

## O 41: Inorganic/Organic Interfaces

Time: Tuesday 18:15–21:00

Location: Poster B

O 41.1 Tue 18:15 Poster B

**LEED-IV-Analysis of large planar molecules on Ag surfaces** — ●INA KRIEGER<sup>1,3</sup>, JOHANNES INGENMEY<sup>1</sup>, GEORG HELD<sup>2</sup>, CHRISTIAN KUMPF<sup>3</sup>, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — <sup>2</sup>Department of Chemistry, University of Reading, Whiteknights, Reading, RG6 6AD, and Diamond Light Source, Didcot, OX11 0DE, UK — <sup>3</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428 Jülich, Germany

The atomic coordinates of large aromatic molecules adsorbed on surfaces are of great interest in the context of understanding the details of interaction and chemical bonding between the molecules and the substrate. Normal incidence X-ray standing waves (NIXSW) is considered to be the only technique which can provide this information with sufficient precision. Here we report on an alternative, namely the I(V)-analysis of low energy electron diffraction (LEED-IV) on two model molecules, which have been investigated by NIXSW before. The intention was to gain additional structural information by LEED-IV and to test the potential of LEED-IV for larger molecules.

We present results on PTCDA/Ag(100) showing an encouraging agreement with those from DFT and NIXSW studies. We obtained a good Pendry R-factor of 0.19 and derive additional structure information on the internal geometry of the molecules, in particular regarding vertical distortions of the perylene core, as well as the buckling of the substrate surface. In addition, we will present first results of a LEED-IV study on the adsorption of NTCDA on Ag(111). Supported by the DFG.

O 41.2 Tue 18:15 Poster B

**Confinement of surface state electrons by molecular self-assembled networks** — ●JUN LI, STEFANO GOTTARDI, JUAN CARLOS MORENO LOPEZ, LEONID SOLIANYK, and MEIKE STÖHR — Zernike Institute for Advanced Materials, University of Groningen, Netherlands

The controlled tuning of material properties on the nanometer scale is a central goal in nanoscience. Artificial nanostructures can be built atom by atom with scanning tunneling microscopy (STM). Corral structures built by this technique were shown to confine the surface state electrons and to locally modify the electronic surface properties. However, the manipulation process is impractical to change the electronic properties of the entire surface. On the other hand, molecular self-assembly offers the possibility to build well-ordered and defect-free nanostructures due to its intrinsic error-correction. By using different molecular building blocks, networks of different sizes and symmetries can be formed, which allows for tuning the electronic structure not only locally but surface wide. Here, we report on confining the surface state electrons of Au(111) by a porous molecular network, which was formed by self-assembled 1,3,5-benzenetribenzoic acid. STM and STS were performed to spatially characterize the electronic properties and to analyze the confinement of the surface state electrons in the pores of the molecular network

O 41.3 Tue 18:15 Poster B

**Comparison of Electronic Transport Measurements on Carbon Nanomembranes using Conductive Probe Atomic Force Microscopy and Ga<sub>2</sub>O<sub>3</sub>/EGaIn Top Electrodes** — ●EMANUEL MARSCHEWSKI, XIANGHUI ZHANG, PAUL PENNER, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

Aromatic self-assembled monolayers (SAMs) can be cross-linked via irradiation with low energy electrons and convert to carbon nanomembranes (CNMs). We compare the electronic transport measurements on pristine and cross-linked self-assembled monolayer of 4'-nitro-1,1'-biphenyl-4-thiol (NBPT) on polycrystalline Au(111)/mica and Au/Si by using two techniques. The conductance along with friction force mapping of pattern arrays of non-cross-linked and cross-linked NBPT-SAMs is conducted by using conductive probe atomic force microscopy (CP-AFM), where the cross-linked regions clearly show lower conductance and lower friction force. The application of soft Ga<sub>2</sub>O<sub>3</sub>/EGaIn top electrodes allows for a quantitative analysis of conductance and transition voltages (TVs) of molecular junctions incorporating NBPT-

SAMs and NBPT-CNMs, respectively. The conductance reduces more than one order of magnitude, despite the fact that the layer thickness reduces slightly upon electron irradiation. The reduction of the TV by  $\sim 0.5$  V is also found in the NBPT-CNM based junctions. In addition, a suppression of conductivity in CP-AFM measurements implies that there could exist a certain amount of highly conducting pinholes, which may explain the discrepancy between the two techniques.

O 41.4 Tue 18:15 Poster B

**On the adsorption behavior of the ionic liquid [BMP][TFSA] on TiO<sub>2</sub> (110), Cu(111) and Ag(111) and the interaction with Li** — ●MARAL HEKMATFAR<sup>1,2</sup>, BENEDIKT UHL<sup>1,2</sup>, FLORIAN BUCHNER<sup>1,2</sup>, DOROTHEA ALWAST<sup>1,2</sup>, and R. JÜRGEN BEHM<sup>1,2</sup> — <sup>1</sup>Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — <sup>2</sup>Helmholtz-Institute Ulm (HIU) Electrochemical Energy Storage, D-89069 Ulm, Germany

The ionic liquid n-butyl-n-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide [BMP][TFSA] is particularly interesting for the application in electrolytes for Li-ion batteries. In this model study we aim at a detailed understanding of the electrode|electrolyte interface at the molecular scale. In a first step [BMP][TFSA] was vapor deposited on Cu(111), Ag(111) and TiO<sub>2</sub>(110) under ultra-high vacuum conditions. At 80 K [BMP][TFSA] adsorbs intact on all surfaces which was verified by XPS measurements; different molecular arrangements were observed by STM, which will be discussed. Upon co-deposition of Li to mimic electrolyte, decomposition of mainly the anion into, e.g., LiF and Li<sub>2</sub>S was found on Cu(111) even at 80 K, while on Ag(111) and TiO<sub>2</sub> the IL is little or nearly not affected. Interestingly, on TiO<sub>2</sub>(110) a new Ti<sup>3+</sup> species is observed in the Ti 2p region, which points toward the reaction of Li with the surface. In contrast, on Cu(111) we assume that a surface mediated decomposition of [BMP][TFSA] with Li takes place. As the electrode|electrolyte interface strongly determines the functionality of a battery, we believe that our model study gives very new insights.

O 41.5 Tue 18:15 Poster B

**Templated Protein Adsorption on Cu<sub>2</sub>N** — ●SEBASTIAN KOSLOWSKI<sup>1</sup>, DANIEL P. ROSENBLATT<sup>1</sup>, SABINE ABB<sup>1</sup>, STEPHAN RAUSCHENBACH<sup>1</sup>, KLAUS KERN<sup>1,2</sup>, and UTA SCHLICKUM<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

In recent investigations of the protein Cytochrome-C (CytC) deposited on metallic substrates by electrospray ion beam deposition (ES-IBD) it has been shown that the adsorption conformation of the unfolded protein is strongly influenced by surface mobility and the charge state of the gas phase protein ion [1]. The length and the flexibility of the peptide chain allows for a large conformational freedom in the gas phase as well as on homogenous surfaces. Here we present scanning tunneling microscopy (STM) investigations of the conformation of single CytC molecules deposited by ES-IBD on a Cu<sub>2</sub>N monolayer. Cu<sub>2</sub>N forms an adlayer with a square grid-like superstructure on the underlying Cu(100) substrate and acts as a template for the deposited proteins. This reduces their conformational freedom. We analyzed the surface conformations of CytC using models, which describe polymer adhesion on a grid with and without the assumption of memory of the gas phase conformation. The acquired data are best described by a model, in which elongated molecules try to reach the pure Cu rows with minimal movement.

[1] Z. Deng et al., Nano Lett. 12 (2012) 2452-2458

O 41.6 Tue 18:15 Poster B

**From hydrogen bonding to metal-coordination and back: porphyrin derivatives on Ag(111)** — ●KATHRIN MÜLLER<sup>1</sup>, FLORIAN STUDENER<sup>1</sup>, NICOLAS MARETS<sup>2</sup>, VÉRONIQUE BULACH<sup>2</sup>, MIR WAIS HOSSEINI<sup>2</sup>, and MEIKE STÖHR<sup>1</sup> — <sup>1</sup>Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — <sup>2</sup>Laboratoire de Tectonique Moléculaire, Institut Le Bel, Université de Strasbourg, France

The formation of well-ordered molecular networks on surfaces has gained increasing attention over the last decades from a fundamen-

tal point of view as well as for their potential application in organic devices like organic photovoltaics or organic field effect transistors. In our studies we used a porphyrin derivative, which is functionalized at the meso positions with two pyridyl groups and two pentyl chains in trans configuration. We used scanning tunneling microscopy (STM) in order to investigate the self-assembly of this molecule on Ag(111). For submonolayer to monolayer coverage, a close-packed rhombic network is observed, which is stabilized via hydrogen bonding. Upon deposition of Co atoms, a porous hexagonal network forms by coordination of the pyridyl groups to the cobalt atoms. Upon thermal annealing at 450 K the hexagonal network is transformed into a second close-packed structure. We assign these structural changes to the Co-metalation of the porphyrin core. For an excess of Co atoms the porous hexagonal network is stable up to 600 K. These results are compared to a similar porphyrin derivative with a Ni core.

O 41.7 Tue 18:15 Poster B

**Interaction of Ethylene Carbonate and Propylene Carbonate with Lithium on a Cu(111) Model Electrode** — ●MARAL BOZORGCHENANI<sup>1,2</sup>, FLORIAN BUCHNER<sup>1,2</sup>, JOHANNES SCHNAIDT<sup>1,2</sup>, HANIEH FARKHONDEH<sup>1,2</sup>, BENEDIKT UHL<sup>1,2</sup>, and R. JÜRGEN BEHM<sup>1,2</sup> — <sup>1</sup>Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — <sup>2</sup>Helmholtz Institute Ulm, 89081 Ulm, Germany

Li-ion battery electrolyte is composed of lithium (Li) salts and a mixture of solvents. Ethylene carbonate (EC) is the key solvent in Li-ion battery; however, EC is solid at room temperature (RT) and has to be solved in other solvents such as propylene carbonate (PC). In order to understand the role of these solvents in the formation of solid-electrolyte interphase (SEI), which determines the function of a battery, it is important to understand how the molecules interact with the electrode and with Li. In the present work, the adsorption behavior and reaction of EC and PC on a Cu(111) model electrode was investigated by scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and Fourier transformation infrared spectroscopy (FTIR) under ultrahigh vacuum (UHV) condition between 80 - 300 K. EC as well as PC desorb and decompose well below RT. The possible decomposition products as potential species of the SEI will be discussed. Additionally, co-adsorption of Li and EC / PC was investigated at 80 K. Li induced changes compared to EC and PC on bare Cu(111) are discussed.

O 41.8 Tue 18:15 Poster B

**Femtosecond time-resolved two-photon photoemission spectroscopy of C<sub>6</sub>H<sub>5</sub>X/D<sub>2</sub>O/Cu(111)** — ●ISHITA AGARWAL, ISABELLA AVIGO, SAMAD ABDUL SAYED, MANUAL LIGGES, VESNA MIKŠIĆ TRONTL, PING ZHOU, and UWE BOVENSIEPEN — University of Duisburg-Essen, Duisburg, Germany

The electron dynamics at a metal-molecule interface is studied with time-resolved two-photon photoemission. We report here energies, workfunction changes and lifetimes of excited electronic states in amorphous D<sub>2</sub>O/Cu(111) and coadsorbed C<sub>6</sub>H<sub>5</sub>F systems after optical excitation with 3.8 eV + 1.9 eV femtosecond laser pulses. We observe a decrease in lifetime of the solvated electron state from 90 ± 5 fs for bare D<sub>2</sub>O to 60 ± 5 fs for coadsorbed C<sub>6</sub>H<sub>5</sub>F. Further, after a total estimated exposure to 0.5 × 10<sup>6</sup> photons per C<sub>6</sub>H<sub>5</sub>F molecule, a workfunction change of 200 ± 50 meV was observed. Due to the absence of photo-induced workfunction changes in the single stack D<sub>2</sub>O/Cu(111) and C<sub>6</sub>H<sub>5</sub>F/Cu(111), this change is concluded to be mediated by solvated electrons. Additional experiments on C<sub>6</sub>H<sub>5</sub>Cl/D<sub>2</sub>O/Cu(111) were performed and an even larger photoinduced workfunction change was observed. The increase in workfunction is explained by the formation of F<sup>-</sup>/Cl<sup>-</sup> as a photo-chemical dissociation product [1,2]. We conclude to have identified the charge transfer to C<sub>6</sub>H<sub>5</sub>F/Cl and a fingerprint of its photoinduced dissociation. Future experiments aim to systematically change the UV photon energy and the molecule acceptor level.

[1] S. Ryu, et al., *J. Am. Chem. Soc.*, **128**, 3500 (2006)

[2] M. Bertin, et al., *Faraday Discuss.*, **141**, 293, (2009)

O 41.9 Tue 18:15 Poster B

**Inelastic Excitations in Rare-Earth-Based Metal-Organic Complexes** — ●DANIELA ROLF<sup>1</sup>, PAUL STOLL<sup>1</sup>, TOBIAS R. UMBACH<sup>1</sup>, JANINA N. LADENTHIN<sup>1</sup>, MATTHIAS BERNIEN<sup>1</sup>, CONSTANTIN CZEKELIUS<sup>1,2</sup>, WOLFGANG KUCH<sup>1</sup>, and KATHARINA J. FRANKE<sup>1</sup> — <sup>1</sup>Freie Universität Berlin — <sup>2</sup>Heinrich-Heine-Universität Düsseldorf

Rare-earth atoms with a partially filled f shell exhibit interesting

magnetic properties due to their large magnetic anisotropy. Embedded in a molecular environment, they are prime examples of single-molecule magnets. The Dy-(aquo)-tris(1,1,1-trifluoro-4-(2-thienyl)-2,4-butanedionate) (Dy-t-TTB) molecule is a 3-dimensional complex, in which the Dy center is coordinated by three organic ligands. Within this complex, Dy has the oxidation state +3, leading to a total angular momentum of  $J = 15/2$ . Due to magnetic anisotropy, the degeneracy of the different  $M_J$  levels of the ground state is partially lifted, allowing for transitions between the sublevels. Employing low-temperature STM we show that Dy-t-TTB on a Au(111) surface forms densely packed self-assembled islands. Tunneling spectra show an inelastic step at ±7.7 meV. To identify the origin of this feature, we compare to spectra taken on Gd-t-TTB, showing inelastic steps at the same energy. Gd<sup>3+</sup> has a half-filled f shell and is not expected to show any magnetic anisotropy. Hence, we conclude that the inelastic step is not due to transitions between the anisotropy-split spin states, but can be explained by the excitation of vibrations. Furthermore, we observe the tip-induced rotation of the upper ligand of Dy-t-TTB and Gd-t-TTB.

O 41.10 Tue 18:15 Poster B

**First steps on the way to a superconductive organic layer** — ●FALKO SOJKA, TOBIAS HUEMPFNER, CHRISTIAN ZWICK, ROMAN FORKER, and TORSTEN FRITZ — Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

Since solid coronene was recently discovered to exhibit superconductive properties by intercalation with potassium, we investigated the potassium doping of ultrathin coronene layers in the (sub-) monolayer regime on Ag(111). The doping process was controlled using in situ differential reflectance spectroscopy (DRS) during the preparation. We show that before the formation of monoanions starts, a primary phase seems to appear which shows a stronger hybridization than the undoped molecules. Higher potassium concentration leads to the occurrence of dianions. Trianions or higher doped species were never observed. After stopping the potassium deposition the dianions decay into monoanions and into molecules in the primary phase. All species up to monoanions are stable and could be further investigated electronically via scanning tunneling microscopy / spectroscopy (STM, STS). While the potassium atoms are not resolved in the STM images, the doping process is evidenced by characteristic features in the related STS data we want to show. We also observed a new well-ordered structure of undoped coronene on Ag(111) for a coverage below 1ML determined by low energy electron diffraction (LEED) and STM.

O 41.11 Tue 18:15 Poster B

**Investigation of the growth of terephthalic and benzoic acids on Au(111) and oxidized Aluminum** — ●MARCEL MARSCHEWSKI<sup>1</sup>, HARUN TAS<sup>2</sup>, OLIVER HÖFFT<sup>3</sup>, WOLFGANG MAUS-FRIEDRICHS<sup>1</sup>, and ANDREAS SCHMIDT<sup>2</sup> — <sup>1</sup>Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Institut für Organische Chemie, Technische Universität Clausthal, Leibnizstr. 6, 38678 Clausthal-Zellerfeld, Germany — <sup>3</sup>Institut für Elektrochemie, Technische Universität Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany

The adsorption behavior of benzoic acids on metal interfaces is of high interest for metal-substrate interactions for catalysis and the construction of metal-organic frameworks. Here we present our results on the growth of thin films of 4-R-benzoic acid (R stands for hydroxyl-, methoxy-, propoxy-, pentoxy- and decyloxy-chains) and terephthalic acid (TPA) on Au(111) and oxidized aluminum. The adsorption was studied with metastable induced electron spectroscopy (MIES) and ultraviolet photoelectron spectroscopy (UPS(HeI)). For the monolayer on Au(111) we find hints for a flat orientation of the molecules. For the growth on an oxidized aluminum foil we suppose a more upstanding arrangement. The TPA molecules show a similar growth behavior for both surfaces.

O 41.12 Tue 18:15 Poster B

**A light-microscope for samples under ultra-high vacuum conditions** — ●CHRISTIAN MARQUARDT, NILS ROHBOHM, ALEXANDER PAULHEIM, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn, Deutschland

Talking about microscopy in the field of surface science, most people would think about scanning probe microscopy (SPM) or low energy electron microscopy (LEEM). However, there is less than a handful of publications dealing with conventional light microscopy and samples

under UHV-conditions. Such a microscope can be a direct tool to image surfaces prepared inside the UHV. Besides, it may be adapted to observe fluorescence from molecules adsorbed on these.

We modified a Nikon incident light microscope and combined it with our UHV-chamber. Due to the requirements of UHV, which are vacuum and bake-out stability, we place all optical components outside the vacuum and observe our sample through a window at the end of a glass tube. Using this technique, we are able to image our sample at a pressure of  $1 \cdot 10^{-10}$  mbar and temperatures down to 6 K directly after preparation.

First images of our Ag(100) crystal show a macroscopic corrugation of the surface with a typical structure size of 10-50  $\mu\text{m}$  that is not expected from STM or LEED data. Supported by DFG.

O 41.13 Tue 18:15 Poster B

**Structural and electronic properties of metal-organic networks on Pb(111)** — ●GELAVIZH AHMADI and KATHARINA J. FRANKE — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany.

Metal-organic networks provide an interesting playground with flexible building blocks to explore different bonding structures, confinement of electronic states and magnetic properties. The latter are particularly interesting on superconducting substrates, where the competition of superconducting pairing and magnetic interactions can be detected with high energy resolution. Here we employ low-temperature scanning tunneling microscopy and spectroscopy to characterize the structure and electronic properties of metal-organic networks of the organic acceptor tetracyanonaphtho-quinodimethane (TNAP) and metal atoms (Na, Pb). Adsorption of TNAP at 170 K leads to the formation of highly ordered hydrogen bonded islands. Annealing to room temperature results in a distinctly different arrangement, where four cyano-groups point towards each other. This bonding motif can only be explained by incorporation of Pb atoms into this windmill-like structure. Co-deposition of Na from NaCl leads to a rectangular structure, where the Na atoms are surrounded by four cyano-groups. This suggests the formation of an ionic bond by charge transfer of the 3s electron from Na to TNAP. However, we detect no sign of magnetic interaction with the underlying superconductor.

O 41.14 Tue 18:15 Poster B

**Reactive Coupling and Self-Assembly of Tetraphenylporphyrins on Cu(111)** — ●MALTE ZUGERMEIER, MIN CHEN, MARTIN SCHMID, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany

Monolayer films of metalloporphyrins on metal substrates combine the chemical versatility of the tetrapyrrole macrocycle with a well ordered, quasi-crystalline arrangement of the molecules. The structural features and robustness of porphyrin layers may be further modified by the formation of strong chemical bonds between the individual molecules, for example by means of Ullmann coupling reactions. To understand the processes which are involved in the molecular arrangement before the formation of covalent porphyrin networks, we prepared (sub-)monolayers of nickel(II)-tetraphenylporphyrin (NiTPP) and its brominated counterpart nickel(II)-tetrakis-(4-bromophenyl)porphyrin (NiTBrPP) on Cu(111); the resulting layers were examined with XPS and STM. While the structure of NiTPP molecules on the Cu(111) surface is exclusively determined by van der Waals forces, the situation is more complex for NiTBrPP. There, the interaction with the Cu(111) surface results in the selective cleavage of all C-Br bonds already at room temperature, and accordingly, the coexistence of chemisorbed Br atoms and surface-stabilized radicalic moieties. The influence of the co-adsorbed Br atoms on the morphology and chemical state of the layers before and after Ullmann coupling will be discussed in comparison to the reference system NiTPP/Cu(111).

O 41.15 Tue 18:15 Poster B

**Dynamic control of STM-induced luminescence by a single molecule** — CHRISTOPH GROSSE<sup>1</sup>, ALEXANDER KABAKCHIEV<sup>1</sup>, THERESA LUTZ<sup>1</sup>, ROMAIN FROIDEVAUX<sup>1,4</sup>, FRANK SCHRAMM<sup>2</sup>, MARIO RUBEN<sup>2,3</sup>, MARKUS ETZKORN<sup>1</sup>, UTA SCHLICKUM<sup>1</sup>, ●KLAUS KUHNKE<sup>1</sup>, and KLAUS KERN<sup>1,4</sup> — <sup>1</sup>Max Planck Institut für Festkörperforschung, Stuttgart, Germany — <sup>2</sup>Karlsruhe Institut für Technologie, Eggenstein-Leopoldshafen, Germany — <sup>3</sup>Université de Strasbourg, Strasbourg, France — <sup>4</sup>Ecole Polytechnique Fédérale de Lausanne, Switzerland

The electronic states of a molecule in a double tunnel junction can con-

trol the plasmonic light emission. We locate a single Ir(ppy)<sub>3</sub> molecule adsorbed on a fullerene bilayer within the tunnel junction between metallic substrate and metallic tip of a low temperature (4K) ultra high vacuum scanning tunneling microscope. Using the ability to precisely control charging and discharging of the molecule, we demonstrate the gating of plasmonic luminescence. Two mechanisms contribute to the gating: A local one is due to the bias-controlled onset of tunnel current passing through the molecular electronic state. A second, non-local one, is due to the extended band bending in the fullerene layer in proximity to the charged molecule. We measure the delay between bias voltage pulses and light pulses and find a charge transfer time below one nanosecond. The double tunnel junction can be operated as a fast plasmon-emitting field-effect transistor with the molecule fulfilling the transistor function. The luminescence on/off ratio is of several orders of magnitude for a bias amplitude of only a few mV.

O 41.16 Tue 18:15 Poster B

**The adsorption geometry and electronic structure of TCNQ and TCNQ + Mn on Ag(001) and Cu(001) surfaces** — ●MARTIN GRAUS<sup>1</sup>, VITALIY FEYER<sup>2</sup>, PASCAL NIGGE<sup>1</sup>, GIOVANNI ZAMBORLINI<sup>2</sup>, ROBERT G. ACRES<sup>3</sup>, ACHIM SCHÖLL<sup>1</sup>, FRIEDRICH REINERT<sup>1</sup>, and CLAUD M. SCHNEIDER<sup>2,4</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VII — <sup>2</sup>Research Center Jülich, 52425 Jülich, Germany — <sup>3</sup>Sincrotrone Trieste, 34012 Basovizza, Trieste, Italy — <sup>4</sup>Universität Duisburg-Essen, 47048 Duisburg, Germany

Molecular beam deposited epitaxial monolayers of TCNQ on Cu(001) and Ag(001) were examined by LEED and photoelectron momentum mapping with respect to adsorption geometry and electronic structure. For Ag(001), two commensurate superstructures depending on the organic coverage were found, whereas the superstructure formed on Cu(001) is incommensurate. Subsequent deposition of Mn on top of TCNQ/Ag(001) creates a commensurate metal-organic array with long-range order. Comparing angle resolved photoemission data of the TCNQ LUMO with DFT calculations allows identifying the azimuthal orientation of the TCNQ molecules in the particular unit cells. We furthermore observe a charge transfer from the substrate resulting in filling of the TCNQ LUMO for all investigated interfaces. In case of Mn coadsorption the TCNQ HOMO and LUMO shift by 230 meV towards higher binding energy compared with TCNQ/Ag(001). A detailed analysis of the angle-resolved photoemission data showed no significant lateral band dispersion.

O 41.17 Tue 18:15 Poster B

**Ab initio thermodynamical study of thiolate adsorption on Au(111) using the vdW-DF-CX functional** — ●JOAKIM LÖFGREN, HENRIK GRÖNBECK, KASPER MOTH-POULSEN, and PAUL ERHART — Chalmers University Of Technology, Gothenburg, Sweden

Adsorption of alkylthiolates on Au(111) and the formation of self-assembled monolayers (SAMs) has been extensively studied for several decades and is important for many applications in e.g., sensing and nanofabrication. In the years, understanding of the interface and adsorption geometry has been elucidated by the combined efforts of experiment and density functional theory (DFT) calculations. One of the key challenges for DFT calculations of SAMs is the description of van-der-Waals type interactions, which are not captured in conventional exchange-correlation (XC) functionals. As a result, DFT studies have struggled to describe alkylthiolate SAMs with longer hydrocarbon chains. Here, we present DFT calculations based on the recently developed vdW-DF-CX functional, which properly accounts for dispersive interactions while providing an excellent description of both the late transition metals and covalently-bonded systems. We investigate several adsorption geometries suggested in the literature and show that the CX functional gives results that are consistent with experimental findings for short alkyl chains while, in contrast to e.g., generalized-gradient XC functionals, also yields excellent results for chain-chain and chain-substrate interactions for longer alkyl chains. We further examine the relative stability of striped and standing-up phases at different coverages as a function of the chemical environment.

O 41.18 Tue 18:15 Poster B

**ARPES study of the electronic structure and light-induced spin-state switching in Fe(II) spin-crossover films on Au(111)** — ●SEBASTIAN ROHLF<sup>1</sup>, ERIC LUDWIG<sup>1</sup>, HOLGER NAGGERT<sup>2</sup>, MATTHIAS KALLÄNE<sup>1</sup>, ERIK KRÖGER<sup>1</sup>, ALEXANDER BANNWARTH<sup>2</sup>, ARNDT QUER<sup>1</sup>, KAI ROSSNAGEL<sup>1</sup>, LUTZ KIPP<sup>1</sup>, and FELIX TUCZEK<sup>2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — <sup>2</sup>Institut für Anorganische Chemie, Universität

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Coordinative Fe(II) complexes are model systems for organic molecules whose optical, electronic, and magnetic properties can be manipulated by external stimuli. Moreover, the temperature- and irradiation-dependent spin transitions observed in a number of these materials may provide a suitable testbed toward the development of future spintronic devices. Here, we present an angle-resolved photoelectron spectroscopy (ARPES) study of thin films of the spin-crossover complex Fe(H<sub>2</sub>bpz)<sub>2</sub>(phen) adsorbed on Au(111) [1]. The photoemission results provide detailed insight into the connection between spin transitions and the valence electronic structure at different temperatures and varying irradiation conditions. In particular, evidence is found for a VUV-induced spin-state trapping effect at low temperatures. Furthermore, the results show that a high optical photon flux can stabilize the metastable high-spin state far above the LIESST transition temperature, allowing us to determine the relaxation rates after photoexcitation as a function of temperature.

[1] E. Ludwig *et al.*, *Angew. Chem. Int. Ed.* **53**, 3019 (2014).

O 41.19 Tue 18:15 Poster B

**Development of a Soft-Landing for Electrospray Deposition** — ●MICA ELSEBACH<sup>1</sup>, MACIEJ BAZARNIK<sup>1</sup>, BERNHARD BUGENHAGEN<sup>2</sup>, ANNIKA FRANK<sup>2</sup>, MARC H. PROSENC<sup>2</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, University of Hamburg, D-20355 Hamburg, Germany — <sup>2</sup>Institute of Inorganic Chemistry, University of Hamburg, D-20146 University of Hamburg, Germany

"Electrospray Deposition (ESD)" is a technique to prepare clean samples of large molecules on metal substrates. Some of the molecules are fragmented when they land on the substrate. The "Soft-Landing-ratio" gives the proportion of the intact landed molecules in comparison to the total number of deposited molecules.

In order to improve this ratio we used an electric field to slow down the molecules right before they hit the substrate. When the ionized molecules arrive at the sample they lose their charge. This induces a current flow from the sample to a readout. An electric circuit was implemented to provide a simultaneous measurement of this current and to apply a bias voltage onto the sample producing the electric deceleration field. The effect of this field is tested by depositing triphenylamine molecules on a Au(111)-surface. By the use of STM the SL-ratio was determined in dependence of the electric field strength.

It has been found that the SL-ratio can be improved by the deceleration field. Up to a threshold value of 7.5 eV per charge, for the energy of the molecules, it increases. Additionally, a simulation gives an insight into the electric field's shape.

O 41.20 Tue 18:15 Poster B

**STM Imaging of Sequence Controlled Polymers** — ●IVAN PENTEGOV<sup>1</sup>, BOGDANA BORCA<sup>1</sup>, VERENA SCHENDEL<sup>1</sup>, SABINE ABB<sup>1</sup>, PETER WAHL<sup>1,4</sup>, UTA SCHLICKUM<sup>1</sup>, STEPHAN RAUSCHENBACH<sup>1</sup>, TAM TRINH<sup>3</sup>, JEAN-FRANCOIS LUTZ<sup>3</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne — <sup>3</sup>Institut Charles Sadron, F-67034 Strasbourg — <sup>4</sup>School of Physics & Astronomy, University of St. Andrews, Fife KY16 9SS, St. Andrews

Sequence controlled polymers (SCP) have recently attracted great interest because of their possible application as information storage platform. The SCP can encode a secondary molecular structure which could be used to define the properties of the molecule. A long oligomer sequence consisting of just two single monomers, which could be associated with a «0» and «1» bit is one possible way to realize SCP. The read-out of such a memory device presents a challenge on the atomic scale. Scanning Tunneling Microscopy (STM) is a promising nondestructive approach providing the necessary spatial resolution. We deposited several oligotriamines (OTA), each containing 3 monomers on a Cu(100) surface with electrospray Ion Beam Deposition (ES-IBD) technique under ultra-high vacuum conditions and transferred it in a vacuum suitcase to a low temperature STM, to probe the sequence of monomers in OTA and study its impact on properties of the whole oligomer chain as conductivity and structure. We were able to distinguish between the «1» and «0» monomer and observed that each OTA adsorbs in 2 different conformations on the surface.

O 41.21 Tue 18:15 Poster B

**Modelling X-ray Photoemission Spectra using Density Functional Theory** — ●THOMAS CHRISTOPH TAUCHER<sup>1</sup>, DAVID ALEXANDER EGGER<sup>1,2</sup>, MICHAEL ZHARNIKOV<sup>3</sup>, and EGBERT ZOJER<sup>1</sup> —

<sup>1</sup>Institute of Solid State Physics, Graz University of Technology, NAWI Graz, Austria. — <sup>2</sup>Department of Materials and Interfaces, Weizmann Institute of Science, Israel. — <sup>3</sup>Applied Physical Chemistry, Heidelberg University, Germany.

In this contribution, we investigate the applicability of slab-type density functional theory-based band structure calculations to quantitatively model X-ray photoemission (XPS) core-level shifts at metal-organic interfaces. Applying the GADGET [1] tool in conjunction with the Vienna Ab Initio Simulation Package (VASP) [2], we compare the performance of the initial state approach (neglecting screening effects) and the final state approach (with screening). Furthermore, the contribution of chemically induced shifts versus electrostatic effects to the overall position of a photoemission line is investigated. The simulations are done mainly for partially fluorinated alkylthiolates on a Au(111) surface for which high-resolution XPS experiments [3] reveal five distinct features in the energy range of the C 1s core levels. Overall, very good agreement with the available experimental data is obtained supporting the original assignment of the observed peaks.

[1] T. Bučko, J. Hafner, and J. Ángyán, *J. Chem. Phys.*, 2005, 122, 124508/1-10. [2] G. Kresse and J. Hafner. *Phys. Rev. B*, 1993, 47:558. [3] Hao Lu *et al.*, *J. Phys. Chem. C*, 2013, 117, 18967-18979.

O 41.22 Tue 18:15 Poster B

**Crystallization of Tris-HCl on gold and mica surfaces** — ●SEYMA NAYIR, MERVE ALTAY, TOPRAK AYAZ, ILKER OZTOPRAK, and OGUZHAN GURLU — Istanbul Technical University, Istanbul, Turkey

Tris molecule crystallizes in the orthorhombic system with a layered structure. Previously we have shown that precipitates from Tris-EDTA-HCl buffer solution crystallize on Au surfaces by forming hexagonal structures. We had shown that Tris-HCl, a component of Tris-EDTA-HCl buffer solution, was the main reason of such crystallites. In this study we investigated the crystallization behavior of Tris-HCl on mica, Au/mica and Au/Cr/mica surfaces from different solutions with various molarities. The samples were prepared by drop-casting of the solution on to surfaces and they were investigated by optical and probe microscopy techniques. Our data indicated that surface roughness directly affects the crystallization behavior of Tris-HCl from the drying droplet, and formation of hexagonal structures depends on the roughness and hydrophobicity of the surfaces. We have observed that the crystallization starts mostly on the rough edges/surfaces and the completed crystallites cover the underlying surface roughness totally. On the other hand we rarely observed hexagonal crystals on initially flat and smooth gold surfaces while they formed on freshly cleaved mica surfaces. We speculate that formations of such structures are strongly related to the electrostatic landscape of substrates used which we investigated by means of Kelvin Probe Microscopy.

O 41.23 Tue 18:15 Poster B

**Optical, electronic, and structural properties of lead phthalocyanine on graphene** — ●MATTHIAS MEISSNER<sup>1</sup>, NORIKAWAKITA<sup>2</sup>, CHRISTIAN ZWICK<sup>1</sup>, ANDREAS MASEK<sup>1</sup>, TAKASHI YAMADA<sup>2</sup>, HIROYUKI S. KATO<sup>2</sup>, ROMAN FORKER<sup>1</sup>, TOSHIKI MUNAKATA<sup>2</sup>, and TORSTEN FRITZ<sup>1</sup> — <sup>1</sup>Friedrich Schiller University, Institute of Solid State Physics, Jena 07743, Germany — <sup>2</sup>Department of Chemistry, Graduate School of Science, Osaka University, Osaka 560-0043, Japan

Lead phthalocyanine (PbPc) thin films on graphite have shown remarkable electronic behavior in ultraviolet photoelectron spectroscopy (UPS) and two photon photoemission (2PPE) measurements [Phys. Rev. B 77, 115404 (2008), Phys. Rev. B 75, 121305 (2007)]. Interestingly, PbPc exhibits a strong electronic intermolecular interaction resulting in a split of the highest occupied molecular orbital (HOMO) in layers of more than one monolayer. We present a detailed analysis of the thickness-dependent optical absorption of PbPc on graphene using differential reflectance spectroscopy (DRS). Additionally, the evolution of the film structures for various film thicknesses was determined by low energy electron diffraction (LEED) and low temperature scanning tunneling microscopy (LT-STM), refining the structural models for a range of substrate temperatures and coverages. Our findings are discussed in relation to the well-established electronic structure of this system. By means of scanning tunneling spectroscopy (STS) we found indications for a splitting of the lowest unoccupied molecular orbital for PbPc monolayer domains similar to 2PPE results.

O 41.24 Tue 18:15 Poster B

**Unveiling the Structure Evolution of CO Adsorption on**

**Ru(0001) and O/Ru(0001) by High-Resolution STM** — ●QIWEI CHEN and KAI WU — BNLMS, College of Chemistry and Molecular Engineering, Peking University, Beijing, China

CO adsorption on metal/metal oxide is one of the most basic and extensively focused questions in the study of gas-solid interaction. It serves as fundamental background for many related heterogeneously catalytic and electrochemical processes. Here, we present a scanning tunneling microscope (STM) study of CO adsorption on both bare and oxygen pre-adsorbed Ru(0001) surface. With the aid of CO modified tip, the structure evolution of CO adsorption on bare surface is unambiguously resolved from individual molecule to  $\langle\sqrt{3}\times\sqrt{3}\rangle$ -R30o structure and finally to the  $\langle 2\sqrt{3}\times 2\sqrt{3}\rangle$ -R30o superstructure. On oxygen pre-adsorbed surface, CO adsorption is induced to form  $\langle 2\times 2\rangle$  structure by the preformed structure of oxygen. It is also suppressed by oxygen adsorption that leads to a much lower saturation coverage at room temperature. Our real time investigation unveils scheme of CO adsorption on Ru(0001) and O/Ru(0001) at various coverage in ultrahigh vacuum condition.

O 41.25 Tue 18:15 Poster B

**Investigation of molecular hydrogen in a tunneling junction using STS** — ●SIMON RÖGER, MATTHIAS STOCKER, and BERNDT KOSLOWSKI — Universität Ulm, Ulm, Germany

Functionalization of probes is widely used in Scanning Probe Microscopy to enhance the spatial resolution of the instrument. This is especially important when determining the intramolecular structure of adsorbed molecules. In Scanning Tunneling Microscopy, molecular hydrogen physisorbed at the sample surface can be exploited to enhance the lateral contrast greatly. However, the physical origin of that phenomenon is not really understood, yet. We use Scanning Tunneling Spectroscopy to elucidate the specific influence of hydrogen on tunneling electrons. We speculate that the hydrogen modifies the electromagnetic environment of tunneling electrons by its dynamic properties.

O 41.26 Tue 18:15 Poster B

**Synthesis and characterization of bulk heterojunction solar cells based on nanoporous templates** — ●SVEN HILKE<sup>1</sup>, STEFAN OSTENDORP<sup>1</sup>, CHRISTIAN STRASSERT<sup>2</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institut für Materialphysik, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — <sup>2</sup>Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

The well-known system ZnPc:C60 (Zn-Phthalocyanine:Fullerene) as a model system of bulk-heterojunction solar cells has been chosen to analyze the effect of a nanoporous pre-structuring on the applicability of the resulting hetero molecular mixture. In this context, the basis of the pre-structuring are Anodic Aluminum Oxide (AAO) membranes made of aluminum oxide constructed by electrochemical processes. The thermal deposition of the ZnPc and C60 is done in an HV-environment so that clean layers are generated and precipitate in the membrane. Obviously, the pre-structuring directly influences the morphology on the nanometer scale. The presented work consists of the controlled growth of the nanoporous templates to obtain regular pore structures with equal and uniformly distributed surface area in the hetero intersection. In addition, every single nanopore is individually functional so that the failure of a single nanopore does not cause the destruction of the whole solar cell because each pore is able to operate by itself. Optical and electrical characterizations are used to analyze the obtained structures.

O 41.27 Tue 18:15 Poster B

**Diindenoperylene film formation on Cu(111)** — ●HAZEM AL-DAHHAK, WOLF GERO SCHMIDT, and EVA RAULS — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

The formation of diindenoperylene (DIP) thin films on metal substrates has been intensively investigated in the context of the miniaturization of organic optoelectronic devices, due to the high charge carrier mobilities, good film forming properties and thermal stability of the molecules [1, 2]. Thereby an interesting, terrace \*width dependent adsorption characteristics has been observed on Cu(111): On narrow terraces (<15nm), the DIP molecules assemble in a co-directionally oriented adsorption pattern, the symmetry of which is not dictated by the hexagonal substrate symmetry [3]. On wider terraces, in contrast, completely different adsorption patterns with a short-range order determined by the underlying substrate are observed. We performed first principles calculations and investigated the balance between intermolecular and molecule-substrate interactions of DIP molecules on pla-

nar surfaces and near step-edges. A detailed analysis of the potential-energy surface is presented. Our calculations show a strong influence of the substrate on the geometric and the electronic properties of single molecules and indicate an important role of the step-edges for molecular self-assembly and film growth.

[1] Zhang et al., *Surface Science*, 603(2009) 3179. [2] De Oteyza et al., *Journal of Physical Chemistry C* 112, 18 (2008) 7168. [3] De Oteyza et al., *Phys. Chem. Chem. Phys.* 11, 8741 (2009).

O 41.28 Tue 18:15 Poster B

**STM Study of the structural formation of cobalt naphthalocyanine on Au(111)** — ●LOTHAR BROSDA and CARSTEN WESTPHAL — Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund

The class of phthalocyanine (Pc) and its derivatives such as naphthalocyanine (Nc) has received considerable attention within the recent years. Especially the tunability of their electrical and optical properties via a central metal atom provides promising results for their integration in organic devices like light-emitting diodes, thin film transistors, solar cells, or single molecule electronic devices. The performance of such a device is particularly dependent on the quality of the self-assembled monolayer (SAM) and the metal-organic interface. Therefore, a detailed knowledge about the adsorption and the structural formation of the molecules on different substrates is required. Here, the CoNc SAMs were prepared via evaporation under ultra high vacuum (UHV) conditions and investigated by means of room temperature scanning tunneling microscopy (RT-STM). On this poster our results of the structural formation of CoNc will be discussed.

O 41.29 Tue 18:15 Poster B

**Self-assembled monolayers of shape-persistent macrocycles on graphite: interior design and conformational polymorphism** — JOSCHA VOLLMEYER, FRIEDERIKE EBERHAGEN, SIGURD HÖGER, and ●STEFAN-SVEN JESTER — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Three shape-persistent naphthylene-phenylene-acetylene macrocycles of identical backbone structures and extraannular substitution patterns but different (empty, apolar, polar) nanopore fillings are self-assembled at the solid/liquid interface of graphite (HOPG) and 1,2,4-trichlorobenzene. Submolecularly resolved images of the resulting two-dimensional crystalline monolayer patterns are obtained by scanning tunneling microscopy. A concentration-dependent conformational polymorphism is found, and open and more dense packing motifs are observed. For all three compounds alike lattice parameters are found, therefore the intermolecular macrocycle distances are mainly determined by their size and symmetry. This is an excellent example that the graphite acts as a template for the macrocycle organization independent from their specific interior. [1] J. Vollmeyer, F. Eberhagen, S. Höger, S.-S. Jester *Beilstein J. Org. Chem.* **2014**, *10*, 2774.

O 41.30 Tue 18:15 Poster B

**Quantum interference in tunneling through a molecular Kondo system** — ISABEL FERNANDEZ-TORRENTE<sup>1</sup>, ●MICHAEL RUBY<sup>1</sup>, TOBIAS R. UMBACH<sup>1</sup>, BENJAMIN W. HEINRICH<sup>1</sup>, JOSE I. PASCUAL<sup>2</sup>, and KATHARINA J. FRANKE<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>CIC nanoGUNE and Ikerbasque, Basque Foundation for Science, Tolosa Hiribidea 78, Donostia-San Sebastian 20018, Spain

The Kondo effect results from a virtual spin scattering process between an unpaired spin of a magnetic impurity and the surrounding spins of the conduction electrons. This leads to a sharp resonance around zero bias in Scanning Tunneling Spectroscopy (STS) spectra at the location of the unpaired spin. Its line-shape depends on the interference between different tunneling pathways in the tip-impurity-surface junction. It is described by a Lorentzian curve for the case of a preferential tunneling into the Kondo state, and shows an increasing asymmetry for higher contributions of direct tunneling paths into the surface.

A prerequisite to study the variation of the line-shape in a molecular network is to have a single electron in a delocalized orbital. An ideal model system for this is a charge transfer monolayer formed by Na atoms and TNAP (tetracyanonaphthoquinodimethane) molecules on an Au(111) surface. The electron donated by the Na atoms is localized in the singly occupied molecular orbital (SOMO) of the acceptor TNAP. We observed intramolecular changes in the shape and intensity of the resonance along the TNAP backbone, with a symmetry change at the nodal planes of the SOMO.

O 41.31 Tue 18:15 Poster B

**Photoswitching Kinetics of Azobenzene SAMs on Gold(111)** — •THOMAS MOLDT, DANIEL PRZYREMBEL, WIBKE BRONSCH, LARISSA BOIE, DANIEL BRETE, CORNELIUS GAHL, and MARTIN WEINELT — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Mixed self-assembled monolayers (SAMs) formed of azobenzene-functionalized alkanethiols and alkanethiol spacers show reversible photoisomerization [1]. Here we examined the photoisomerization kinetics of that system using near edge X-ray absorption fine structure and optical differential reflectance spectroscopy. We determined the photoisomerization cross sections as well as the thermal *cis-trans* isomerization rate and estimated the ratios of *trans* vs. *cis* components in the photostationary states. While in the dark the *cis* isomer is stable for hours under ambient atmosphere, in vacuo it switches back within minutes.

[1] Moldt et al., submitted.

O 41.32 Tue 18:15 Poster B

**Including depolarization effects in molecular dynamics simulations of self-assembled monolayers** — •IRIS HEHN<sup>1</sup>, MANUEL VIEDER<sup>1</sup>, OTELLO M. ROSCIONI<sup>2</sup>, SWEN SCHUSTER<sup>3</sup>, MICHAEL ZHARNIKOV<sup>3</sup>, CLAUDIO ZANNONI<sup>2</sup>, and EGBERT ZOJER<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — <sup>2</sup>Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Italy — <sup>3</sup>Applied Physical Chemistry, Heidelberg University, Germany

In a regular, ordered arrangement of molecules with aligned electric dipole moments depolarization effects take place and the individual molecular dipoles get reduced. This effect can be quite significant often reducing dipole moments to a small fraction of their original values. Depolarization should also be considered, when determining the non-bonding Coulomb interactions in molecular dynamics (MD) simulations, which are, however, typically based on calculating atomic charges of isolated molecules. Instead, to account for the depolarization we calculate the atomic charges for a molecule surrounded by a cluster of point charges that reproduces the electric field in the self-assembled monolayer (SAM), where the embedding charge distribution has to be determined self-consistently. In a second self-consistency cycle also the geometry of the molecules in the SAM is optimized considering the depolarized charge distribution in the MD runs. We test our approach on SAMs consisting of cyano-substituted biphenylthiol and a mid-chain ester functionalized alkanethiol, which differ both in the rigidity of the backbones and the orientation and location of the dipoles.

O 41.33 Tue 18:15 Poster B

**Structural and Electronic Properties of Thiophene-based Supramolecular Architectures on the Metal Surface** — •ZECHAO YANG<sup>1,2</sup>, KATHARINA J. FRANKE<sup>1</sup>, and JOSE I. PASCUAL<sup>1,3</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>Department für Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany — <sup>3</sup>CIC nanoGune, 20018 Donostia-San Sebastián, Spain

We investigated the structural and electronic properties of dicyanovinyl-hexathiophenes (DCV6T), a prototype molecule for organic electronics, on Au(111) by using low temperature STM and AFM. DCV6T self-assembles in organic islands and chains simultaneously, stabilized by hydrogen bonding. Interestingly, the molecule is deformed to an energetically unfavorable configuration by the intermolecular interaction upon self-assembly of chains, which can be interpreted by the \*Induced Fit Theory\*. Moreover, the intermolecular hydrogen-bonds induce an energetic downshift of the lowest unoccupied molecular orbital of molecules within assemblies compared to isolated molecules on the surface. In addition to the organic motifs, metal-organic chains with incorporation of Au atoms are also formed. Here, the coordination modifies the molecular orbital energy alignment and spatial distribution within individual molecules depending on the bonding structure. Our results demonstrate that one can manipulate the molecular structural configuration and electronic geometry by tuning its chemical environments with site-specific.

O 41.34 Tue 18:15 Poster B

**Ultrafast Exciton Dynamics in Thin Sexithiophene Films** — WIBKE BRONSCH, MALTE WANSLEBEN, KRISTOF ZIELKE, •CORNELIUS GAHL, and MARTIN WEINELT — Freie Universität, Berlin, Deutschland

Sexithiophene (6T) is one of the model systems for organic semiconductors. Therefore we are interested in the details of exciton formation and decay in thin 6T films [1]. As it is known the S1 absorption band of sexithiophene strongly depends on the mutual orientation of the molecules [2]. This allowed us to study the coverage-dependent orientation of 6T on the Au(111) surface by means of UV-vis spectroscopy. Following up these results we investigated the influence of the excitation energy on the exciton dynamics in this system by means of two-photon-photoemission spectroscopy.

[1] Varene et al., Phys. Rev. Lett. 109 (2012), 207106

[2] Egelhaaf et al., Synthetic Metals, 61 (1993), 143

O 41.35 Tue 18:15 Poster B

**Tuning Molecular Electronic "Set Screws" to Realize Deep-Blue Triplet Emitters - an STM/STS study** — •PASCAL RAPHAEL EWEN<sup>1,3</sup>, JAN SANNING<sup>1</sup>, NIKOS DOLTSINIS<sup>2</sup>, CRISTIAN ALEJANDRO STRASSERT<sup>2</sup>, and DANIEL WEGNER<sup>3</sup> — <sup>1</sup>Physikalisches Institut & CeNTech, Münster, Germany — <sup>2</sup>Institut für Theoretische Physik, Münster, Germany — <sup>3</sup>Institute for Molecules and Materials, Nijmegen, The Netherlands

State-of-the-art organic light emitting diodes (OLEDs) are still under intense investigation both in fundamental research and development as challenges, e.g. efficient deep-blue emitters, are still unsolved. Moreover, the physical and electronic behavior on the nanoscale after thermal sublimation at the molecule-substrate interface is often unknown but can drastically determine the device performance. Using low-temperature scanning tunneling microscopy (STM) and spectroscopy (STS) we study the adsorption and electronic structure of new types of Pt(II) complexes on Au(111). These molecules exhibit photoluminescent quantum yields up to 65% and are used in prototype devices. By mapping frontier orbitals of systematically varied organometallic complexes we are able to evaluate and control the impact of the ligands on the HOMO-LUMO gap which basically determines the emitted wavelength. Our findings provide a strategy to characterize and tailor organometallic molecules with targeted properties. Furthermore, we show that potential dissociation during the deposition is an important issue.

O 41.36 Tue 18:15 Poster B

**Self-assembly of thienothiophene based molecules and C<sub>60</sub> on Au(111)** — •JULIA LÄGER<sup>1</sup>, CHRISTIAN LOTZE<sup>1</sup>, NILS KRANE<sup>1</sup>, LEI ZHANG<sup>2</sup>, ALEJANDRO L. BRISEÑO<sup>2</sup>, and KATHARINA J. FRANKE<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Department of Physics, Berlin, Germany — <sup>2</sup>University of Massachusetts, Department of Polymer Science and Engineering, Amherst, USA

Thiophene-containing molecules and fullerenes can form a donor-acceptor heterojunction for use in organic solar cells. The charge transfer between the two compounds and thus the efficiency depends on the interface of the junction and the morphology of the molecules on the surface.

Submonolayer of BTTT were adsorbed on Au(111). We used a combined LT-STM and AFM to examine the resulting structure. We observed two ordered, planar phases and molecular configurations: a windmill-like arrangement with interdigitation of the dodecyl chains on areas with high coverage, and a parallel alignment with lower molecular density and closer proximity of the thiophene rings. The major contribution to the self-assembly is likely to be van der Waals interaction between the alkyl chains. Two isomers with different configurations of the sulfur atoms could be identified in STM and AFM images. Subsequently, we deposited C<sub>60</sub> on the submonolayer preparation and find islands on clean Au(111) as well as on the BTTT islands.

O 41.37 Tue 18:15 Poster B

**Spectroscopic study of self-assembled monolayers on a Co(0001) surface** — •RUNYUAN HAN, DAVID A. DUNCAN, JOHANNES BAUER, PETER FEULNER, and FRANCESCO ALLEGRETTI — Physics Department e20, TU München, Germany

Self-assembled monolayers (SAMs) are systems of high technological relevance and thiolate-bonded SAMs on gold and other coinage metal surfaces have been regarded as prototypical systems for fundamental understanding [J.C. Love et al., Chem. Rev. 105, 1103]. Currently, there is an increasing demand for application of SAMs on more reactive transition metals, such as Pt, Ni and Fe [Z. Mekhalif et al., Langmuir 19, 637; P. G. Hoertz et al., J. Am. Chem. Soc. 130, 9763], however the increased strength of the sulfur-metal interaction poses strong limitations to the stability of these systems. Here, we test benzoate-bonded SAMs as possible candidates for room temperature stable monolayer-

ers and compare the adsorption behavior of a 4-fluorobenzoic acid molecule onto the Co(0001) surface to that of 4-fluorothiophenol by employing a combination of X-ray photoelectron spectroscopy and X-ray absorption spectroscopy with synchrotron radiation. We show that the benzoate SAMs exhibit a much higher thermal stability and lead to well-defined layers. Moreover, by resonant photoemission we investigate the charge transfer dynamics from the end group and head group to the substrate. Supported by the DFG (MAP B.1.3 & B.1.4), Helmholtz-Zentrum Berlin and China Scholarship Council.

O 41.38 Tue 18:15 Poster B

**Ab-initio Calculation of Scanning Tunneling Spectra of Tin-Phthalocyanine Multilayer Structures** — ●FELIX SCHWARZ<sup>1</sup>, YONGFENG WANG<sup>2</sup>, RICHARD BERNDT<sup>3</sup>, ERICH RUNGE<sup>1</sup>, and JÖRG KRÖGER<sup>1</sup> — <sup>1</sup>Technische Universität Ilmenau, D-98693 Ilmenau — <sup>2</sup>Department of Electronics, Peking University, Beijing 100871, China — <sup>3</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

Tin-Phthalocyanine molecules on Ag(111) represent archetypical molecular switches [1]. Two conformations, which are characterized by the central Sn ion pointing towards vacuum and towards the surface have reversibly been interchanged by electron injection from a scanning tunnelling microscope (STM) tip. Using density functional theory the electronic structure of the different conformations has been determined. STM images and spectra of the differential conductance have been simulated and compared to experimental data. Contributions of inelastic electron tunnelling to the spectra due to excitation of molecular vibrations are discussed.

[1] Y. F. Wang, J. Kröger, R. Berndt, W. A. Hofer, J. Am. Chem. Soc. 131, 3639 (2009)

O 41.39 Tue 18:15 Poster B

**On-surface reactions of porphyrin molecules on Au(111)** — ●NINO HATTE, SONJA SCHUBERT, BENJAMIN W. HEINRICH, and KATHARINA J. FRANKE — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

Chemical reactions on surfaces are a key ingredient on the route towards molecular electronics. Yet, reactions on surfaces differ from gas- or liquid-phase reactions, as the surface may act catalytically or selectively, thereby changing the reaction barrier, the yield or the product. Porphyrin is the parent compound of the porphyrines and has a simple structure, consisting of a conjugated tetrapyrrole macrocycle.

Here, we present a scanning tunneling microscopy/spectroscopy (STM/STS) study of free-base porphyrin adsorbed on Au(111). Annealing the system to 620 K leads to the formation of covalently linked dimers, as was previously observed for porphyrin on Ag(111) [1]. We identify three different types of porphyrin dimers. Furthermore, we use on-surface metalation [2,3] to produce Fe-porphyrin and metalized dimers on Au(111). Using STS, we probe the electronic and magnetic properties of the free-base porphyrin, as well as the metalized porphyrin monomers and dimers.

[1] A. Wiengarten, et al., J. Am. Chem. Soc. 136, 9346 (2014)

[2] J.M. Gottfried, et al., J. Am. Chem. Soc. 128, 5644 (2006)

[3] W. Auwärter, et al., ChemPhysChem 8, 250 (2007)

O 41.40 Tue 18:15 Poster B

**Properties of self-assembled monolayers formed by triarylamine derivatives on metal and insulator substrates** — ●MARTIN GURRATH<sup>1</sup>, CHRISTIAN STEINER<sup>2</sup>, SABINE MAIER<sup>2</sup>, and BERND MEYER<sup>1</sup> — <sup>1</sup>Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg — <sup>2</sup>Department of Physics, FAU Erlangen-Nürnberg

The atomic and electronic structure of homo- and bi-molecular networks of triarylamine derivatives with either diaminotriazine (ADTPA) or carboxylic (CDTPA) end-groups, which were observed by low-temperature STM and AFM to form on Au(111) and KBr(001) substrates, were studied by density-functional theory (DFT) calculations. Both molecules exhibit three-fold rotational symmetry. While the carboxylic end-groups of CDTPA can form only one type of contact with other molecules in a flat geometry, the amine groups of ADTPA allow for three different hydrogen bonding motifs, which can be either flat or tilted. First, for all possible combinations the molecule-molecule interaction strength for the different hydrogen bonding motifs was determined by calculation of the dimerization energies. Then, monolayer arrangements were derived from the dimer structures. Preliminary calculations of molecules on a KBr(001) surface give insights into why different monolayers form on metal and insulator substrates. Finally,

charge transfers and the mutual influence on the electronic structure were analyzed.

O 41.41 Tue 18:15 Poster B

**Growth and vibrational properties of ultra-thin TiOPc films on Ag(111)** — LAURA FERNÁNDEZ, SEBASTIAN THUSSING, SEBASTIAN FLADE, and ●PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

The coverage dependent growth of titanyl-phthalocyanine (TiOPc) ultra-thin films on a Ag(111) surface has been studied using IR Spectroscopy, SPA-LEED, and TDS. In the monolayer regime three different phases were found: a 2D-gas phase in the low coverage regime ( $\theta < 0.7\text{ML}$ ), a commensurate  $(4\sqrt{3}\times 7)\text{rect}$  phase for 0.8-0.9 ML, and finally, a point-on-line phase when the coverage approaches saturation. While the IR spectra of the monolayer phases vary only slightly, the vibrational modes corresponding to the mono- and bilayers of TiOPc/Ag(111) are distinctly different, so that the transition from the ML to the BL regime is clearly defined. Thermal desorption spectroscopy measurements reveal a high thermal stability of the TiOPc bilayer, which requires temperatures above 500K to desorb from the Ag(111) surface. Similarly, the stacked (TiOPc bilayer on PTCDA)/Ag(111) structure displays exceptional stability of the organic heterolayer interface. Only for temperatures above 470K indications of intermixing or degradation of the underlying PTCDA/Ag(111) layer are observed.

O 41.42 Tue 18:15 Poster B

**Probing non-planar porphyrin molecules with nc-AFM** — FLORIAN ALBRECHT<sup>1</sup>, ●FELIX BISCHOFF<sup>2</sup>, YUANQIN HE<sup>2</sup>, WILLI AUWÄRTER<sup>2</sup>, JOHANNES BARTH<sup>2</sup>, and JASCHA REPP<sup>1</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — <sup>2</sup>Technische Universität München, Department of Physics, E20, 85748 Garching, Germany

Small amplitude, nc-AFM has been established as advanced imaging tool in scanning probe microscopy. Its capability to determine molecular bond characteristics allows a direct identification of molecular structures, conformation and changes therein caused by chemical reactions. However nc-AFM investigations of surface-confined molecules have so far mainly been applied to planar species. Herein we investigate non-planar porphyrins on metal substrates and compare free-base to metalated species. The substrate-induced saddle-shape conformation and the orientation of molecular moieties can be clearly visualized. However, in a direct comparison of 2H-TPP to CuTPP on Cu(111), a flattening of the macrocycle of Cu-TPP, as reported in literature, could not be unambiguously confirmed. On the other hand, a conformational change of the macrocycle caused by the formation of an SAT-complex can clearly be observed for 2H-TPCN on Ag(111). nc-AFM therefore provides the potential to identify (and quantify) the orientation of sub-molecular units within non-planar molecules in real space and might present a possible alternative to space averaging methods such as NEXAFS.

O 41.43 Tue 18:15 Poster B

**Forced assembly of functional molecules** — ●KNUD SEUFERT<sup>1,2</sup>, FELIX BISCHOFF<sup>1</sup>, YUANQIN HE<sup>1</sup>, AUWÄRTER WILLI<sup>1</sup>, JOHANNES V. BARTH<sup>1</sup>, and LEONHARD GRILL<sup>2</sup> — <sup>1</sup>Physik-Department, Technische Universität München, Deutschland — <sup>2</sup>Institut für Chemie, Karl-Franzens-Universität Graz, Österreich

The self-assembly of molecules is essential en route to ordered and utile organic structures - a groundwork of molecular electronics. An archetype of such a functional building block is the porphyrin as it plays a key role in several fundamental processes in nature.

Here we present a study on porphyrin molecules, the parent compound of all porphyrins, adsorbed on smooth noble metal single crystals. A partial filling of the lowest unoccupied molecular orbital (LUMO) results in a charge redistribution at the porphyrin/Ag(111) interface and a dominating repulsive intermolecular interaction [1]. This repulsion can be overcome by coadsorption or a modification of the substrate. In the first case well-ordered mixed layers can be produced where small gas molecules between the porphyrins stabilize a self-assembly process via dipole-dipole interaction [2]. A reduced interaction to the metal surface can be achieved by adding a thin insulating interlayer or a complete exchange of the support resulting in the lack of charge transfer. This leads to a suppression of the main repulsive intermolecular force and the formation of islands.

[1] Bischoff et al., ACS Nano (2013) 3139-3149

[2] Buchner et al., ACS Nano (2009) 1789-1794

O 41.44 Tue 18:15 Poster B

**Structural analysis of ordered monolayers of the ladder-type molecule DBP on Ag(100) via STM and LEED** — ●TIMO HEPPENSTRICK, YIFEI ZHANG, INA KRIEGER, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn

We investigated the perylene derivate ladder-type molecule DBP (dibenzotetraphenylperiflanthene). It consists of a stiff body and four rotatable phenyl groups on the edges. DBP has recently been used as an electron donor in organic solar cells [1]. We investigated the adsorption on the Ag(100) surface via STM and LEED at room temperature. From LEED images we found one incommensurate structure with a quadratic unit cell of 2.98 nm side length containing two molecules each. It exhibits a p4g symmetry with two symmetry equivalent rotation domains. The molecule forms large islands on the substrate, which can be observed by STM.

[1]D. Fujishima et al. *Solar Energy Mat. and Solar Cells* 93, 1029, (2009).

O 41.45 Tue 18:15 Poster B

**Ordering and Electronic Properties of Porphine on Graphene/Ag(111)** — ●JACOB DUCKE, YUANQIN HE, FELIX BISCHOFF, MANUELA GARNICA, JOHANNES BARTH, and WILLI AUWÄRTER — Physik Department E20, Technische Universität München, James Franck Straße 1, 85748 Garching, Germany

Bonding and organization of functional molecules at interfaces is strongly affected by the interaction with the support. By switching from metal surfaces to sp<sup>2</sup>-bonded monolayer templates an electrical decoupling of the molecules from their support is possible that recently attracted significant interest [1,2]. This decoupling provides new possibilities to order and structure components at the nanometer scale. Here we focus on the interactions and the electronic modification of free-base porphine (2H-P), a prototype tetrapyrrole compound, on graphene/Ag(111). In STS measurements pronounced peaks corresponding to LUMO and HOMO orbitals appear. Furthermore, the repulsions between 2H-P previously identified on Ag(111) are diminished [3]. Our findings are put into perspective with results for electronically decoupled 2H-P on BN/Cu(111) and 2H-P on bare Ag(111). All measurements were conducted with a low temperature STM. [1] Joshi, Sushobhan, et al. *Nano letters* 12.11 (2012): 5821-5828. [2] Jaervinen, Paeivi, et al. *Nano letters* 13.7 (2013): 3199-3204. [3] Joshi, Sushobhan, et al. *ACS Nano* 8 (2014) 430

O 41.46 Tue 18:15 Poster B

**Controlling Coordination Reaction and Assembly on an Insulating Boron Nitride Monolayer** — JOSÉ I. URGEL<sup>1</sup>, ●MARTIN SCHWARZ<sup>1</sup>, MANUELA GARNICA<sup>1</sup>, DAPHNÉ STASSEN<sup>2</sup>, DAVIDE BONIFAZI<sup>2</sup>, DAVID ECIJA<sup>3</sup>, JOHANNES V. BARTH<sup>1</sup>, and WILLI AUWÄRTER<sup>1</sup> — <sup>1</sup>Physik Department E20, Technische Universität München, Germany — <sup>2</sup>Department of Chemistry and Namur Research Center, Belgium — <sup>3</sup>IMDEA Nanoscience, Madrid, Spain

Two-dimensional metal-organic coordination networks presenting organized arrays of metal centers and functional molecular linkers [1] have not been achieved to date on a highly relevant class of materials, namely atomically thin sp<sup>2</sup>-bound sheets as boron nitride (BN) or graphene. Here, we report the formation of a metal-organic network on a BN/Cu(111) template [2, 3] by co-deposition of carbonitrile-functionalized porphyrin derivatives (2H-TPCN) with Co atoms in an ultra-high vacuum environment. The resulting metallosupramolecular structure explored by scanning tunneling microscopy and spectroscopy features a distinct four-fold coordination motif. Furthermore, we demonstrate an in-situ metalation of the tetrapyrrole macrocycles with co-adsorbed Co yielding Co-TPCN directly on the BN sheet. Our results provide perspectives for the formation of coordination networks on BN and related systems featuring structural, electronic and magnetic properties unachievable on conventional metallic supports.

[1] Barth, J. V. *Annu. Rev. Phys. Chem.* 2007, 58, 375-407

[2] Joshi, S. et. al. *Nano Lett.* 2012, 12, 5821-5828

[3] Joshi, S. et. al. *ACS Nano*, 2014, 8, 430-442

O 41.47 Tue 18:15 Poster B

**Light-induced ring-closure isomerization of a diarylethene derivate in direct contact with surfaces** — ●FABIAN NICKEL<sup>1</sup>, MATTHIAS BERNIEN<sup>1</sup>, SANDRO WRZALEK<sup>1</sup>, MARTIN HERDER<sup>2</sup>,

PANTELIS CHITTAS<sup>1</sup>, KAI KRAFFERT<sup>1</sup>, LUCAS M. ARRUDA<sup>1</sup>, LALMINTHANG KIPGEN<sup>1</sup>, STEFAN HECHT<sup>2</sup>, and WOLFGANG KUCH<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — <sup>2</sup>Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2, 12489 Berlin

The photochromic isomerization of molecules in direct contact with solid surfaces can be important for the further miniaturization of molecular electronic devices. A potential candidate for this purpose is T-DAE, a diarylethene derivate with attached phenyl groups. This molecule can be switched reversibly between two metastable states in solution. In the closed-ring configuration, a conjugated conduction path through the molecule exists, making it interesting for photochromic switching of the electronic interaction between two attached end groups. In-situ X-ray photoelectron spectroscopy (XPS) and near-edge X-ray absorption fine structure (NEXAFS) experiments performed on T-DAE adsorbed on Bi(111), Au(111), and highly oriented pyrolytic graphite (HOPG) revealed a UV-light-induced ring-closure reaction on Bi(111) and HOPG. Spectroscopy of the sulfur 2p core electrons shows the existence of three different species of molecules after light exposure, pointing towards the presence of a byproduct that is known to exhibit no reversible switching.

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O 41.48 Tue 18:15 Poster B

**STM investigations of functional platform adlayers on Au(111) surfaces** — ●TALINA RUSCH<sup>1</sup>, SONJA LEMKE<sup>1</sup>, SANDRA ULRICH<sup>2</sup>, HANNE JAKOB<sup>3</sup>, FELIX TUCZEK<sup>3</sup>, RAINER HERGES<sup>2</sup>, and OLAF MAGNUSSEN<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel — <sup>2</sup>Institut für Organische Chemie, Christian-Albrechts-Universität Kiel — <sup>3</sup>Institut für Anorganische Chemie, Christian-Albrechts-Universität Kiel

The controlled assembly of functional molecules on metal surfaces is an important research topic. We have introduced the so called platform approach, where the Triazatriangulenium (TATA) [1,2,3] or Trioxatriangulenium (TOTA) [4] ions are used as molecular platforms which can be functionalized at the central carbon atom as well as by alkyl side chains to control their steric demand. Using this versatile concept, it is possible to control the orientation and distance of the functional group with respect to the surface and the intermolecular distance. Here, detailed STM investigations of TATA adlayer structures as a function of alkyl side chain length are presented as well as structural investigations of new azobenzene functionalized TATA adsorbate layers, namely methoxy-azobenzene-octyl-TATA adlayers. Additionally, we present the reversible switching of these adlayers by infrared reflection absorption spectroscopy [5] as well as UV/Vis spectroscopy.

[1] Baisch et al., *J. Am. Chem. Soc.* (2009), 131, 442. [2] Kuhn et al., *PCCP* (2010), 12, 4481. [3] Kubitschke et al., *Eur. J. Org. Chem.* (2010), 5041. [4] Kuhn et al., *Chem. Commun.*, 2011, 47, 8880-8882 [5] Jacob et al., *Phys. Chem. Chem. Phys.*, 2014, 13, 22643

O 41.49 Tue 18:15 Poster B

**Hierarchical and charge transfer effects in a bimolecular network of structurally related scaffolds** — ●CHRISTIAN STEINER<sup>1</sup>, MAXIMILIAN AMMON<sup>1</sup>, BETTINA GLIEMANN<sup>2</sup>, UTE MEINHARDT<sup>2</sup>, MARTIN GURRATH<sup>3</sup>, BERND MEYER<sup>3</sup>, MILAN KIVALA<sup>2</sup>, and SABINE MAIER<sup>1</sup> — <sup>1</sup>Department of Physics, Universität Erlangen-Nürnberg, Germany — <sup>2</sup>Department of Chemistry and Pharmacy, Universität Erlangen-Nürnberg, Germany — <sup>3</sup>Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, Universität Erlangen-Nürnberg, Germany

Functional electron donor-acceptor networks on metal surfaces are integral parts of organic optoelectronic devices such as solar-cells. Understanding and controlling the formation of multi-component molecular self-assemblies is important for the design of efficient donor-acceptor networks. Here, we present a scanning tunneling microscopy and spectroscopy study of a bimolecular network assembled from triarylaminines with carboxylic and diaminotriazine functional groups on Au(111). The molecules form a perfectly intermixed honeycomb network via N ··· H-O hydrogen bonds. Density functional theory (DFT) calculations reveal that mainly geometrical aspects lead to the intermixing as opposed of an increase in binding strength. The HOMO-LUMO gap in the mixed network is defined by the two types of molecules, typical for a charge donor-acceptor scheme. The charge transfer process in the intermixed network will be discussed based on DFT calculations.