

SYSA 2: Organic Interface Structure and Growth

Time: Tuesday 10:45–13:00

Location: H 0105

Invited Talk SYSA 2.1 Tue 10:45 H 0105
Organic film growth and organic-metal interfaces — ●NORBERT KOCH — Humboldt-Universität zu Berlin, Institut f. Physik, Berlin, Germany

The structure, morphology, and electronic properties of thin films formed by conjugated organic molecules are key factors determining the function and efficiency of organic (opto-) electronic devices. Molecules chemisorbed on metal surfaces can undergo significant conformation changes, often facilitated by a hybridization of molecular and metal electron wavefunctions. The resulting energy levels at such interfaces are determined by a complex interplay of molecular orientation, charge transfer, and conformation dependent dipoles, which will be exemplified for strong electron acceptor molecules on coinage metal surfaces. The modification of metal surfaces with electron acceptors can be used to control the energy level alignment of subsequently deposited organic layers. Thin organic films on insulating substrates are of interest for organic field effect transistors. Co-deposited rod-like conjugated molecules can form new crystalline intercalated structures with electronic properties significantly different from those of the pure materials. It will be shown that the appropriate combination of two different molecules facilitates (i) control over the energy levels, and (ii) widely tunable charge transport properties.

SYSA 2.2 Tue 11:15 H 0105
Growth analysis at the contacts of nanoscale oligothiophene field effect transistors — ●ARNE HOPPE, TORSTEN BALSTER, and VEIT WAGNER — Jacobs University Bremen, School of Engineering and Science 28725 Bremen

Decreasing the size of bottom contact organic field effect transistors (OFETs) to the nanoscale in order to achieve high performance devices with enhanced integration density leads to new challenges such as contact resistance and modified growth modes on nanostructured surfaces. The growth behavior of dihexyl-substituted oligothiophenes is investigated by in-situ electrical characterisation and by AFM topography analysis. DH4T, DH5T, and DH6T show oscillations in the charge carrier mobility with layer thickness reflecting the length of the individual molecules. Downscaling of the channel length to the sub-micrometer region allows the direct analysis of the contact resistance and reveals that oscillations occur not only in the mobility, but in the contact resistance as well. Typical mobility values for micrometer devices are as high as 6×10^{-2} cm²/Vs despite contact resistance. With further shrinking of the channel length we find the suppression of the oscillations observed before. By a growth analysis by AFM, we attribute this behaviour to the disturbed growth close to the contacts due to lateral material diffusion, i. e. due to a step-flow growth mode. Due to this diffusion we find excess organic material in the channel for channel lengths below 500 nm. These findings indicate that nanoscale transistors below a critical channel length can exploit the step-flow growth mode to suppress the mobility drops caused by fractional monolayers.

SYSA 2.3 Tue 11:30 H 0105
Growth and Electronic Structure of Pentacene on Pd & Pt Surfaces — ●DANIEL KÄFER and GREGOR WITTE — Physikalische Chemie I, Ruhr-Universität Bochum, Germany

Due to its high charge carrier mobility pentacene is a promising molecular semiconductor for the fabrication of organic field effect transistors (OFETs). While gold has been commonly used as electrode material in pentacene based thin film transistors recent studies have shown improved device characteristics for Pd electrodes.

In this study the growth and structures of pentacene films on single-crystalline and polycrystalline Pd and Pt surfaces has been investigated by means of SEM and NEXAFS spectroscopy. Significant differences were found for the molecular orientation in multilayer films grown on both substrates, which is important for the realization of OFETs in view of the large anisotropy of charge carrier mobility in crystalline pentacene. In addition a rather different film morphology was observed for the various substrates ranging from a quasi layer-by-layer fashion to extreme dewetting. The interaction strength of pentacene with both metal surfaces was further characterized by TDS measurements. Moreover, by using UPS the electronic structure of pentacene thin films on Pd and Pt has been analyzed in detail. These results reveal a different electronic coupling between the metal substrate and

the first monolayer on the one hand, and between the first layer and pentacene multilayers on the other hand, which has to be taken into consideration for an understanding and optimization of charge injection in such devices.

SYSA 2.4 Tue 11:45 H 0105
X-ray standing wave study of pentacene and perfluorinated pentacene on Cu(111) — ●A. GERLACH¹, F. SCHREIBER¹, S. DUHM², N. KOCH², A. VOLLMER³, T. SUZUKI⁴, and J. ZEGENHAGEN⁵ — ¹Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ³Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung, Albert-Einstein-Str. 15, 12489 Berlin, Germany — ⁴Institute for Molecular Science, Myodaiji, Okazaki 444-8787, Japan — ⁵European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

The adsorption geometry of pentacene (PEN) and perfluorinated pentacene (PFP) on Cu(111) is studied using the X-ray standing wave technique. The element specific structural information derived from the C(1s) and F(1s) photoelectron signals demonstrate the different bonding mechanism of both molecules.

While PEN interacts strongly with the copper substrate and adsorbs with an average bonding distance of only 2.34 ± 0.02 Å, the carbon core of the PFP molecule is located at 2.98 ± 0.07 Å. Despite the relatively weak interaction of PFP with the substrate the molecules experience a mild distortion upon adsorption with the fluorine atoms being slightly above the molecular plane at 3.08 ± 0.04 Å. Based on the XSW results we discuss the influence of the intramolecular dipole on the charge transfer across the interface.

Invited Talk SYSA 2.5 Tue 12:00 H 0105
Molecular n-doping of organic semiconductors — ●ANTOINE KAHN and CALVIN CHAN — Princeton University, Princeton, NJ, USA

Chemical doping of organic molecular films is a powerful way to improve charge injection and transport in organic devices, and to enhance device functionality. However, n-type doping is challenging, often hindered by the energetic requirements of transferring an electron from the dopant HOMO to the host low lying LUMO. We recently demonstrated efficient n-doping of the electron transport material tris{2,5-bis(3,5-bis-trifluoromethyl-phenyl)-thieno}[3,4-b,h,n]-1,4,5,8,9,12-hexaazatriphenylene (THAP), which has a 4.59 eV electron affinity (EA), with cobaltocene (CoCp, IE = 4.07 eV). We now introduce a stronger n-dopant, i.e. decamethylcobaltocene (CoCp*2), and demonstrate n-doping of copper phthalocyanine (CuPc, EA = 3.25 eV). CoCp*2 is found to have a remarkably low IE of 3.30 eV. N-doping is evidenced by a large upward swing of the Fermi-level in the gap of CuPc, and confirmed by current-voltage (I-V) measurements. A 10^4 to 10^7 -fold increase in current density of the interface-doped device as compared to the undoped CuPc device is due to enhanced injection. An additional 10^3 -fold increase in current density is observed for the uniformly doped device and is attributed to enhanced conductivity of the bulk film. The application of p- and n-doping of CuPc to an organic homojunction p-i-n diode with a 1.47 eV built-in potential is demonstrated.

SYSA 2.6 Tue 12:30 H 0105
Electronic structure of the CuPc/BPE-PTCDI donor/acceptor hetero interface of organic solar cells for varied O2 and TCNQ doping concentrations — CORINNA HEIN, ●ERIC MANKEL, JOHANNA HÄRTER, THOMAS MAYER, and WOLFRAM JAEGERMANN — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstr. 23, 64287 Darmstadt

The bilayer hetero junction model solar cell of Copper phthalocyanine (CuPc) / BPE-PTCDI, a perylene derivative, shows a low efficiency of 0.8% only. With synchrotron induced photoemission (SXPS) in the course of interface formation we find the development of potential barriers due to band bending, hindering charge collection. To overcome the formation of the barrier we test p-doping of the CuPc layer by oxygen or by TCNQ, which are strong electron acceptors. Oxygen doping of CuPc was performed by evaporation in O₂ atmosphere at pressures in the range from 10-8mbar to 10-3mbar which leads to oxygen con-

centrations less than 1%. A shift of the CuPc Fermi level by 200meV was achieved. TCNQ doping was performed by coevaporation. With increasing TCNQ content in the percent region, a shift of the CuPc Fermi level up to 450meV has been achieved. The doping mechanism has been analyzed by performing SXPS on the TCNQ/CuPc interface. In the course of CuPc deposition we find a shift of the CuPc HOMO by 450 meV indicating electron transfer. In addition an interface dipole of 320 meV is formed.

SYSA 2.7 Tue 12:45 H 0105

Ambipolar organic semiconductor blends for photovoltaic cells — ●ANDREAS OPITZ, MARKUS BRONNER, JULIA WAGNER, MARCEL GÖTZENBRUGGER, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, Germany

Blends of organic semiconducting materials, so-called bulk-heterojunctions, are widely used in ambipolar field-effect transistors and as photoactive films in solar cells. One particularly interesting material system is a mixture of n-conducting fullerene (C₆₀)

and p-conducting copper-phthalocyanine (CuPc) prepared by coevaporation.

The electronic properties of these blends were analysed by X-ray and ultraviolet photoelectron spectroscopy in dependence on the mixing ratio [1]. A common vacuum level is observed suggesting that a phase separation of the two materials in the blends occurs only on the nanometer scale. The HOMO and the core level spectra show no evidence for a charge transfer or a chemical reaction among the materials in the ground state. These results also indicate a reduced energy offset between the HOMO of the donor and the LUMO of the acceptor in bulk heterojunctions in comparison to planar heterojunctions. As a consequence photovoltaic cells reveal higher built-in and open circuit voltage for the bilayered system. Nevertheless, photovoltaic cells using mixtures yield higher photocurrents due to the presence of donor/acceptor interface in the whole active film [2].

[1] A. Opitz et al., *Appl. Phys. Lett.* **90** (2007) 212112.

[2] W. Brütting et al., *Macromol. Symp.* (2007), accepted.