

## DS 23: Organic Thin Films III

Time: Wednesday 14:45–16:15

Location: GER 38

DS 23.1 Wed 14:45 GER 38

**Adsorption of bay-substituted perylene bisimide dyes on Ag(111) investigated by PES and NEXAFS** — ●MARKUS SCHOLZ<sup>1</sup>, STEFAN KRAUSE<sup>1</sup>, RÜDIGER SCHMIDT<sup>2</sup>, MARC HÄMING<sup>1</sup>, ACHIM SCHÖLL<sup>1</sup>, FRANK WÜRTHNER<sup>2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — <sup>2</sup>Universität Würzburg, Institut für Organische Chemie, 97074 Würzburg — <sup>3</sup>Gemeinschaftslabor für Nanoanalytik, Forschungszentrum Karlsruhe, 76021 Karlsruhe

Perylene tetracarboxylic acid bisimides (PBI) are among the best available n-conducting organic materials. Halogen substituents attached to the perylene bay positions change the molecular structure by introducing a twist angle into the usually planar perylene backbone. This influences the optical properties, the stacking of the molecules, as well as the electronic properties. Moreover, the molecular conformation is also expected to effect the interaction with metal contacts, an aspect of crucial importance for electronic devices. We report on a high resolution photoemission (PES) and x-ray absorption (NEXAFS) study of the electronic structure and the molecular orientation of ultra-thin films of the planer *PBI-H<sub>4</sub>*, and the core twisted *PBI-Cl<sub>4</sub>* on Ag(111) substrates. In the monolayer regime, substantial changes in the UPS and XPS data with respect to the bulk samples clearly indicate a covalent interaction at the interface. In the valence regime charge transfer induced occupied states are observed at the Fermi-level. This is corroborated by the NEXAFS results, which allow probing a possible change of the molecular conformation due to the interfacial interaction.

DS 23.2 Wed 15:00 GER 38

**Correlating bonding distance and interfacial electronic structure: The role of molecular side groups** — ●STEFFEN DUHM<sup>1,2</sup>, ALEXANDER GERLACH<sup>3</sup>, GEORG HEIMEL<sup>1</sup>, BENJAMIN BRÖKER<sup>1</sup>, TAKUYA HOSOKAI<sup>3</sup>, TIEN-LIN LEE<sup>4</sup>, JENS PFLAUM<sup>5</sup>, SATOSHI KERA<sup>2</sup>, NOBUO UENO<sup>2</sup>, FRANK SCHREIBER<sup>3</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Germany — <sup>2</sup>Chiba University, Japan — <sup>3</sup>Universität Tübingen, Germany — <sup>4</sup>European Synchrotron Radiation Facility, Grenoble, France — <sup>5</sup>Universität und ZAE Würzburg, Germany

The interplay of energy level alignment and bonding distance of conjugated organic adsorbates on metal substrates is not yet fully understood. We studied the interfaces formed between pentacene (PEN) and its oxo-derivatives pentacenequinone (PQ) and pentacenetetrone (PT) on Ag(111) using X-ray standing waves (XSW) and ultraviolet photoelectron spectroscopy (UPS). A strong correlation could be found between the XSW and UPS results: The interaction of PEN and PQ with Ag(111) is rather weak, which is reflected in larger bonding distances and almost identical electronic structures for mono- and multilayer. In contrast, PT is strongly chemisorbed on Ag(111) through a charge transfer reaction leading to a metallic monolayer and a partial filling of the lowest unoccupied molecular orbital. This strong interaction results in a rather low bonding distance of PT on Ag(111) and an additional bending of the oxygen atoms towards the metal substrate.

DS 23.3 Wed 15:15 GER 38

**Diindenoperylene on rutile TiO<sub>2</sub> (110)** — ●BRITT-ELFRIEDE SCHUSTER, MARIA BENEDETTA CASU, HEIKO PEISERT, and THOMAS CHASSÉ — Institute for Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany

In order to optimize device performance, a comprehensive knowledge of the electronic, structural and morphological properties of organic materials is indispensable. In this regard, a crucial aspect in this field is the growth because the understanding of growth phenomena is extremely significant for many technical applications dealing with systems ranging from thin films to single crystals. Diindenoperylene (DIP) is a perylene-based aromatic hydrocarbon that exhibits besides its good film forming properties a very high hole mobility already in thin films and high thermal stability. In this work we present X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) measurements taken on thin DIP films (nominal thicknesses: 1-90 Å) on rutile TiO<sub>2</sub>(110). Diindenoperylene was deposited onto the well-characterized TiO<sub>2</sub>(110) substrate with a (1x1) reconstruction using strictly controlled evaporation conditions (evaporation rate: 3Å/min, substrate temperature 298K). The decrease of the FWHM of the C1s

peak with increasing film thickness indicate a different intermolecular interaction in the monolayer regime. By analyzing the attenuation of the substrate XPS signal, we find evidence for a Stranski-Krastanov growth mode (layer plus islands) under these preparation conditions. This observation is corroborated by AFM measurements showing a distinctive island formation.

DS 23.4 Wed 15:30 GER 38

**Structure and Lateral Conduction in a monolayer of molecular nanographenes** — ●ASIF BASHIR<sup>1</sup>, CARSTEN BUSSE<sup>1,2</sup>, XI DOU<sup>3</sup>, DANIEL KÄFER<sup>1</sup>, ZHIHONG WANG<sup>1</sup>, GREGOR WITTE<sup>1,4</sup>, KLAUS MÜLLEN<sup>3</sup>, and CHRISTOF WÖLL<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Germany — <sup>2</sup>Physikalisches Institut, Universität zu Köln, Germany — <sup>3</sup>Max Planck Institute for Polymer Research Mainz, Germany — <sup>4</sup>AG Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany

The molecular nanographenes hexa-peri-hexabenzocoronene (HBC) and HBC-derivatives can self-assemble in form of columnar film structures, which have recently attracted a paramount interest in connection with one-dimensional charge transport. The fabrication of such columnar system was carried out by using thiolated HBC-derivatives, where one-dimensional monomolecular columns are formed by the self organization of HBC molecules modified by thiol (-SH) anchors upon adsorption on Au(111) substrates. The HBC self-assembled monolayer (SAMs) are found to form long range ordered domains consisting of equidistant paired rows with closely stacked HBC units. Data from scanning tunneling microscopy (STM) and near-edge x-ray absorption spectroscopy (NEXAFS) allows to derive a detailed structural model. The charge transport along the columns within the SAM is investigated by embedding the thiolated HBC-derivates into a matrix of alkanethiols (C<sub>10</sub>-SH). The temperature dependence of apparent height on the HBC-thiol-islands and the electronic coupling between closely packed aromatic molecules exhibited by the lateral transport will be presented.

DS 23.5 Wed 15:45 GER 38

**Formation of a Polymer-Metal Interface: Deposition of Ca on Poly(3-hexylthiophene) Films** — ●FABIAN BEBENSEE<sup>1</sup>, JACK HESS BARICUATRO<sup>2</sup>, JUNFA ZHU<sup>3</sup>, WANDA LEW<sup>2</sup>, HANS-PETER STEINRÜCK<sup>1</sup>, J. MICHAEL GOTTFRIED<sup>1</sup>, and CHARLES T. CAMPBELL<sup>2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg — <sup>2</sup>Department of Chemistry, University of Washington — <sup>3</sup>National Synchrotron Radiation Laboratory, University of Science and Technology of China

The interface between Ca and poly(3-hexylthiophene) (P3HT) belongs to the technologically important class of interfaces between low work function metals and semiconducting polymers, which can be found in many applications in the rapidly developing field of organic electronics. We used various complementary techniques, including ISS and HR-XPS, to study the morphology, the chemical composition, and the electronic structure of this interface. In addition, we applied adsorption microcalorimetry to quantitatively study the energetics of Ca adsorption on the polymer, a measurement that has only recently become technically feasible. We find a strong interaction between Ca and P3HT, as indicated by a high initial heat of adsorption (629 kJ/mol). Furthermore, the appearance of a new peak doublet in the S2p XP spectra indicates that Ca interacts mainly with the sulphur in the polymer. The XPS data also allow for the determination of the penetration depth of Ca into P3HT, which is between 2.7 and 3.7 nm. Support by the DAAD, the NSF, and the Excellence Cluster "Engineering of Advanced Materials" is gratefully acknowledged.

DS 23.6 Wed 16:00 GER 38

**Ionic Liquids at the Solid-Liquid Interface - Monolayer Systems Studied Using ARXPS** — ●KEVIN ROBERT JOHN LOVELOCK<sup>1</sup>, CLAUDIA KOLBECK<sup>1</sup>, TILL CREMER<sup>1</sup>, FLORIAN MAIER<sup>1</sup>, NATALIA PAAPE<sup>2</sup>, MATTHIAS SCHMIDT<sup>2</sup>, BASTIAN ETZOLD<sup>2</sup>, PETER WASSERSCHIED<sup>2</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — <sup>2</sup>Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs), molten salts with a melting point below 100 °C, are promising candidates for many applications such as electrochemistry, separation, lubrication and catalysis. Many of the processes for

these applications are governed by the solid-liquid interface. Two different approaches have been used to study this interface, both using angle-resolved X-ray photoelectron spectroscopy (ARXPS). Firstly, an IL vapour deposition process has been established capable of producing sub-monolayer coverages. Investigations of specific IL-substrate

interactions, surface modification and film growth modes are therefore possible. Results will be presented for a range of surfaces. Secondly, the ex-situ covalent attachment of a functionalised IL to a silicon substrate has been investigated as a model system for microreactors. Such systems can be used for supported ionic liquid phase (SILP) catalysis.