technische Universität Ilmenau, Ilmenau, Germany — ²Institute for

Solid State Physics and Optics, Wigner Research Center for Physics, Budapest, Hungary

Using the tip of a STM chemical reactions are induced in organic 5,10,15,20-tetrakis(4-bromophenyl)-porphyrin-cobalt molecules adsorbed on superconducting Pb(111). Two chemical reactions, the dehalogenation and dephenylation of the molecules are presented. Yu-Shiba-Rusinov bound states occur in the superconductor energy gap only after the entire dephenylation of the molecule. The presence of the intragap resonances is related to an unoccupied molecular orbital that is confined to the atomic magnetic center (Co) of the porphyrin. From the energy position and spectral weight of these intragap resonances, a weak interaction between the molecular magnetic moment and the Cooper pair condensate is inferred. The electron-hole asymmetry of the bound states exhibits a spatial oscillation with a wavelength that evidences the exchange coupling of the molecular magnetic moment to the sp-sheet of the Fermi surface. The very low binding energy of the Yu-Shiba-Rusinov levels is consistent with the observed absence of the Kondo effect. Funding by the DFG through KR 2912/10-1 and KR 2912/10-3 is acknowledged.

O 55.5 Wed 18:00 P4

Pentacene on prototypical antiferromagnets: A photoemission study — ●VALENTIN MISCHKE, DAVID JANAS, GIOVANNI ZAMBORLINI, JONAH E. NITSCHKE, and MIRKO CINCHETTI — Department of Physics, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

In the last years, so-called molecular spinterfaces have been intensively studied because of the novel spin properties raising from the molecule-metal hybridization [1]. Recently, antiferromagnets have been considered as an alternative to their ferromagnetic counterparts for the engineering of spinterfaces with novel spin properties. Here, we present the preliminary characterization of a single layer of pentacene atop two prototypical antiferromagnets, namely nickel oxide NiO(111) and iron oxide FeO(100). Both thin films have been grown in-situ, under UHV conditions, by depositing Ni and Fe in a O₂ background atmosphere onto Au(111) and oxygen-passivate Fe(100), respectively. The resulting interfaces have been characterized with low energy electron diffraction and momentum microscopy. In addition, photoemission tomography was employed to determine the energy level alignment of the molecular orbitals at the interface.

[1] Cinchetti, Dediu, Hueso, *Nature Materials* 16, 507 (2017)

O 55.6 Wed 18:00 P4

Systematically mapping the distance-dependent tip-sample interaction for the PTCDA/Ag(111) system — ●TIM DIERKER and PHILIPP RAHE — Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, 49076 Osnabrück, Germany

Scanning probe microscopy (SPM) has been continually improved by establishing a number of controlled tip functionalizations [1]. In particular, the attachment of a single 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) molecule to the apex of a metallic tip enables mapping of the electrostatic potential near sample surfaces by so called scanning quantum dot microscopy [2,3]. In order to reliably apply this technique, the expedient pick-up of a single molecule is required [4]. Here, the tip-molecule interaction between a metallic tip and surface-adsorbed molecules is investigated by means of systematic scanning tunneling (STM) and atomic force (AFM) microscopy measurements. In particular the vertical dependencies of the STM tunneling current and the AFM frequency shift are mapped along different axes of single PTCDA molecules embedded in the molecular film on Ag(111). Fingerprints for the dynamic behavior of the molecules are clearly revealed and guide the vertical manipulation for molecular pick-up.

[1] L. Gross, *Nat. Chem.* 3, 273 (2011)

[2] C. Wagner et. al., *PRL* 115, 026101 (2015)

[3] M. F. B. Green et. al., *JJAP* 55, 08NA04 (2016)

[4] M. F. B. Green et. al., *Beilstein J. Nanotech.* 5, 1926 (2014)

O 55.7 Wed 18:00 P4

Photoemission and Raman Spectroscopic Studies of n-GaAs(100) Surface Passivation with Thioglycolic Acid — ●ALEXANDER EHM, OLEKSANDR SELYSHCHEV, and DIETRICH R. T. ZAHN — Semiconductor Physics, TU Chemnitz, Chemnitz D-09107,

Germany

Gallium arsenide is one of the most investigated inorganic semiconductors and used in a vast variety of applications and prospective for new high-performance devices. A challenge in constructing such devices is a surface of native oxides causing a high surface density of states, which leads to the mid-gap pinning of the surface Fermi level, band bending, and the formation of a surface depletion layer. Sulphur passivation yields a significant reduction of the depletion layer and related effects but requires several treatment steps [1].

We report a new simple approach utilizing thioglycolic acid (TGA) to provide a one-step effective removal of surface oxides and protection from reoxidation compared to etching with inorganic acids. This effect is confirmed by X-ray photoemission spectroscopy and the reduction of the depletion layer is confirmed by Raman spectroscopy results. n-GaAs(100)/poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) solar cells show improved performance for such passivated n-GaAs(100) surfaces.

[1] V. N. Bessolov, M.V. Lebedev, D. R. T. Zahn: J. Appl. Phys. 82 (5) (1997)

O 55.8 Wed 18:00 P4

Vibrational quanta of single melamine on Cu(100) — ●REBECCA CIZEK, NICOLAS NÉEL, and JÖRG KRÖGER — TU Ilmenau Melamine adopts an up-standing adsorption geometry on Cu(100) and can be tautomerized by the local injection of electron from the tip of a scanning tunneling microscope [1]. Here, we compare inelastic electron tunneling spectroscopy (IETS) of intact and tautomerized melamine. Two low-energy vibrational quanta are observed for both molecules. The tautomer exhibits an energy shift and enhancement of one of the excitations. These findings are moreover complemented by IETS and tautomerization of the deuterated molecule.

[1] R.-P. Wang et al., J. Phys. Chem. Lett. 12, 1961 (2021)

O 55.9 Wed 18:00 P4

Photoemission orbital tomography of NiTPP molecules deposited on the passivated Fe(100)-p(1x1)O surface — ●MICHAEL GUTNIKOV¹, DAVID JANAS¹, JONAH NITSCHKE¹, MIRA ARNDT¹, VITALIY FEYER², GIOVANNI ZAMBORLINI¹, and MIRKO CINCHETTI¹ — ¹Department of Physics, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — ²Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Leo-Brandt-Straße, 52425 Jülich, Germany

Recently, it was shown that a single layer of oxygen is sufficient to decouple nickel porphyrins from a ferromagnetic surface, thus, preserving most of the electronic features of the pristine molecules [1]. However, distortions of the molecular structure, e.g. upward-bent phenyl-rings, can make the interpretation of surface imaging techniques like STM extremely challenging.

Additional information can be gained by photoemission tomography (PT), which combines angle-resolved photoelectron spectroscopy (ARPES) with ab-initio calculations of the gas phase molecules to interpret the orbital arrangement of thin molecular layers.

This work provides a characterization of NiTPP molecules on an oxygen passivated Fe(100)-p(1x1)O surface using PT, focusing not only on the energy level alignment but also on their azimuthal orientation with respect to the substrate.

[1] G. Albani et al. Micromachines 12, 191 (2021)

O 55.10 Wed 18:00 P4

Surface Chemical Bond of Alternant vs. Non-Alternant Aromatic Isomers — ●FLORIAN MÜNSTER¹, LUKAS RUPPENTHAL¹, LEONARD NEUHAUS¹, JAN HERRITSCH¹, JON HENRICK BOTH¹, PENGCAI LIU², XING-YU CHEN², JIAWEN CAO², XIAO-YE WANG², and J. MICHAEL GOTTFRIED¹ — ¹Fachbereich Chemie, Philipps-Universität Marburg, Germany — ²College of Chemistry, Nankai University, Tianjin, China

The different effects of the topology of pyrene and cyclohepta[*fg*]acenaphthylene (acepleiadylene) on the occupied and the unoccupied electronic states as well as on the desorption process from the Cu(111) surface are studied using PES, NEXAFS and TPD. Both molecules are aromatic but differ in their topology. While pyrene has an alternating structure, its constitutional isomer acepleiadylene has a non-alternating one. With TPD, we showed that the desorption of acepleiadylene begins at about 340 K, 40 K higher than for pyrene, indicating a stronger bond to the Cu(111) surface. Using the modified leading edge analysis we find a desorption energy of 152 kJ/mol for

acepleiadylene compared to 108 kJ/mol for pyrene, each at monolayer coverage. Furthermore, combining PES and NEXAFS, we were able to assess the energy needed in the excitation process of electrons originating from occupied valence orbitals into unoccupied ones. Here we find a 0.5 eV smaller energy difference for the non-alternating species in comparison to the alternating species.

O 55.11 Wed 18:00 P4

New Photon Scanning Tunnelling Microscope for studying electrically driven single photon emitters in the GHz range — ●ANDREAS REUTTER^{1,2}, MIKE STUMMVOLL^{1,2}, NEDA NOEI¹, MARKUS ETZKORN^{1,2}, and UTA SCHLICKUM^{1,2} — ¹Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, 38106 Braunschweig — ²Laboratory for Emerging Nanometrology, Langer Kamp 6a/b, 38106 Braunschweig

Single atoms and molecules have always been an interesting research area. An important tool for investigating such is scanning tunnelling microscopy (STM) which has become a widely used method to characterize not only the surface density states and vibrational excitations but also electrical excitations and recombination processes of individual atoms and molecules by STM-induced luminescence (STML).

We would like to present a state-of-the-art, self-build, low-temperature, ultra-high vacuum STM with the possibility for STML measurements and for the time-resolved probing of electrically driven single photon emitters with a band width of up to around 20 GHz. This allows for instance the investigation of charge transfer in molecules below the nanosecond range and further insight into its exciton decay.

O 55.12 Wed 18:00 P4

Anchoring *p*-terphenyl-based thiols to top-layer sulphur defects on MoS₂/Au(111) — J. RIKA SIMON¹, DMITRII MAKSIMOV², ●JUAN PABLO GUERRERO FELIPE¹, PAUL WIECHERS¹, CHRISTIAN LOTZE¹, ANA M. VALENCIA^{3,4}, CATERINA COCCHI^{3,4}, BJÖRN KOBIN⁴, STEFAN HECHT⁴, MARIANA ROSSI², and KATHARINA J. FRANKE¹ — ¹Freie Universität Berlin, Germany — ²MPI for the Structure and Dynamics of Matter, Hamburg, Germany — ³Carl von Ossietzky Universität Oldenburg, Germany — ⁴Humboldt-Universität zu Berlin, Germany

Systems consisting of transition metal dichalcogenides (TMDCs) and organic molecules is a field gathering much interest in recent years. By using a scanning tunneling microscope (STM), it is possible to explore these systems in detail, where the TMDC layer works as a decoupling layer between the adsorbate and metal substrate. In our experiments, we investigate a monolayer of MoS₂ on Au(111) where interesting results occur once a sulphur defect on the top-layer is created. It gives rise to a localized resonance around the Fermi energy, not present in pristine MoS₂. Here we show experimental and theoretical comparisons where the thiol-based molecule CF₃-3P-SH (4^{tr}-(trifluoromethyl)-[1,1':4',1'']-terphenyl)-4-thiol) is anchored to a sulphur top-layer defect, creating a chemical bond between the molecule and MoS₂. We observe a characteristic Kondo resonance due to the interaction between molecule and substrate. Additionally, we have mapped out the spatial distribution of the electronic states as well as explored the vibronic states of the molecule.

O 55.13 Wed 18:00 P4

On-Surface Transmetalation of a Lead-Porphyrin on the Cu(111) surface — ●JAN HERRITSCH, STEFAN R. KACHEL, QITANG FAN, MARK HUTTER, LUKAS J. HEUPLICK, FLORIAN MÜNSTER, and J. MICHAEL GOTTFRIED — Philipps-Universität Marburg

Starting from porphyrin complexes, highly ordered nanostructures can be assembled on surfaces in which reactive metal centers are firmly anchored in a defined environment. Such structures have enormous potential in various areas of modern technology. A reaction in which there is an exchange of the central atom by another element leads to a drastic change in the properties of the functionalized surface. Here, we report on a thermally induced Pb/Cu metal exchange of lead(II)-tetraphenylporphyrin (Pb(TPP)) on the Cu(111) surface. Using temperature-dependent XPS, we were able to track this exchange reaction and the accompanying change of the Pb oxidation state by probing the Pb 4f level. The reaction starts already below 380 K and is completed at 600 K. In parallel, partial desorption of a monolayer occurs above 430 K. In a temperature-programmed reaction experiment (TPR), the desorbing species are unambiguously identified as the product, Cu(TPP), of the metal exchange by mass spectrometry. By STM, the adsorbate structure of Pb(TPP) on Cu(111) were revealed and individual free Pb atoms, which are formed in the course of the

Pb/Cu metal exchange, were observed. Moreover, side-reactions of the peripheral phenyl substituents occur due to dehydrogenative coupling reactions.

O 55.14 Wed 18:00 P4

Tip-enhanced Raman Spectroscopy of a lifted single PTCDA molecule — ●RODRIGO CEZAR DE CAMPOS FERREIRA¹, JIŘÍ DOLEŽAL^{1,2}, SOFIA CANOLA¹, PROKOP HAPALA¹, PABLO MERINO³, and MARTIN ŠVEC¹ — ¹Institute of Physics, Czech Academy of Science, Czech Republic — ²Faculty of Mathematics and Physics, Charles University, Czech Republic — ³Instituto de Ciencia de Materiales de Madrid; CSIC, Madrid, Spain

Advanced scanning probe techniques in the research of molecular adsorbates on surfaces have been instrumental in unveiling fundamental quantum phenomena with high sensitivity and spatial resolution at the nanoscale level. Such advances impact areas of molecular electronics, nanophotonics, and near-field spectroscopies. Tip-enhanced Raman spectroscopy (TERS) is a technique that provides access to vibrational modes of individual molecules via the extremely confined plasmonic field at the STM tip apex. This can be also used as a probe to chemically scrutinize single bonds with subnanometer precision. In this work, the STM-controlled TERS technique in a UHV environment at low temperature was performed for the perylene tetracarboxylic dianhydride molecule (PTCDA), in which we measured the Raman fingerprint for an array of PTCDA on Ag(111) as well as for a single molecule. Moreover, we were able to simultaneously follow the conductance spectrum of the system while lifting a single PTCDA from the surface. The observed transition in the Raman spectra correlates with the differential conductance showing the transition of the system from S=0 neutral to S=1/2 anion state.

O 55.15 Wed 18:00 P4

Electronic properties of CuPc/TiSe₂ heterostructures — ●HIBIKI ORIO^{1,2}, KIANA BAUMGÄRTNER^{1,2}, CHRISTIAN METZGER^{1,2}, MARKUS SCHOLZ^{3,4}, KAI ROSSNAGEL^{4,5}, and FRIEDRICH REINERT^{1,2} — ¹Universität Würzburg Experimentelle Physik VII, Würzburg, Germany — ²Würzburg-Dresden Cluster of Excellence ct.qmat, Würzburg Dresden, Germany — ³European XFEL Facility, Schenefeld, Germany — ⁴Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — ⁵KiNSIS, Universität Kiel, Kiel, Germany

Transition metal dichalcogenides (TMDC) are a class of quasi-2D materials that exhibit a variety of electronic properties including su-

perconductive, excitonic insulator, and charge-density wave (CDW) phases. TiSe₂ is one of the most prominent TMDC because it has intriguing CDW properties. The physical process of the CDW is not fully understood, however, and is attributed to either be purely electron-electron or jointly electron-electron and electron-phonon mediated. To gain more insight into the CDW buildup, modulating the intrinsic physical properties is useful [1]. For this purpose, we have used organic molecules as several interactions such as charge transfer or a rearrangement of the electron density can modulate the electronic properties at the organic/TMDC interface. We have evaporated copper phthalocyanine (CuPc) on TiSe₂ single crystals. We report the perturbed electronic characteristics of the resulting CuPc/TiSe₂ heterostructure examined with angle-resolved and X-ray photoelectron spectroscopy.

[1] K. Baumgärtner et al., submitted.

O 55.16 Wed 18:00 P4

Chirality-induced electron spin filtering in chiral helicene mono-, double- and multilayers — ●RUWEN QUENTER¹, PAUL VALERIAN MÖLLERS¹, KARL-HEINZ ERNST², and HELMUT ZACHARIAS¹ — ¹Center for Soft Nanoscience, WWU Münster, Germany — ²Empa, Dübendorf, Switzerland

The transmission yield of electrons through molecules with chiral structure can depend on the electron spin. This phenomenon is established as chirality-induced spin selectivity (CISS).¹ While initial demonstrations of CISS were conducted with, e.g., short DNA strands,² studies with simpler molecules such as helicene potentially allow for a better insight into the mechanism. Previous work³ on CISS in ordered monolayers of heptahelicene ([7]H) demonstrated that while the preferentially transmitted spin orientation depends on the helicity of the molecules, no major influence of the substrate is evident. Since the CISS increases with the number of helical turns, we investigate how it evolves for double and multilayers of [7]H adsorbed on a Cu(332) surface. Photoelectrons were excited from the substrate by deep-UV laser pulses and transmitted through [7]H mono-, double or multilayers. Subsequently, the average spin polarization of the photoelectrons was measured via Mott scattering. With a [7]H monolayer a spin polarization of $P \approx 8\%$ was shown earlier³ and reproduced now. For the double and multilayers no increased spin polarization magnitude was found. ¹ D. H. Waldeck et al., APL Mater. **9**, 040902 (2021) ² B. Göhler et al., Science **331**, 894 (2011) ³ M. Kettner et al., J. Phys. Chem. Lett. **9**, 2025 (2018)