

## HL 52: Organic Electronics and Photovoltaics: Electronic Properties I (jointly with DS, CPP, O)

Time: Wednesday 9:30–11:15

Location: H 2032

HL 52.1 Wed 9:30 H 2032

**Design of novel dielectric surface modifications for perylene thin-film transistors** — ●CHRISTIAN EFFERTZ<sup>1</sup>, INGOLF SEGGER<sup>1</sup>, PHILIP SCHULZ<sup>1</sup>, ARNO CLASSEN<sup>2</sup>, CARSTEN BOLM<sup>2</sup>, and MATTHIAS WUTTIG<sup>1,3</sup> — <sup>1</sup>I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen — <sup>2</sup>Institut für Organische Chemie (IOC), RWTH Aachen, 52056 Aachen — <sup>3</sup>JARA FIT, Forschungszentrum Jülich, 52425 Jülich

Dielectric surface modifications (DSMs) can improve the performance of organic thin-film transistors (OTFTs) significantly. To gain a deeper understanding of this performance enhancement and to facilitate high mobility transistors, perylene based OTFTs utilizing novel dielectric surface modifications have been produced. Novel DSMs, which are based on derivatives of tridecyltrichlorosilane (TTS) with different functional end-groups have been applied to tailor the adhesion energy of perylene. The resulting samples were characterized by electronic transport measurements, scanning probe microscopy and x-ray diffraction (XRD). Measurements of the surface free energy of the modified dielectric enabled the calculation of the adhesion energy of perylene upon these novel DSMs by the equation-of-state approach. These calculations demonstrate the successful tailoring of the adhesion energy. The insight gained in this study was used to carefully choose further novel DSMs based on polymers. Utilizing these novel DSMs, perylene thin-films and TFTs with a superior film quality, in terms of crystallinity and morphology, as well as performance, in terms of mobility, have been produced[1]. [1]: Effertz, C., et. al. (2011), Adv. Func. Mater. doi: 10.1002/adfm.201101299

HL 52.2 Wed 9:45 H 2032

**Intermolecular hybridization governs molecular electrical doping** — ●INGO SALZMANN<sup>1</sup>, GEORG HEIMEL<sup>1</sup>, STEFFEN DUHM<sup>2</sup>, MARTIN OEHZELT<sup>3</sup>, PATRICK PINGEL<sup>4</sup>, BENJAMIN GEORGE<sup>3</sup>, ALEXANDER SCHNEGG<sup>3</sup>, KLAUS LIPS<sup>3</sup>, RALF-PETER BLUM<sup>1</sup>, AN-TJE VOLLMER<sup>3</sup>, and NORBERT KOCH<sup>1,3</sup> — <sup>1</sup>Humboldt Universität zu Berlin, Germany — <sup>2</sup>Chiba University, Japan — <sup>3</sup>Helmholtz Zentrum Berlin, Germany — <sup>4</sup>Universität Potsdam, Germany

Strong molecular acceptors in organic semiconductor (OSC) films are typically used for molecular electrical p-type doping assuming electron transfer from OSC to dopant. Positive polarons in the fundamental OSC gap are thus expected and could be observable in ultraviolet photoelectron spectroscopy (UPS) as emission feature at, or close to the Fermi Energy ( $E_F$ ) with reduced ionization energy (IE), which, however, has not been observed to date. We present a study on the prototypical OSC/p-dopant pair pentacene (PEN) and tetrafluorotetracyano-quinodimethane (F<sub>4</sub>-TCNQ) up to 1:1 ratio [1]. The IE of 1:1 mixed (amorphous) films is *increased* and larger than possible for pure PEN, while all states occur well below  $E_F$  in UPS. We suggest OSC/dopant frontier molecular orbital hybridization forming a doubly occupied bonding and an empty anti-bonding supramolecular hybrid orbital with reduced fundamental gap, which is in fact found by optical absorption measurements and corroborated by density-functional theory (DFT) calculations. Based on similar results for various OSCs, common doping-related observations are discussed within this framework. [1] I. Salzmann, G. Heimel et al., *Phys. Rev. Lett.*, in press.

HL 52.3 Wed 10:00 H 2032

**Effect of molecular p-doping on hole density and mobility in P3HT and MEH-PPV** — ●PATRICK PINGEL and DIETER NEHER — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitry. Recently, p-doping of conjugated polymers with the strong molecular acceptor tetrafluorotetracyanoquinodimethane, F<sub>4</sub>TCNQ, has been introduced.

Here, we present a detailed study of the doping efficiency and carrier mobility in thin layers of poly(3-hexylthiophene), P3HT, and poly(2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene), MEH-PPV, doped with F<sub>4</sub>TCNQ over a wide range of concentrations. Investigation of these layers with impedance spectroscopy in a metal-insulator-semiconductor (MIS) geometry allowed us to determine both charge carrier density and mobility as a function of doping

ratio.

We show that the density of mobile holes increases strictly linearly with increasing F<sub>4</sub>TCNQ concentration, but the mobilities in P3HT and MEH-PPV exhibit non-monotonic dependencies on doping concentration. This behavior can be fully explained by a model originally developed by Arkhipov et al. [Phys. Rev. B **72**, 235202 (2005)], which predicts that the Coulomb potential of a doping-induced negative counterion acts as a trapping center for holes. Thus, energetical disorder in the polymer layer is effectively increased upon chemical doping.

HL 52.4 Wed 10:15 H 2032

**Investigation of the degradation processes in small molecule solar cells using impedance spectroscopy** — ●ANDRÉ DÖRING, LORENZO BURTON, MARTIN HERMENAU, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The purpose of this work is to correlate the impedance spectra (IS) of different solar cell structures - composed of small molecules - with the degradation processes that take place under different aging conditions.

The materials chosen for the optically active bulk-heterojunction layer are ZnPc as donor and C<sub>60</sub> as acceptor, often used in small-molecule solar cells. In addition to the bulk-heterojunction, doped electron and hole transport layers forming a p-i-n structure are used. Concomitant with the measurement of the IS, the characteristic parameters of the device (i.e.  $j_{sc}$ ,  $V_{oc}$ , FF, PCE, EQE) are monitored during the degradation and correlated to the changes in the IS.

Analyzing the IS gives the possibility to identify different electrical processes that take place in the device. At the beginning of the aging process, we observe an initial improvement of the solar cell parameters, in conjunction with a decreasing trap response in the IS spectra. To investigate in more details the role of trap states for the solar cell performance, simplified structures are prepared. We identify in this way the trap location, type and density inside the solar cell structure. The devices are also exposed to controlled atmospheric conditions to investigate whether oxygen or water vapor is more responsible for the observed change in the electrical properties of the solar cell.

HL 52.5 Wed 10:30 H 2032

**IR spectroscopic investigation of the MoO<sub>3</sub> doping efficiency in CBP** — ●TOBIAS GLASER<sup>1,4</sup>, SVEN TENGELER<sup>1,4</sup>, SEBASTIAN BECK<sup>1,4</sup>, DANIELA DONHAUSER<sup>2,4</sup>, BERND LUNKENHEIMER<sup>3,4</sup>, ANDREAS KÖHN<sup>3,4</sup>, and ANNEMARIE PUCCI<sup>1,4</sup> — <sup>1</sup>Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — <sup>2</sup>Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstraße 22, 38106 Braunschweig — <sup>3</sup>Universität Mainz, Institut für Physikalische Chemie, Jakob-Welder-Weg 11, 55128 Mainz — <sup>4</sup>InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

A major challenge towards high-efficiency and low-voltage organic electronic devices such as OLEDs is to overcome the low bulk conductivity of the organic films. P-type doping with transition-metal oxides like tungsten oxide and molybdenum oxide has proven to increase the charge carrier concentration in hole transporting materials. But the doping efficiency of only a few percent is rather low and the reason for the low efficiency is not fully understood yet. We investigated doping of the ambipolar charge transport material 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) with MoO<sub>3</sub> using FTIR-spectroscopy in ultrahigh-vacuum. Comparison of the measured spectra of films with different MoO<sub>3</sub>-concentration to DFT-calculations reveals the amount of charge transfer from CBP to MoO<sub>3</sub> but also shows that most of the CBP molecules are still in the neutral state. Also the impact of substrate temperature during the evaporation process is investigated.

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HL 52.6 Wed 10:45 H 2032

**Agglomeration of MoO<sub>3</sub> doped into organic thin films studied by TEM-spectroscopy and Tomography** — ●DANIELA DONHAUSER<sup>1,2</sup>, KATRIN SCHULTHEISS<sup>1,2</sup>, LEVIN DIETERLE<sup>1,2</sup>, MARTIN PFANNMÖLLER<sup>3</sup>, RASMUS R. SCHRÖDER<sup>3</sup>, TOBIAS GLASER<sup>4,2</sup>, BERND LUNKENHEIMER<sup>5,2</sup>, MICHAEL KRÖGER<sup>1,2</sup>, and WOLFGANG

KOWALSKY<sup>1,2</sup> — <sup>1</sup>Institut für Hochfrequenztechnik, Technische Universität Braunschweig — <sup>2</sup>InnovationLab GmbH, Heidelberg — <sup>3</sup>CellNetworks, Universität Heidelberg — <sup>4</sup>Kirchhoff-Institut für Physik, Universität Heidelberg — <sup>5</sup>Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz

Electrochemical doping is essential to overcome limitations in organic devices imposed by low intrinsic conductivity and high injection barriers at the contacts. Materials with very deep lying HOMO-levels like CBP (4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) can be doped with transition metal oxides, e.g. MoO<sub>3</sub>. In such systems a very low doping efficiency has been found for which the physical origin is not understood. With TEM spectroscopy we could show that agglomeration of MoO<sub>3</sub> in the CBP-matrix is most likely the reason for the low doping efficiency. Using TEM tomography we observed that MoO<sub>3</sub> forms filament-like structures perpendicular to the substrate. Combining our results with FTIR-measurements, which indicate a charge carrier localization at single molecules, we can model the charge transport to occur at the interface of the MoO<sub>3</sub> filaments and the organic matrix.

HL 52.7 Wed 11:00 H 2032

**Depth Profiling of Organic Electronic Materials by Gas Cluster Ion Beam** — ●ANDREY LYAPIN — Physical Electronics GmbH, Fraunhoferstr. 4, D-85737, Ismaning, Germany

The development of new electronic devices incorporating organic materials, such as Organic Light Diodes (OLED) and Organic Photovoltaics (OPV) is rapidly increasing. To control quality, performance and lifetime of these devices, it is necessary to characterize the layered structures and the dopant distributions in the thin organic materials. Conventional surface analysis techniques such as XPS and ToF-SIMS, combined with mono-atomic ion beam sputtering, have been widely used for chemical depth profiling of inorganic thin films. However, this approach has not been successful for the depth profiling of organic materials due to the loss of chemical information during the sputtering process. Recent cluster ion beam developments utilizing C<sub>60</sub><sup>+</sup> ions have also had limited success for the depth profiling of OLED and OPV structures due to similar modification of chemical and molecular information as a function of sputter depth. The use of surface-sensitive techniques will be discussed for chemical and molecular characterization of OLED and OPV materials in combination with newly developed Gas Cluster Ion Beam (GCIB) source to achieve non-destructive chemical/molecular characterization beyond the surface and through the device. The GCIB source with an average of 2500 Ar atoms per single charged ion has shown dramatic results that both simplify and improve upon the analysis of OLED and OPV materials with a C<sub>60</sub><sup>+</sup> cluster ion beam.