

## DS 4: Organic Thin Films

Time: Monday 16:15–17:30

Location: H 2013

DS 4.1 Mon 16:15 H 2013

**PTCDA on an alkali-halogenide layer: adsorption or formation of a complex?** — ●HATICE KARACUBAN, SASCHA KOCH, THORSTEN WAGNER, and ROLF MÖLLER — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1-21, 47057 Duisburg

The initial growth of 3,4,9,10 perylene tetracarboxylic dianhydride (PTCDA) on a thin layer of NaCl was studied by means of scanning tunnelling microscopy (STM) in ultra high vacuum. The alkali-halogenide layer with a average coverage of 1.5 monolayer was prepared by thermal evaporation while the Cu(111) substrate held was at 345K. The local height of NaCl varies between 0, 2 and 3 layers. This thin insulating layer on Cu(111) still allows to establish a tunnelling current without dipping the tip into the surface. PTCDA was adsorbed on this surface. At a mean coverage of 0.04 monolayer, it was possible to image individual molecules attached to  $\langle 011 \rangle$  steps of the NaCl which are presumably sodium terminated. The alignment of the molecules at these steps can be explained by the partial charges of the molecules interacting with the steps. On terraces which are not covered by NaCl and at a coverage of 0.4 monolayers, three phases are dominant where the molecules align parallel in rods. The rod phases contradict a simple Coulomb interaction between the molecules. However, this adsorption geometry can be explained by a complex formed between PTCDA molecules and sodium atoms.

DS 4.2 Mon 16:30 H 2013

**Charged Molecules on Insulators: Optical Spectroscopy of PTCDA Ions** — ●THOMAS DIENEL, ANDREAS KRAUSE, ROMAN FORKER, and TORSTEN FRITZ — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

It has been shown that the performance of organic-based devices can be improved considerably by doping [1]. However, on the molecular scale the mechanisms of doping are still not fully understood. Here, optical spectroscopy comes in handy as valuable tool for material characterization. By applying *in situ* optical spectroscopy to (sub-)monolayer thick organic films during the actual doping process, insight in the successive development of the charged states can be gained.

In our contribution we present differential reflectance spectroscopy (DRS) [2] on perylene-3,4,9,10-tetracarboxylic-dianhydride (PTCDA) layers doped by potassium. From the spectral development with increasing potassium concentration we conclude the occurrence of different charged states and give reasons for their assignment.

[1] K. Walzer et al., Chem. Rev. **107** (2007), 1233.

[2] H. Proehl et al., Phys. Rev. B **71** (2005), 165207.

DS 4.3 Mon 16:45 H 2013

**Electronic properties of thin halogenated perylene bisimide films on Ag(111).** — ●MARKUS SCHOLZ<sup>1</sup>, STEFAN KRAUSE<sup>1</sup>, RÜDIGER SCHMIDT<sup>2</sup>, FRANK WÜRTHNER<sup>2</sup>, ACHIM SCHÖLL<sup>1</sup>, FRIEDRICH REINERT<sup>1</sup>, and EBERHARD UMBACH<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>Forschungszentrum Karlsruhe, 76021 Karlsruhe

A majority of organic semiconductors exhibit p-channel behavior. For complementary circuits both p-type and n-type semiconductors are necessary. Perylene tetracarboxylic acid bisimides (PBI) are not only considered to be among the best n-type organic semiconductors available, but also their structural properties, e.g. the twist angle of the perylene core as well optical and electronic properties can be tuned by proper substituents at the perylene core.

While previous investigations on bay-substituted perylene bisimides were performed in solution or addressed the electron mobility in thin

films, we focused on the electronic structure of thin condensed films of PBI-H4, core chlorinated PBI-Cl4, and core fluorinated PBI-F2 on Ag(111) substrates with x-ray and UV photoelectron spectroscopy (XPS/UPS) and inverse photoemission spectroscopy (IPES). Particular respect was given to the influence of different bay-substituents, which allow to vary the twist angle of the perylene core and thus possibly the intermolecular  $\pi$ -overlap. Additionally, the attenuation behavior of the substrate peaks allows conclusions about the growth mode.

DS 4.4 Mon 17:00 H 2013

**Direct spectroscopic evidence for the  $\pi$ - $\pi$ -interaction between heteroaromatic molecules** — ●F. HOLCH<sup>1</sup>, D. HÜBNER<sup>1</sup>, R. FINK<sup>2</sup>, A. SCHÖLL<sup>1</sup>, F. REINERT<sup>1</sup>, and E. UMBACH<sup>1</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II — <sup>2</sup>Universität Erlangen/ICMM, Physikalische Chemie II

High-resolution near-edge x-ray absorption fine structure (NEXAFS) spectroscopy is a very sensitive tool to analyse the electronic structure of condensed, liquid, and gaseous samples. Moreover, it provides local information due to the localized core hole excitation. We have utilized the potentials of this technique to probe the localisation of the  $\pi$ -interaction within aggregates of organic molecules.

An analysis of the intermolecular interaction requires a comparison of high-quality spectroscopic data of gaseous and condensed organic molecules. On the example of the heteroaromatic molecules 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) and 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) we present spectroscopic evidence which allows us to confine the intermolecular interaction to the  $\pi$ -system of the aromatic core. The NEXAFS spectra show a consistent shift of all resonances of the naphthalene ring system towards lower energy upon condensation, while such a shift can not be observed for the functional group. These experimental findings can be interpreted in terms of a  $\pi$ - $\pi$ -interaction induced delocalisation of the naphthalene  $\pi$ -system leading to a lowering of the respective orbital energy.

This project is financed by the BMBF under contract 05KS4WWC/2

DS 4.5 Mon 17:15 H 2013

**Organic field effect transistors based on n-conducting PTCDI derivatives** — ●DANIEL LEHMANN and DIETRICH R.T. ZAHN — Chemnitz University of Technology, Semiconductor Physics, D-09107 Chemnitz, Germany

Perylenetetracarboxylic diimide (PTCDI) is a  $\pi$ -conjugated planar perylene derivative. Being used as a red dye pigment in industry, PTCDI is highly available, and due to its n-conducting properties it is a subject of interest as an organic semiconductor for organic field effect transistors (OFETs). We present a comparative study on the electrical properties of top contact OFETs based on different PTCDI derivatives: DiMethyl-PTCDI, DiPhenyl-PTCDI, DiMethoxyethyl-PTCDI, as well as Di3Pentyl-PTCDI. The gate oxide for the devices is a 100 nm thick layer of SiO<sub>2</sub> on a highly doped Si(100) substrate. The thickness of the organic layer is in all cases 20 nm. The top contacts were made by depositing gold through a shadow mask. Channel length and width are  $L = 17 \dots 186 \mu\text{m}$  and  $W = 3 \text{ nm}$ , respectively. While the initial electron mobility measured *in situ* is between  $10^{-4} \text{ cm}^2/\text{Vs}$  and  $10^{-8} \text{ cm}^2/\text{Vs}$  depending on the molecule, an annealing of the sample at about 100°C leads to an increase in mobility typically up to one order of magnitude. This mobility is stable and not influenceable by further bias stress. Furthermore, we report on the influence of air exposure, which leads to a breakdown of the mobility by several orders of magnitude.