

## O 47 Organic films IV

Time: Friday 11:15–13:00

Room: PHY C213

O 47.1 Fri 11:15 PHY C213

**Comparison of the vertical bonding distances of PTCDA on Ag(111) and Au(111)** — ●S. K. M. JÖNSSON<sup>1</sup>, O. BAUER<sup>1</sup>, A. HAUSCHILD<sup>2</sup>, T.-L. LEE<sup>3</sup>, M. SOKOLOWSKI<sup>2</sup>, and F. S. TAUTZ<sup>1</sup> — <sup>1</sup>School of Engineering and Science, International University Bremen, P.O. Box 750561, 28725 Bremen, Germany — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, University of Bonn, 53115 Bonn, Germany — <sup>3</sup>European Synchrotron Radiation Facility, Bote Postale 220, 38043 Grenoble Cedex, France

The model molecule PTCDA adsorbs on the Au(111) and Ag(111) surfaces in a planar configuration forming long range ordered superstructures. However, from different electron spectroscopies, STM and LEED data there is evidence that the bonding strength of PTCDA on Ag(111) is stronger than on Au(111). Hence the question arises, whether this also leads to a change of the vertical bonding distance of PTCDA with respect to the underlying surface. For this purpose we have measured the vertical distance of the carbon skeleton of PTCDA with respect to both surfaces using the normal incidence standing wave technique (NIXSW). Interestingly, we find that the bonding distance on Au(111) is by 0.4 Å (or 15 %) larger than on Ag(111), in agreement with the expectation on the basis of a weaker bonding. This work was supported by the DFG and the ESRF.

O 47.2 Fri 11:30 PHY C213

**LEED-IV for the structural investigation of the EC4T monolayer on Ag(111)** — ●JOHANNES ZIROFF<sup>1</sup>, CHRISTIAN KUMPF<sup>1</sup>, AZZEDINE BENDOUNAN<sup>1</sup>, WOLFGANG MORITZ<sup>2</sup>, and FRIEDRICH REINERT<sup>1</sup> — <sup>1</sup>Experimentelle Physik II, Physikalisches Institut, Univ. Würzburg — <sup>2</sup>Sektion Kristallographie, Department für Geo- und Umweltwissenschaften, LMU München

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

We report on a LEED-IV study of a well ordered monolayer of EC4T on Ag(111), the so called relaxed monolayer structure. Important geometric parameters like the position of the molecule (height above the surface and adsorption site) as well as possible bending and deformation of the molecule down to the variation of single atomic positions were investigated. The data are compared with results from other experimental methods (e.g., NIXSW, SXRD, NEXAFS), and the effect of radiation damage will be addressed. A structural model for EC4T on Ag(111) is presented.

O 47.3 Fri 11:45 PHY C213

**Structural investigation of SnPc on Ag(111) using NIXSW** — ●C. STADLER, F. POLLINGER, S. HANSEN, C. KUMPF, and E. UMBACH — Exp. Physik II, Univ. Würzburg

The investigation of the interaction of organic molecules with inorganic substrates is a key issue for understanding interface effects. We report on NIXSW measurements of two different superstructures of flat-lying tin-phthalocyanine (SnPc) molecules on Ag(111): an incommensurate monolayer at room temperature with one molecule per unit cell and a commensurate submonolayer (at 150K) with two molecules per unit cell. Precise information about the vertical bonding distance of different atomic species in the molecule with respect to the substrate is obtained. This results in a model for the RT structure with the Sn atom 0.75Å below the plane of carbon and nitrogen atoms, i.e., the molecules lie "tin-down" on the surface. The Sn-Ag distance is 2.44Å, which is very close to the Ag-Ag layer distance. In contrast, for the 150K phase a mixture of "tin-down" and "tin-up" orientations is formed. This is based on a strongly reduced coherent fraction of 0.42 for the Sn3d signal, which can be explained by two Sn-adsorption sites with a height of 2.37Å and 3.91Å respectively.

O 47.4 Fri 12:00 PHY C213

**Adsorption behavior of the amino acid DOPA on single crystalline Au(110) surfaces** — ●MIRKO WEINHOLD<sup>1</sup>, RUSLAN TEMIROV<sup>2</sup>, SERGUEI SOUBATCH<sup>2</sup>, and STEFAN TAUTZ<sup>2</sup> — <sup>1</sup>Universität Bremen — <sup>2</sup>International University Bremen

In investigations of proteins which are responsible for strong mussel adhesion, an unusually frequent appearance of the otherwise rare amino acid 3-(3,4-Dihydroxyphenyl)-L-alanine (DOPA) has been observed. This amino acid is thought to play a major role in the mechanism of mussel adhesion. Here we report an investigation of the molecule-substrate interaction between DOPA and the Au(110) surface. Several spectroscopic techniques (HREELS, LEED, XPS, IR) have been applied. Although DOPA decomposes close to the sublimation point, vapour deposition of the intact molecule without additional contamination turns out to be possible. DOPA molecules form a commensurate superlattice on Au(110). The chirality of the molecule leads to a one-domain chiral surface. Vibrational spectroscopy in conjunction with density functional calculations proves that DOPA adsorbs on Au(110) in its zwitter-ionic state. Annealing a DOPA/Au(110) monolayer to 550 K leads to partial desorption of the monolayer as well as catalyzed oxidation of DOPA to DOPAquinone.

O 47.5 Fri 12:15 PHY C213

**Comparative UHV-STM study of adsorption structures formed from a family of oligo-(phenylene ethynyls) with systematic variation of geometry and functional groups** — ●CHRISTIAN BOMBIS<sup>1</sup>, CARSTEN BUSSE<sup>1</sup>, SIEGRID WEIGELT<sup>1</sup>, MARTIN NOERGAARD<sup>1</sup>, MARTIN KNUDSEN<sup>2</sup>, KURT V. GOTHELF<sup>2</sup>, EVA RAULS<sup>1</sup>, BJOERK HAMMER<sup>1</sup>, FLEMMING BESENBACHER<sup>1</sup>, and TROLLE R. LINDEROTH<sup>1</sup> — <sup>1</sup>Department of Physics and Astronomy, and iNANO, University of Aarhus, 8000 Aarhus C, Denmark — <sup>2</sup>Department of Chemistry, and iNANO, University of Aarhus, 8000 Aarhus C, Denmark

Using scanning tunneling microscopy we have systematically explored the influence of the geometry of molecules and the chemical nature of their functional groups on formed adsorbate structures. For this purpose we utilized compounds from a family of organic molecules, oligo-(phenylene ethynyls), which have been deposited on the Au(111) surface under ultra high vacuum conditions. The elementary member of this family consists of a highly conjugated linear backbone functionalized with aldehyde, hydroxyl and bulky tert-butyl groups while compounds with bent and three-spoke geometries represent geometrical variants. The study with systematic variation of the endgroup chemistry supports the hypothesis, that only in the case, where intermolecular hydrogen bonds can form, does a more open network phase form instead of a close packed structure held together by non-specific Van-der-Waals interactions. Theoretical modelling based on the DFT-B method is currently being performed to further illuminate this observation.

O 47.6 Fri 12:30 PHY C213

**STM and LEED study on the Influence of Different Substituents on the Growth of Quaterylene Derivatives on Gold.** — ●CHRISTIAN WAGNER<sup>1</sup>, ROBERT FRANKE<sup>1</sup>, SEBASTIAN FRANKE<sup>1</sup>, THOMAS DIENEL<sup>1</sup>, STEFAN MANNFELD<sup>2</sup>, and TORSTEN FRITZ<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik; TU-Dresden; George-Bähr-Straße 1; 01069 Dresden — <sup>2</sup>Department of Chemical Engineering; Stanford University; 381 North South Mall; Stanford, CA 94305-5025

The possibility to tailor and control organic molecules for special purposes opens a new field of possible applications. There is a general interest in the question how even minor modifications e.g. different substituents change the behavior of a class of molecules. In highly ordered monolayers, the influence of the substituents can be studied in a well defined environment. As perylene derivatives [1] have already been studied intensively, we have now grown highly ordered monolayers of the larger IR absorbing quaterylene derivatives, quaterylene (QT) and quaterylenebisdicarboximide (QTCDI) on Au in UHV. The structure of QT has been studied by STM and LEED and fits nicely to state-of-the-art potential calculations [2] for the growth of large QT domains on gold. Due to the presence of imide groups the structure of QTCDI differs strongly from QT. Three different phases have been found which can be explained by the formation of hydrogen bonds. The capability of the potential calculations is demonstrated as all three phases are predicted.

[1] H. Proehl, T. Dienel, R. Nitsche und T. Fritz, PRL. 93 (2004)

097403 [2] S.C.B. Mannsfeld and T. Fritz, PRB 93 (2004) 075416 & PRB 71 (2005) 235405

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**Aromatic selenolates as an attractive alternative to the respective thiulates** — ●ANDREY SHAPORENKO<sup>1</sup>, PIOTR CYGANIK<sup>2</sup>, MANFRED BUCK<sup>2</sup>, ANDREAS TERFORT<sup>3</sup>, and MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — <sup>2</sup>School of Chemistry, St Andrews University, North Haugh, St Andrews, KY16 9ST, United Kingdom — <sup>3</sup>Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

Self-assembled monolayers (SAMs) formed from bisbiphenyl-4-yl diselenide (BBPDSe) on Au(111) and Ag(111) substrates have been characterized by several complementary spectroscopic and microscopic techniques. BBPDSe was found to form contamination-free, densely-packed, and well-ordered biphenyl selenolate (BPSe) SAMs on both Au and Ag. Spectroscopic data suggest very similar packing density, orientational order, and molecular inclination in BPSe/Au and BPSe/Ag. STM data give a similar intermolecular spacing of 5.3 Å on both Au and Ag, but exhibit differences in the exact arrangement of the BPSe molecules on these two substrates. There is strong evidence for adsorbate-mediated substrate restructuring in the case of Au, whereas no clear statement on this issue can be made in the case of Ag. The film quality of the BPSe SAMs is superior to their thiolate analogues, which is presumably related to a better ability of the selenolates to adjust the surface lattice of the substrate to the most favorable 2D arrangement of the adsorbate molecules. This implies that aromatic selenolates represent an attractive alternative to the respective thiulates.