

## CPP 41: Organic Photovoltaics III

Time: Friday 10:30–13:15

Location: ZEU 222

CPP 41.1 Fri 10:30 ZEU 222

**Characterization of electroactive polymers and block copolymers with potential application in organic solar cells** —

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Organic solar cells represent a new type of solar cells based on composites of an electron-donor (p-type) and an electron-acceptor (n-type) material. The low consumption of material and the application of efficient production techniques offer great potential for cost-efficient production of these solar cells.

In my talk I will show results on the electrochemical characterization of redox polymers bearing triarylamine as pendant electroactive units and on conjugated polymers, e.g. poly(para phenylene vinylenes). We use electrochemically-gated transistors to study the electronic properties of these p-type polymers, in particular the potential of doping and the intrinsic conductivity.

Block copolymers consisting of the above-mentioned polymers and neutral, sacrificial polylactides were further polymerized and characterized. Block copolymers are particularly interesting because they typically self assemble into ordered microdomain morphologies with length scales of about 5-50 nm. Upon degradation of the sacrificial block after structure formation polymer films with nanopores can be obtained. Ultimately these nanoporous polymer films shall be employed as templates for the deposition of semiconducting inorganic materials.

CPP 41.2 Fri 10:45 ZEU 222

**Bipolar substituted spiro-bifluorenes for organic solar cells?**— •CORNELIA M. BRENDDEL<sup>1</sup>, FERNANDO DIAS<sup>2</sup>, ANDY P. MONKMAN<sup>2</sup>, and JOSEF SALBECK<sup>1</sup> — <sup>1</sup>Macromolecular Chemistry and Molecular Materials, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany — <sup>2</sup>Durham Photonic Materials Institute, Department of Physics, Durham University, South Road, Durham DH1 3LN, U.K.

Substituted spiro-bifluorenes are frequently being employed in optoelectronic devices due to their tendency to build amorphous layers. Donor-acceptor compounds with a spiro-bifluorene unit as bridge have already been employed in phototransistors and have potential for application in organic solar cells.

To test their suitability for organic solar cells and clarify the role bipolar substituted spiro-bifluorenes play in phototransistors we investigated these compounds more closely by spectroscopic methods. Bipolar substituted spiro-bifluorenes show strong solvatochromism of about 100 nm when cyclohexane is exchanged by more polar solvents, e. g. methyl-THF or acetone, indicating charge-transfer emission. Charge separation by photoexcitation happens within some hundred picoseconds and has a lifetime of up to 50 ns.

We will discuss the interplay of the locally excited and the charge-transfer state on the basis of temperature dependent measurements of fluorescence and absorption as well as measurements of the fluorescence lifetime. We will also go into detail about the origin of triplet emission and its connection with the charge transfer state.

CPP 41.3 Fri 11:00 ZEU 222

**Tuning the ionization energy of organic-semiconductor films: The role of intramolecular polar bonds** —•INGO SALZMANN<sup>1</sup>, STEFFEN DUHM<sup>1</sup>, GEORG HEIMEL<sup>1</sup>, MARTIN OEHZELT<sup>2</sup>, ROBERT KNIPRATH<sup>1</sup>, ROBERT L. JOHNSON<sup>3</sup>, JÜRGEN P. RABE<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — <sup>2</sup>Institut für Experimentalphysik, Johannes Kepler Universität, Linz, Austria — <sup>3</sup>Institut für Experimentalphysik, Universität Hamburg, Hamburg, Germany

For the prototypical conjugated organic molecules pentacene and perfluoropentacene, we demonstrate that the surface termination of ordered organic thin films with intramolecular polar bonds (e.g., -H versus -F) can be used to tune the ionization energy. The collective electrostatics of these oriented bonds also explains the pronounced orientation dependence of the ionization energy. Furthermore, mixing of differently terminated molecules on a molecular length scale allows continuously tuning the ionization energy of thin organic films between the limiting values of the two pure materials. Our study shows that surface engineering of organic semiconductors via adjusting the polar-

ity of intramolecular bonds represents a generally viable alternative to the surface modification of substrates to control the energetics at organic/(in)organic interfaces.

CPP 41.4 Fri 11:15 ZEU 222

**Textile electrodes as substrates in the electrochemical growth of porous ZnO for application in dye-sensitized solar cells** —•THOMAS LOEWENSTEIN<sup>1</sup>, MARKUS MINGEBACH<sup>1</sup>, MELANIE RUDOLPH<sup>1</sup>, KERSTIN STRAUCH<sup>1</sup>, YVONNE ZIMMERMANN<sup>2</sup>, ANDREAS NEUDECK<sup>2</sup>, and DERCK SCHLETTWEIN<sup>1</sup> — <sup>1</sup>Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, D-35392, Gießen. — <sup>2</sup>Textilforschungsinstitut Thüringen-Vogtland e.V., D-07973, Greiz.

The use of textile substrates for solar active electrodes is of interest in view of future applications of textile based electronics. Active structures prepared below 150 °C are needed. An approach using dye sensitized solar cells is useful for the achievable electrode distances in the micrometer range. Deposition of semiconductor films from solutions appears as an optimum technique. We will discuss the results of cathodic electrodeposition of porous ZnO films from aqueous zinc salt solutions with a structure directing agent (SDA) on metal-coated polyamide fibers leading to well-oriented single crystalline particles of ZnO with a high internal surface area. Individual fibers showed characteristics of microelectrodes and hence increased deposition rates were obtained relative to traditional planar electrodes. The modification of the diffusion layer by hydrodynamic flow or pulsed deposition had a strong effect on the morphology of the grown ZnO. Following the dissolution of the SDA in aqueous KOH, a porous ZnO structure was obtained. Sensitization studies will be presented to show the feasibility of the chosen approach. Lit.: T. Loewenstein et al. *Phys.Chem.Chem.Phys.*, 10, 1844 (2008)

CPP 41.5 Fri 11:30 ZEU 222

**Doping of organic absorbers for application in solar cells**

— •CORINNA HEIN, ERIC MANKEL, THOMAS MAYER, and WOLFRAM JAEGERMANN — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, 64287 Darmstadt, Germany

The band alignment of the absorbing layers of an organic bilayer heterojunction solar cell was determined by synchrotron induced photoemission (SXPS). As donor type material copper phthalocyanine (CuPc) was used, the acceptor layer consists of BPE-PTCDI (a perylene derivate). At the CuPc/BPE-PTCDI interface a band bending is induced that retains the generated charge carriers leading to recombination and a low photo current of 2.4 mA/cm<sup>2</sup>. P-doping is suggested to reverse the electric field. As dopant WO<sub>3</sub> was used, known to be a strong electron acceptor. Doping was successfully performed by co-evaporation of the CuPc matrix and the dopant showing high doping efficiency and limit. The Fermi level shifts gradually with the concentration of dopant up to 690 meV. The doping mechanism was additionally investigated by layer by layer photoemission studies. Assuming phase separation the doping limit can be explained by an interface dipole. Using the doped CuPc the field at the bilayer heterojunction was reversed to the beneficial direction.

CPP 41.6 Fri 11:45 ZEU 222

**LEEM and X-PEEM investigations of diindenoperylene on Au(100)** —•MARIA BENEDETTA CASU<sup>1</sup>, BRITT-ELFRIEDE SCHUSTER<sup>1</sup>, TEVFIK ONUR MENTES<sup>2</sup>, MIGUEL ANGEL NINO<sup>2</sup>, ANDREA LOCATELLI<sup>2</sup>, and THOMAS CHASSÈ<sup>1</sup> — <sup>1</sup>ITPC, University of Tuebingen, Auf der Morgenstelle 8, 72076 Tuebingen, Germany — <sup>2</sup>Sincrotrone Trieste S.C.p.A., 34012 Basovizza, Trieste, Italy

Diindenoperylene (DIP) thin films can give rise to different film phases depending essentially on the substrate, including its local morphology, and preparation conditions. By using a combination of microscopic imaging and diffraction techniques with structural and chemical sensitivity, we studied the growth of DIP on Au(100), willing to compare the results with what previously obtained on polycrystalline gold. DIP thin films were grown on Au(100) by organic molecular beam deposition at room temperature (RT) and at very low evaporation rate (~ 0.1 Å/min). The growth and structure of DIP films of different thickness was monitored in situ and in real time by LEEM. Our investigations showed the occurrence of a Stranski-Krastanov growth mode, also establishing the influence of the local substrate morphol-

ogy. Micro-LEED evidenced the different structure of the wetting layer and the islands, confirming a different molecular arrangement depending on the film thickness. Domains of different molecular orientation were identified by dark-field LEEM, following their evolution during growth. In parallel, XPEEM and micro-XPS provided information about the bond between the molecule and the substrate as well as the chemical environment.

CPP 41.7 Fri 12:00 ZEU 222

**Growth of metal thin films on conductive polymer surfaces** — ●GUNAR KAUNE<sup>1</sup>, MATTHIAS A. RUDERER<sup>1</sup>, EZZELDIN METWALLI<sup>1</sup>, ROBERT MEIER<sup>1</sup>, WEINAN WANG<sup>1</sup>, SEBASTIEN COUET<sup>2</sup>, KAI SCHLAGE<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup> und PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik Department LS E13, James-Franck-Straße 1, 85747 Garching — <sup>2</sup>HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

Type and structure of the metal electrode deposited on top of the active layer of an organic photovoltaic cell have a strong influence on the performance of the device. Therefore it is necessary to understand the structural growth and the interaction with the photoactive polymer layer. We investigate the formation of a metal/polymer interface by deposition of gold on a poly(N-vinylcarbazole) surface [1]. The growth of the gold film is investigated in-situ with grazing incidence small angle x-ray scattering (GISAXS). In-situ GISAXS allows us to follow the spatial growth of the gold clusters from the initial stage to the formation of a continuous layer and to determine the temporal evolution of the cluster morphology. From these observations a growth model is derived, explaining the cluster growth in four steps, with a characteristic process being attributed to each step. Metal incorporation inside the semi-conducting polymer film is revealed with x-ray reflectivity measurements [1]. Finally, the results are compared with the growth of an aluminium layer on a poly(3-hexylthiophene) surface.

[1] G. Kaune et al., ACS Applied Materials and Interfaces, at press

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**Growth and morphology of photoactive small organic molecules on device-relevant substrates** — ●JONATHAN HEIDKAMP<sup>1</sup>, AYSE TURAK<sup>2</sup>, FELIX MAYE<sup>1,2</sup>, and HELMUT DOSCH<sup>1,2</sup> — <sup>1</sup>Universität Stuttgart — <sup>2</sup>Max-Planck-Institut für Metallforschung Stuttgart

Indium-Tin-Oxide (ITO) is a commonly used electrode in organic solar cells. However, the performance of these devices depends crucially on the characteristics of the interface between the ITO and the photoactive organic layer.

To study the interface characteristics, we investigated the growth, morphology, structure and ordering of small organic molecules, diindenoperylene (DIP) and perylene tetracarboxylic di-imide (PTCDI), on SiO<sub>2</sub>, ITO and modified ITO substrates by atomic force microscopy and x-ray measurements.

Both molecules formed well ordered multilayer structures on all investigated substrates. However, only DIP showed a substrate dependence in the growth behaviour and stability, indicating different interfacial interactions for the two molecules. These differences in growth and especially in stability for different substrates can have significant implications for the use of DIP and PTCDI in organic devices.

CPP 41.9 Fri 12:30 ZEU 222

**Excitons in Conjugated Polymers - Do we need a Paradigma Change** — ●WICHARD J. D. BEENKEN — Technische Universität Ilmenau, Institut für Physik, FG Theoretische Physik I, Germany

We have previously shown that both, polymer conformation and dynamics are crucial for the exciton transport in conjugated polymers. Thereby we found that the usual Förster-type hopping transfer model – even if one applies the line-dipole approximation – fall short in two respects: (i) It is still unclear of what kind the site the excitons are transferred between is. We found that the simple model of spectroscopic units defined as segments of the polymer chains separated by structural defects breaking the  $\pi$ -conjugation is only justified for chem-

ical defects like hydrogenated double bonds, or extreme gauche (90°) torsions between the monomers. Both defects are far too rare in a well prepared conjugated polymer to explain the mean spectroscopic unit length of typically 6-7 monomers. In the meanwhile, also the concept of dynamical formation of the spectroscopic units, we had previously suggested, has turned out to fail. (ii) For the ultra-fast anisotropy decay observed in films of polythiophenes, the Förster-rates are far too low. Therefore, the mechanisms resulting in initial turns of the transition-dipoles have to be different from the excitation energy transfer valid on longer time-scales. In the present talk several possible ways out of these problems will be pinpointed. It will turn out that these considerations may lead to simplified concepts for the design of polymer-based organic solar cell, with possibly higher efficiencies and longer life-times than the common polymer-fullerene blends.

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**The nature of charge transfer excitons in conjugated polymer-fullerene blends** — ●ILKA KRIEGEL, ENRICO DA COMO, MARKUS HALLERMANN, STEPHAN HANEDER, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Department of Physics and CeNS Ludwig-Maximilians-Universität, 80799, Munich (Germany)

Blends of conjugated polymers and fullerene derivatives are one of the most promising systems for organic photovoltaics. We have focussed our attention on the nature of the electronic interactions taking place at the heterojunction between the polymer MDMO-PPV and the fullerene PCBM. The presence of charge transfer excitons in these materials has been recently considered and it appears to have important implications for the solar cell efficiency [1]. Here we demonstrate the presence of hybrid ground- and excited-states at the MDMO-PPV:PCBM heterojunction. Evidence for such states is provided by photoluminescence (PL) spectroscopy, where a red-shifted emission is detected in the blend film, in addition to the MDMO-PPV excitonic emission. A comparison with the spectra of the pristine polymer or PCBM indicates that the new emission originates exclusively from a charge transfer exciton forming between the two materials in the blend. In contrast to exciplexes reported in polymer/polymer blends, the emission at 1.4 eV can be directly excited below the gap of the two materials, demonstrating the presence of a ground state [1].

[1] M. Hallermann, S. Haneder, E. Da Como, Applied Physics Letters 93, 053307 (2008)

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**Electronic properties of pristine FePc and CoPc thin films: experiment and calculations** — OLGA MOLODTSOVA<sup>1</sup>, MARTIN KNUPFER<sup>1</sup>, VOLODYMYR MASLYUK<sup>2</sup>, YURI OSSIPIYAN<sup>3</sup>, ALEXANDER CHAIKA<sup>3</sup>, THOMAS BREDOW<sup>4</sup>, INGRID MERTIG<sup>2</sup>, and ●VICTOR ARISTOV<sup>1,3</sup> — <sup>1</sup>IFW Dresden, D-01069 Dresden, Germany — <sup>2</sup>Martin-Luther-Universität Halle-Wittenberg, Fachbereich Physik, D-06099 Halle, Germany — <sup>3</sup>ISSP RAS, Chernogolovka, 142432, Russia — <sup>4</sup>Institute for Physical and Theoretical Chemistry, Bonn University, D-53115 Bonn, Germany

Magnetic transition metal (MTM) phthalocyanines are regarded as objects for the development of low dimensional molecular magnets because they are assumed as possible candidates for potential applications in high-density information storage and quantum computers that gives a strong motivation to characterize and study the electronic structure of MTM phthalocyanine thin films. Moreover this determines also the performance of devices. In this presentation we report the results of extensive investigations of the electronic structure: core-levels and valence band of the organic semiconductors CoPc and FePc in situ grown on Au(001) surface under UHV conditions. The studies were performed by means of direct and resonant photoemission, NEXAFS and DFT calculations. The experimentally obtained electronic states appeared to be in very good agreement with DFT calculations. This work was supported by the DFG under grant no. 436RUS17/52/06 and through the DFG Priority Program 1165., by the SMWK and by RFBR (grant no. 08-02-01170).