O 45 Organische Dünnschichten IV

Zeit: Dienstag 15:45–18:30 Raum: TU EB301

O 45.1 Di 15:45 TU EB301

Molecular distortions and chemical bonding of a large π-conjugated molecule on a metal surface — •F. S. Tautz[1], A. Hauschild[2], K. Karki[1], B.C.C. Cowie[3], M. Rohlfing[1], and M. Sokolowski[2] — [1]International University Bremen, School of Engineering and Science, PO Box 750761, D-28725 Bremen — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn — [3]European Synchrotron Radiation Facility, Bote Postale 220, 38043 Grenoble Cedex, France

We report an experimental and theoretical investigation of the chemical bonding of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). Normal incidence x-ray standing wave experiments and density functional theory reveal that PTCDA chemisorbs on Ag(111) in a non-planar, vertically distorted configuration. The carboxylic O atoms are 0.018 nm closer to the surface than the perylene core. The distortion is related to weak local bonds between carboxylic O atoms and the Ag surface which are coupled - through charge transfer into the former lowest unoccupied molecular orbital - to the primary, extended chemisorption bond via the perylene skeleton.

O 45.2 Di 16:00 TU EB301

Diffusion and Chemical Reaction at the Interfaces between Metals and the PTCDA — •Gianina Gavrila[1], Mihaela Gorgoi[1], Reinhard Scholz[1], Walter Braun[2], and Dietrich R.T. Zahn[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

The electronic and chemical and properties of interfaces in organic devices are decisive for charge carrier injection and transport. Metal/organic interfaces can undergo complex and spatially extended chemical interactions. In and Mg metals were deposited onto 3,4,9,10-perylene tetracarboxylic-dianhydride (PTCDA). The interface formation is analyzed via High Resolution Soft X-ray Photoemission Spectroscopy. The experimentally observed C1s, O1s, In4d and Mg2p core level emission intensities together with the valence band evolution upon metal deposition are compared to data from previous study [1]. Additionally, the differences between the two metals are emphasized and a new model for the formation of the In/PTCDA interface is proposed. The photoemission results are correlated with the near edge X-ray absorption spectroscopy spectra taken at the C K-edge and O K-edge. [1] Y. Hirose, A. Kahn, V. Aristov, P. Soukiassian, Appl. Phys. Lett. 68 (2), 1996.

O 45.3 Di 16:15 TU EB301

Ordered (dppy)BF films grown on Ag(110): From submonolayer to multilayer — •Dingyong Zhong[1], Feng Lin[1], Lifeng Chi[1], Yue Wang[2], and Harald Fuchs[1] — [1]Institute of Physic and Center for Nanotechnology (CeNTech), Universität Münster, Wilhelm-Klemm-strabe 10, 48149 Münster, Germany — [2]Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, College of Chemistry, Jilin University, 130012 Changchun, P. R. China

Ordered molecular films of a blue light-emitting material, 1,6-bis(2-hydroxyphenyl) pyridine boron complex [(dppy)BF], grown on the Ag(110) surface by means of organic molecular beam epitaxy, were investigated by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) under an ultrahigh vacuum. Two commensurate structures exist in the monolayer film grown at 300 K, as found by STM. In the monolayer film, two types of hydrogen bonds are formed between the molecules, which, in addition to the molecule-substrate interaction, essentially determine the monolayer structures. The structural evolution of the (dppy)BF films from submonolayer to 3 monolayers was monitored by LEED in situ and in real time. The results indicate that the growth of the first two monolayers is affected by the periodic potential on the substrate surface, while such a template effect is weakened beyond the second monolayer.

O 45.4 Di 16:30 TU EB301

Structural and spectroscopic investigations of the laterally structured heterorganic system alkanethiol/PTCDA/Ag(111) — •Florian Pollinger, Stefan Schmitt, Christian Kumpf, and Eberhard Umbach — Exp. Phys. II, Univ. Würzburg, 97074 Würzburg

The planar organic molecule 3,4,9,10-perylenetetracarboxylic acid dianhydride (PTCDA) is well known to form commensurate thin films on Ag(111) surfaces. Furthermore, it has been demonstrated that PTCDA induces faceting on vicinal Ag(111) surfaces by step bunching. For an appropriate choice of coverage, self-organization leads to a grating-like morphology with a periodicity down to several nanometres. This enables the use of these surfaces as pre-patterned templates [1].

Other model systems important for designing organic nanostructures are alkanethiols like 1-Decanethiol and 1-Octadecanethiol. They grow as self-assembled monolayers (SAMs) on clean Au and Ag(111) surfaces. In the study presented here, however, we also deposited them on pre-patterned sub-monolayer PTCDA/Ag(111) substrates. These *laterally structured* heterorganic systems were investigated using standard surface characterization techniques, like TPD, XPS and LEED.

[1] X.Ma et al., Appl. Phys. Lett. 84 (2004) 4038

O 45.5 Di 16:45 TU EB301

A standing wave study of the PTCDA-precursor state on the Ag(111) surface — •A. Hauschild[1], R. Temirov[2], M. Sokolowski[1], and F. S. Tautz[2] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]International University Bremen, School of Engineering and Science, PO Box 750 561, 28725 Bremen, Germany

PTCDA deposited on Ag(111) can lead to two different adsorption states: At room temperature (RT) the commonly-known stable chemisorbed state is formed, deposition at temperatures below 160 K, however, yields a meta-stabile "precursor state". This state is also chemisorbed, but no long-range order exists. Photoemission spectroscopy also shows significant differences of the electronic structures of both states [1]. From an earlier normal incidence x-ray standing wave (NIXSW) study, we know that the "RT state" involves a significant distortion of the planar PTCDA molecule. The aim of the present experiment was to investigate the different bonding geometry of the precursor state in comparison to that of the RT state. A first data evaluation actually confirms the existence of differences. However, in contrast to the RT-state, the precursor also undergoes a reversible transition to a second state under exposure to the intensive x-rays, which complicated the experiments. Supported by the DFG. [1] L. Kilian, Doctoral thesis, Universität Würzburg 2002.

O 45.6 Di 17:00 TU EB301

High resolution ARPES study of thin organic films on metallic substrates — •Azzedine Bendounan, Johannes Ziroff, Frank Foster, Felix Schmitt, Eberhard Umbach, Achim Schöll, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We study by high energy and angular resolution photoemission (ARPES) the electronic properties of ultrathin organic films deposited on metal surfaces. Our interest is focused on large π-conjugated planar molecules like 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) and 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NTCDA). On noble metal surfaces, characterized by flat density of states close to the Fermi energy, these molecules form a highly ordered superstructure and grow in layer-by-layer mode. Ag(111), for example, is an ideal substrate since the molecule can diffuse over large distances and form ordered islands. After deposition of one monolayer of PTCDA, the Ag-Shockley surface state disappears and new spectrae features appear. One of these features is associated with the formation of a chemical bond suggesting an hybridization between the metal and the molecule which fills the lowest unoccupied molecular orbital (LUMO). The second feature is described as the highest occupied molecular orbital (HOMO) peak modified also by the bonding. Moreover, we observe an important modification in the photoelectron intensity as function of the emission angle. The observed structures are significantly narrower than in previously published investigations on similar systems.

O 45.7 Di 17:15 TU EB301

Tetracene and pentacene growth on Ag(111) — •Moritz Sokolowski[1], Andreas Langner[1], Annegret Hauschild[1], Russlan Temirov[2], Stefan Tautz[2], Maxim Eremtchenko [3], D. Bauer[3], and Jürgen-A. Schaefer[3] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]School of Engineering and Science, International University Bremen — [3]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau

The growth of the two polyacenes tetracene (Tc) and pentacene (Pc) on Ag(111) was investigated by SPA-LEED, STM, HREELS, XPS, and TPD. Although the two molecules are chemically similar, their growth behaviour on Ag(111) turns out to be significantly different. Tc forms two long-range ordered monolayer structures at temperatures below 230 K, which contain one (planar) and two (slighly tilted) Tc molecules per unit cell, respectively [1]. From the second layer onward, a pronounced cluster-growth occurs. Quite differently, the monolayer of Pc appears to be disordered, possibly due to kinetic limitations. Interestingly, the second layer exhibits a long range ordered structure, whereby the growth directions are templated by surface steps. Supported by the DFG. [1] A. Langner et al., Surf. Science (2004), in press.

O 45.8 Di 17:30 TU EB301

Growth and electronic structure of pentacene films deposited on polycrystalline gold surfaces — •V. Yanev, Ch. Weis, M. Himmerlich, S. Krischok, M. Eremtchenko, and J.A. Schaefer — Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Pentacene is a promising material for organic thin film transistors due to its high carrier mobilities. Therefore, for organic electronics, it is of great interest to gain a basic understanding of the pentacene growth on evaporated or sputtered metal films, similar to the contacts in electronic devices. We examined the structure and electronic properties of pentacene films on evaporated gold surfaces. The molecular layer structure was investigated using atomic force microscopy (AFM). An upright molecular orientation was observed. The structure of the films is compared to that of pentacene grown on Ag(111). The dependence of the grain size on the deposition conditions is discussed. The electronic structure of the molecular-metal interface was investigated using X-ray and ultraviolet photoelectron spectroscopy (XPS and UPS).

O 45.9 Di 17:45 TU EB301

Orientation of substituted phthalocyanines on polycrystalline gold: distinguishing between the first layers and thin films — •Indro Biswas[1], Heiko Peisert[1], Lei Zhang[1], Martin Knupfer[2], Michael Hanack[3], Danilo Dini[3], Thomas Schmidt[4], David Batchelor[4], and Thomas Chassé[1] — [1]Universität Tübingen, IPC, Auf der Morgenstelle 8, 72076 Tübingen — [2]Leibniz Institute for Solid State and Materials Research Dresden, P.O. Box 270116, , D-01171 Dresden — [3]Universität Tübingen, Inst. Organ. Chem., Auf der Morgenstelle 18, D-72076 Tübingen — [4]Universität Würzburg, Am Hubland, D-97074 Würzburg

We have studied the molecular orientation of substituted phthalocyanines (Pc's) grown as ultra-thin films on a polycrystalline gold substrate. For about 10-20 nm thick films of Pc's with small substituents, a high degree of molecular orientation has been observed. Similar to unsubstituted PcCu, the orientation of the molecules is perpendicular to the sample surface. Importantly, however, the molecular orientation is different for low coverages, the molecules lie on the substrate surface. Thus, the orientation of organic molecules directly at the interface cannot be deduced from the orientation in typical thin film systems. The growth mode is discussed in terms of different molecule-molecule and molecule-substrate interactions. We are grateful for helpful discussions and the synthesis of organic materials to M. Cook and I. Chambrier. Financial support by BESSY is acknowledged.

O 45.10 Di 18:00 TU EB301

Structural and Topographic Study of clean Porphyrin films — •Karmen Comanici, Florian Maier, Hubertus Marbach , and Hans-Peter Steinrück — Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

Organic molecules play a prominent role for the development of new materials and molecular devices. An important group of such molecules are porphyrins. Their versatility and distinct chemical and electronic properties makes them promising candidates for tailored catalytic processes and as building blocks for nanoscaled electronic devices.The properties of porphyrins can be modified e.g. by introducing or changing a central metal atom and different ligands. We studied different porphyrins on silver surfaces by means of scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) in ultra high vacuum (UHV). The preparation of the porphyrin layers were done in UHV via sublimation techniques. Ordered porphyrin layers as well as tip induced structural changes in the STM image of the adsorbed fims were observed. One topic to be presented and discussed will be the first time observation of ordered porphyrin layers on an Ag(111) surface.

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O 45.11 Di 18:15 TU EB301

Conjugated organic molecules on Au(111): Effect of molecular geometry and conformational changes — •Carsten Busse[1], Sigrid Terkelsen[1], Lars Petersen[1], Morten Nielsen[2], Kurt V. Gothelf[2], Trolle R. Linderoth[1] und Flemming Besenbacher[1] — [1]Department of Physics and Astronomy and iNANO, University of Aarhus, 8000 Aarhus C, Denmark — [2]Department of Chemistry and iNANO, University of Aarhus, 8000 Aarhus C, Denmark

We have performed a UHV-STM study of structures formed by a family of geometrically different, but chemically similar, molecules adsorbed on Au(111). The molecules consist of a central benzene ring with three or two ethynylene spokes, each terminating in a tert-butyl substituted salicylaldehyde moiety. After adsorption at 300 K a variety of close-packed phases is observed which can be rationalized by a common motif of molecules adsorbed with their backbone parallel to the surface and optimized side-to-side interactions. These results constitute a platform for ongoing experiments where conformational changes of the adsorbed molecules are studied and the molecular parameters governing this flipping process are determined, and where covalent cross-linking is induced through co-adsorption with reactive amines.