

O 27: Metal substrates: Adsorption of organic / bio molecules IV

Time: Tuesday 11:15–13:00

Location: PHY C213

O 27.1 Tue 11:15 PHY C213

Alkali-induced nanopatterning of Ag(110) surface mediated by molecular adsorbate — ●GIUSEPPE MERCURIO^{1,2}, OLIVER BAUER³, MARTIN WILLENBOCKEL^{1,2}, BENJAMIN FIEDLER³, CHRISTIAN WEISS^{1,2}, RUSLAN TEMIROV^{1,2}, SERGEY SUBACH^{1,2}, MORITZ SOKOLOWSKI³, and STEFAN TAUTZ^{1,2} — ¹Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — ²JARA-Fundamentals of Future Information Technology — ³Institute for Physical and Theoretical Chemistry, University of Bonn

It is known for decades that alkali metals initiate the restructuring of fcc metal surfaces resulting in a composite patterned morphology. On the other hand, co-adsorbed metal atoms and organic molecules often form extended 2D networks due to the metal-molecular coordination reaction. Here we report on a new type of structural modification of the molecule-substrate interface, which is not only restricted to self-assembly of the adsorbed metal atoms and molecules, but it also involves significant morphological reorganization of the metallic surface. In the experiments, potassium atoms are deposited on a monolayer of the long-range ordered PTCDA/Ag(110) phase. Subsequent annealing forces potassium atoms to intercalate under the molecular layer partially unbinding PTCDA from the substrate. The complex interaction between potassium, PTCDA and substrate induces a significant silver mass-transfer and leads to the appearance of 1D stripe-structures of K atoms and PTCDA molecules on a nanopatterned silver surface. Structural and electronic properties of this pattern were studied by means of NIXSW, XPS, LEED and LT-STM.

O 27.2 Tue 11:30 PHY C213

Adsorption of Tetrahydroxybenzene on Metal Surfaces — ●FABIAN BEBENSEE¹, CHRISTIAN BOMBIS¹, FEDERICO MASINI¹, SVETLANA KLYATSKAYA², MARIO RUBEN², ERIK LAEGSGAARD¹, FLEMMING BESENBACHER¹, and TROLLE R. LINDEROTH¹ — ¹iNANO, Aarhus University, Aarhus, Denmark — ²Karlsruhe Institute of Technology (KIT), Institut für Nanotechnologie, Karlsruhe, Germany

The synthesis of extended, well-ordered bi-dimensional molecular networks on surfaces has received a great deal of interest over the past years, fueled not least by potential applications such as functionalized surface coatings, sensors and molecular electronics. Here, we employ scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) to study the adsorption of tetrahydroxybenzene (THB) on the Au(111) and Cu(111) surfaces. The molecule shows a complex adsorption behavior despite being structurally rather simple. Depending on post-deposition treatment, coverage and substrate, we find different adsorption structures: a hexagonal close-packed phase and a porous network structure exhibiting a high degree of order. The XPS results reveal that the transformation from the hexagonal close-packed phase to the porous network is linked to a chemical modification of THB, possibly involving dehydrogenation of the molecules. We tentatively propose that the porous network, which was observed solely on the Cu(111) surface, is a metal complexation structure involving native Cu released during post-deposition annealing.

O 27.3 Tue 11:45 PHY C213

Structure of self-assembled monolayers of 1,1'-biphenyl-4-thiols on Au(111): A combined STM, LEED and XPS study — ●DAN G. MATEI, HEIKO MUZIK, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Physik supramolekularer Systeme und Oberflächen, Universität Bielefeld

Self-assembled monolayers (SAMs) of aromatic molecules are in the focus of research due to their applications in nanotechnology ranging from the fabrication of biofunctional surfaces to the generation of free-standing graphene. However, important structural issues of aromatic SAMs on metal substrates are not yet well understood. In this contribution, we report on the structure of 1,1'-biphenyl-4-thiol (BPT) SAMs on Au(111) prepared from solvents and by vapour deposition in vacuum. We analyze molecular resolved scanning tunneling microscopy (STM) images of "as prepared" and annealed samples. Upon vacuum annealing regular molecular superstructures form on Au(111). Their unit cells were investigated by low-energy electron diffraction (LEED). X-ray photoelectron spectroscopy (XPS) was employed to study the chemical composition and effective thickness. We present a comprehensive analysis of these data.

O 27.4 Tue 12:00 PHY C213

Electronic many-body effects at metal-organic interfaces studied with PES, NEXAFS and Resonant Auger Raman Spectroscopy — ●M. HÄMING¹, A. SCHÖLL¹, E. UMBACH², and F. REINERT¹ — ¹Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg, Germany — ²Karlsruhe Institut für Technologie (KIT) D-76021 Karlsruhe, Germany

Electronic many-body and correlation effects have been studied intensively at transition metal compounds with localized d/f electrons. They are related to interesting material properties, e.g. Mott metal-insulator transitions, charge transfer satellites and superconductivity. Recent investigations of graphene,¹ C₆₀,² and TTF-TCNQ³ showed that many-body effects can also be important for organic thin films. We have investigated several organic thin films (PTCDA, PTCDI, BTCDA, BTCDI, SnPc) deposited on a Ag(111) surfaces with photoelectron spectroscopy, NEXAFS and resonant Auger Raman spectroscopy. Our data provide significant indications for electronic many-body effects involving substrate-adsorbate charge transfer, which can be understood by concepts developed for charge transfer compounds. These results give insight into new, interesting aspects of physics at metal-organic interfaces.

¹ I. Gierz *et al.*, Nano Letters **8**, 4603–4607 (2008)² W. Yang *et al.*, Science **300**, 303–307 (2003)³ M. Sing *et al.*, Phys. Rev. B **68**, 125111 (2003)

O 27.5 Tue 12:15 PHY C213

Compensation of the odd-even effects in araliphatic monomolecular films by non-symmetric attachment of the aromatic part — JOHN DAUSELT¹, JIANLI ZHAO², MARTIN KIND¹, ROBERT BINDER¹, ANDREAS TERFORT¹, and ●MICHAEL ZHARNIKOV² — ¹Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany — ²Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

The integrity, chemical identity, packing density, and molecular orientation in SAMs formed by anthracene-substituted alkanethiols (Ant-n) with a variable number of methylene groups (n) in the aliphatic linker on Au(111) and Ag(111) substrates were studied by a combination of several complementary experimental techniques. The Ant-n molecules were found to form well-defined and highly ordered SAMs on these substrates, with very small inclination of the anthracene backbone. In addition, the Ant-n SAMs exhibited odd-even effects, i.e. dependence of the molecular orientation and packing density on the length of the aliphatic linker, with the parity of n being the decisive parameter. Whereas the direction (sign) of this odd-even behavior on gold and silver is the same as for SAMs of biphenyl- and terphenyl-substituted alkanethiols and alkaneselenolates, the extent of the odd-even effects in the Ant-n films is noticeably smaller than in the latter systems. This behaviour can be explained by the additional rotational degree of freedom of the anthracene unit in the case of the Ant-n SAMs due to its non-symmetrical attachment to the adjacent alkyl linker.

O 27.6 Tue 12:30 PHY C213

4,4'-dithiodipyridine on Au(111): An STM and STS study — ●NORBERT MAURER, ANNA TSCHETSCHETKIN, BERNDT KOSLOWSKI, and PAUL ZIEMANN — Institut für Festkörperphysik, Albert-Einstein-Allee 11, University of Ulm, D-89081 Ulm

Driven by the overwhelming possibilities of molecular electronics, systems of inorganic substrates covered with organic materials evolved to a widely investigated field. Promising candidates in this respect are thiols containing heterocyclic groups, e.g. the 4,4'-dithiodipyridine (PySSPy). We prepared PySSPy/Au(111) *in vacuo* at a reduced temperature and investigated the result by scanning tunneling microscopy and spectroscopy with emphasis on *z*-V spectroscopy. PySSPy forms islands on Au(111) exhibiting a $13 \times 3\sqrt{3}$ superstructure where the substrate-induced enantiomeric-excess of the molecules plays an important role. In that structure the LUMO is found to be at 3.2 eV with a slight variation depending on the position/coordination of the PySSPy. By annealing the structure at room temperature, a chain growth can be observed. The LUMO is then found at ~ 2.1 eV. We conclude that the PySSPy dissociates at RT on Au(111) and forms a thiolate.

O 27.7 Tue 12:45 PHY C213

STM-investigations on aza-BODIPYs at low temperatures —

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Scanning Tunnelling Microscopy (STM) is a powerful experimental technique in surface science. It combines atomic resolution imaging with the opportunity to perform nanoscale manipulations. Additionally, STM enable the mapping of the density of states of materials. Here we report investigations on aza-BODIPY adsorbed on metal surfaces with a low-temperature STM/AFM-System. Aza-BODIPY (e.g. 1,3,5,7-tetraphenyl-8-azadipyromethene) are a class of organic fluores-

cent dyes characterised by the same molecular core region consisting of two pyrroles connected by a boronfluorine complex and a nitrogen atom. These molecules exhibit strong chemical stability and highly tuneable, sharp absorption wavelength. Aza-BODIPY has previously been used for immunostaining and photodynamic therapy during the last few years. Recently, electron donor materials for organic photovoltaics (OPVs) has emerged as another field of application, due to aza-BODIPYs strong infrared absorption. In this work we investigated single aza-BODIPY molecules adsorbed on Ag(110) and Au(111) by STM at 77 K and 5 K. We verified the adsorption configuration and geometry and found it to be in qualitative agreement with theoretical simulations. In addition we conducted spectroscopy measurements to determine the electronic structure of the molecule on the surface.