O 31 Organische Dünnschichten III

Zeit: Montag 10:45–13:00 Raum: TU EB420

O 31.1 Mo 10:45 TU EB420

Structural investigation of organic monolayers on Ag(111) using NIXSW — •C. Stadler, A. Schöll, S. Hansen, C. Kumpf, and E. Umbach — Exp. Physik II, Uni Würzburg, Germany

The investigation of the interaction of organic molecules with inorganic substrates is a key issue for the understanding of interface effects. We report on new NIXSW measurements on different organic monolayers with flat lying molecules on Ag(111). Information about the bonding distance of different atomic species in the molecule is obtained. In the case of the relaxed monolayer structure of NTCDA a value of 3.02 Å and 3.08 Å for O and C respectively, was measured, demonstrating that the molecule is truely chemisorbed on the surface, not only weakly physisorbed. For the oxygen atoms we also tried to resolve possible differences in the bonding strength for the two different oxygen species in the molecule by identifying core level shifts in the photoemission signal. Measurements on metallo-phthalocyanines have also been performed in order to study the position of the metallic atom with respect to the molecular plane and the substrate. Non-dipolar contributions to the photoemission yield are taken into account as well as electron induced effects on the Auger yield.

O 31.2 Mo 11:00 TU EB420

Epitaktisches Wachstum in organisch-organischen Heterosystemen: line-on-line-Koinzidenz — •T. Fritz, S.C.B. Mannsfeld und K. Leo — Institut für Angewandte Photophysik, TU Dresden, Germany

Die experimentelle Untersuchung des epitaktischen Wachstums zweier unterschiedlicher molekularer Spezies aufeinander führt zu Überstrukturmatrizen, die ein inkommensurables Wachstum nahe legen [1,2]. Dies steht jedoch im Widerspruch zur Tatsache, dass immer wieder die gleichen Anordnungen beobachtet werden. In unserem Beitrag schlagen wir einen neuen Epitaxietyp, die so genannte line-on-line-Koinzidenz (LOL) vor, mit dem sich z.B. das geordnete Wachstum von PTCDA auf HBC auf Graphit erklären lässt. LOL-Koinzidenz entspricht in soweit der bekannten point-on-line-Koinzidenz (POL), als dass die Moleküle der obersten Schicht alle auf parallelen gleichabständigen Gitterlinien der darunter liegenden Molekülschicht liegen. Der wesentliche Unterschied besteht jedoch darin, dass bei LOL im Gegensatz zu POL diese Linien nicht auf primitive Gitterlinien beschränkt sind. Mittels Potentialberechnungen weisen wir nach, dass dieser neue Epitaxietyp tatsächlich durch ein Minimum des Wechselwirkungspotentials zwischen den beiden Molekülschichten charakterisiert ist [2].

[1] T. Schmitz-Hübsch et al., Surf. Sci. **445**, 358 (2000).
[2] S.C.B. Mannsfeld et al., Phys. Rev. Lett., *submitted* (2004).

O 31.3 Mo 11:15 TU EB420

New insight into the physics of organic materials by the absence of surface core level shifts — •M. B. Casu, Y. Zou, S. Kera, D. Batchelor, Th. Schmidt, and E. Umbach — EPII, Universität Würzburg, Am Hubland, 97074 Würzburg

We present highly resolved X-ray photoemission measurements on various different organic materials taken at different photon energies and at different take-off angles in order to investigate Surface Core Levels Shifts (SCLS). Thin films of perylenetetracarboxylic acid dianhydride, coronene, and metal free phthalocyanine were deposited on Ag(111). Photoemission spectra of the C1s core levels evidence the absence of SCLS in organic thin films. We explain these results in terms of very efficient screening. If the molecular interaction is sufficiently strong, the screening of the created charge by rapid delocalisation is quite efficient. This implies that the influence of polarization on the determination of orbitals and gaps and on the electronic and transport properties of organics must be reconsidered taking this delocalization process into account. The idea of the electronic polarisation playing a major role in their electronic properties has to be rediscuss: the usual values considered for the polarisation energy are too high and not supported by the present SCLS nvestigation. This has a strong implication on the characterisation of interfaces in electronic devices, where concepts like band offsets or charge injection should be reconsidered under these new aspect.

O 31.4 Mo 11:30 TU EB420

The in situ observation of organic growth - a spectro-microscopic study of PTCDA and NTCDA on Ag(111) — •Th. Schmidt[1], U. Groh[1], H. Marchetto[2], R. Fink[3], and E. Umbach[1] for the SMART collaboration — [1]Exp. Physik II, Universität Würzburg, 97074 Würzburg — [2]Fritz-Haber-Institut, 14195 Berlin — [3]Phys. Chemie II, Univ. Erlangen, 91058 Erlangen

The growth of two similar molecules - PTCDA and NTCDA - on a Ag(111) surface has been studied *in situ* by the spectroscopic PEEM instrument SMART, using UV-light and polarized monoenergetic synchrotron radiation. Whereas PTCDA grows in a Frank-van der Merwe fashion bellow 300 K, the growth above room temperature is of the Stranski-Krastanov type in both systems: first two closed layers of molecules are formed, followed by three dimensional (3D) growth of islands. Strong differences are observed in the molecular orientations: whereas the PTCDA molecules are always flat-lying on the substrate, the NTCDA behaves differently: the molecules are also flat-lying in the double layer but tilted by about 45° in the islands. We report on surprising observations like reduced sticking coefficient, metastable layers, internal crystal structures, and dynamic changes within the layers. Differences in the growth and the temperature dependence of the two systems are discussed. Funded by BMBF under contract no. 05KS4WWB/4.

O 31.5 Mo 11:45 TU EB420

High resolution STM images of the PTCDA/Ag(111) interface — •A. Kraft, M. Rohlfing, and F. S. Tautz — School of Engineering and Science, International University Bremen, Campus Ring 8, D-28759 Bremen, Germany

We present a combined experimental and theoretical investigation of the detailed atomic structure of the interface between 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and Ag(111). The herringbone structure of the PTCDA/Ag(111) interface was imaged in a range of different tunneling conditions with a low-temperature scanning tunneling microscope (T =9K). Experimental images are compared to calculated images based on a density functional study of the complete interface. We use the generalized gradient approximation, localized basis orbitals, and a transfer-matrix formalism to evaluate the local density of states above the surface, which corresponds to the tunneling current (Tersoff-Hamann-theory) We find excellent agreement between experiment and calculations. Implications of our results for the precise structure of the interface are discussed.

O 31.6 Mo 12:00 TU EB420

LEED-IV for the structural investigation of the NTCDA monolayer on Ag(111) — •Christian Kumpf[1], Michael Scheuermann[1], Christoph Stadler[1], Eberhard Umbach[1], and Wolfgang Moritz[2] — [1]Experimentelle Physik II, Physikalisches Institut, Univ. Würzburg — [2]Sektion Kristallographie, Fakultät für Geowissenschaften, LMU München

The Low Energy Electron Diffraction-IV (LEED-IV) technique is a powerful tool for obtaining structural information of surfaces and is often used for the investigation of adsorbate systems or surface reconstructions on an atomic level. In the past this technique was frequently applied to inorganic systems. For organic adsorbates there is a severe demand for detailed structural information, like exact atomic coordinates, which would enable, e.g., detailed quantum chemical calculations. Even though the unit cells of organic adsorbates are often very large and beam damage effects may play an essential role, in some favorable cases LEED-IV can be used to investigate organic adsorbate systems.

We report on a LEED-IV study of a well ordered, coherent monolayer of NTCDA on Ag(111) (the so called relaxed monolayer structure). Important geometric parameters like the position of the molecules (height above the surface), their orientation within the unit cell as well as possible bending and deformation of the molecules were investigated. The effect of radiation damage is also addressed. The data are compared with results from other experimental methods (like, e.g., STM, XSW, NEXAFS and XPS).

O 31.7 Mo 12:15 TU EB420

Molecular resolution in non-contact atomic force microscopy: Experiments and force field calculations — •Tobias Kunstmann[1], Regina Hoffmann[2], Markus Fendrich[1], and Rolf Möller[1] — [1]Universität Duisburg-Essen, D-45141 Essen, Germany — [2]Universität Karlsruhe, D-76128 Karlsruhe, Germany

A scanning force microscope operated in the dynamic force mode has been used to analyze the arrangement of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecules on a KBr surface. The molecules do not form a close-packed layer but crystallites with the shape of truncated pyramids. Even after depositing only 0.3 molecular layers of PTCDA, these crystallites have a height of 20-30 molecular layers. We have been able to resolve individual molecules of the top layer and on some of the crystallite's facets. Additionally, molecular force field calculations simulating a silicon tip on a layer of α-PTCDA(102) have been performed. For the frequency shift, we used the formula given by Garcia et al.[1]. The results agree well with the experimental data.

This work was funded by the SFB616 "Energy dissipation at surfaces"of the Deutsche Forschungsgemeinschaft.

[1] Ricardo García, Rubén Pérez, Surf. Sci. Rep. 47 (2002), 197

O 31.8 Mo 12:30 TU EB420

Effect of substrate structure on organic thin film morphology: Oligo-phenylenes on gold. — •Stefan Müllegger[1], Stefan Mitsche[2], Peter Pölt[2], Kathrin Hänel[3], Alexander Birkner[3], Christof Wöll[3], and Adolf Winkler[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria. — [2]Research Institute for Electron Microscopy, Graz University of Technology, Austria. — [3]Physikalische Chemie I, Ruhr Universität Bochum, Germany.

Thin films of organic semiconducting materials are attracting a growing interest both from a scientific and an applications point of view. In particular, the structure and morphology of such films are important, as they influence the (opto)electronic thin film properties. Based on our model systems, oligo-phenylene thin films grown on different Au surfaces by physical vapour deposition under UHV conditions, we demonstrate the significance of the geometric substrate structure for the development of highly anisotropic thin films. This is achieved by applying a properly prepared polycrystalline Au substrate, which comprises a large variety of differently oriented single-crystalline grains. We have applied multiple surface-sensitive techniques like secondary electron microscopy (SEM), electron backscattering diffraction (EBSD) and scanning tunnelling microscopy (STM), in order to reveal the effects of geometric anisotropy of the substrate on the structure and morphology of organic crystal growth. In particular, we could relate the orientation and terrace width of stepped (vicinal) Au surfaces to the orientation of the elongated organic crystals and the corresponding growth mode.

O 31.9 Mo 12:45 TU EB420

Die Wechselwirkung von 1,1'-Diisocyanoferrocen mit Gold: Selbstorganisierte Monolagen und supramolekulare Polymerisation — •T. Weidner[1,2], F. Träger[1,2], C. Bruhn[3,2], D. Rother[3,2], U. Siemeling[3,2], D. Fenske[4], A. Rothenberger[4] und A. Priebe[5] — [1]Institut für Physik, Universität Kassel, 34132 Kassel — [2]Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [3]Institut für Chemie, Universität Kassel, 34132 Kassel — [4]Institut für Anorganische Chemie, Universität Karlsruhe, 76128 Karlsruhe — [5]Kirchhoff Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Isocyanide sind wichtige Liganden in der Koordinations- und in der Oberflächenchemie. Durch unser Interesse an Nanostrukturen redoxaktiver Liganden und sind wir auf das bidentate 1,1'-Diisocyanoferrocene (1) aufmerksam geworden. Wir haben es im Hinblick auf seine Reaktion mit $AuCl(SMe_2)$ und die Adsorption auf Goldoberflächen untersucht. Die Reaktion mit $AuCl(SMe_2)$ ergibt ein unlösliches Koordinationspolymer $[(1)(AuCl)_2]_\infty$. Die $(1)(AuCl)_2$ Moleküle nehmen hierbei eine 3,4-Diaura-[6]ferrocenophan-Konformation ein. Sie aggregieren reissverschlussartig durch aurophile Wechselwirkungen. Die Adsorption von (1) auf polykristallinem Gold führt zur Bildung selbstorganisierter Monolagen. Messungen mit optischer Frequenzverdopplung ergeben eine Langmuirkinetik erster Ordnung. Mehrlagiges Filmwachstum konnte mit Ellispometrie ausgeschlossen werden. FTIR-Spektren zeigen eine Chemisorption beider Isocyanogruppen. Mit einiger Vorsicht kann die Struktur von $[(1)(AuCl)_2]_\infty$ als Modell der Adsorptionsgeometrie dienen.