

## CPP 33: Organic Photovoltaics II

Time: Thursday 14:00–16:00

Location: ZEU 222

CPP 33.1 Thu 14:00 ZEU 222

**Interplay between morphology and energy levels in conjugated polymers: A theoretical view** — ●GEORG HEIMEL<sup>1</sup>, INGO SALZMANN<sup>1</sup>, STEFFEN DUHM<sup>2</sup>, JÜRGEN P. RABE<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489, Berlin, Germany — <sup>2</sup>Graduate School of Advanced Integration Science, Chiba University, Japan

Conjugated polymers are important constituents of organic electronic devices and it is both the bulk properties and the interfaces, which decisively determine device performance. For example, the preparation conditions are known to crucially impact the thin-film morphology of the prototypical  $\pi$ -conjugated polymer region-regular poly(3-hexylthiophene) and, consequently, also the device characteristics of, e.g., organic solar cells based on this material (rr-P3HT). We present first-principles calculations on highly ordered monolayers of rr-P3HT and a fluorinated derivative with the backbone orientations varying continuously from face-on to edge-on. Supported by electrostatic modeling, we find that the backbone orientation importantly influences the energy-level positions in these films due to intra-molecular surface dipoles; we find variations of up to 1.5 eV. As a consequence, also the energy-level alignment at ubiquitous inorganic/organic and organic/organic interfaces can be expected to depend critically on thin-film morphology. Our results provide further insight into the structure-property relationship in an important class of materials and imply novel strategies for molecular, polymer, and device design.

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**Investigation of the preparation process of dye sensitized photovoltaic cells by AFM, Kelvin Probe Force Microscopy and X-ray diffraction** — ●HARALD GRAAF<sup>1</sup>, CARSTEN MÄDLER<sup>1</sup>, MIRKO KEHR<sup>1</sup>, and TORSTEN OEKERMANN<sup>2</sup> — <sup>1</sup>Institute of Physics, University of Technology Chemnitz, 09107 Chemnitz, Germany — <sup>2</sup>Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, 30167 Hannover, Germany

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. Up to now studies concerning the influence of different processing steps on the structure of the ZnO are sparse. We discuss the growth mechanism during film deposition and the crystal structure changes of the ZnO accompanying the desorption process, which is performed in an alkaline aqueous solution. X-ray investigation shows the influence of the dye on the structure of the formed ZnO/dye hybrid film. AFM topography and Kelvin Probe Force Microscopy investigations suggest the following deposition process: at first dye molecules are adsorbed on the electrode followed by ZnO formation within the pores of the organic network. This ZnO, which shows high crystallinity, seems to be oriented with the zinc face up.

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**Nanoscale Near-field Spectroscopic Investigation of the Interplay between Local Film Morphology and the P3HT/PCBM Organic Solar Cell Efficiency** — ●DAI ZHANG<sup>1</sup>, XIAO WANG<sup>1</sup>, KAI BRAUN<sup>1</sup>, HANS-JOACHIM EGELHAAF<sup>2</sup>, and ALFRED J. MEIXNER<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Tuebingen, Germany — <sup>2</sup>Christian-Doppler-Lab for Surface Optical Methods, Johannes-Kepler-University and Konarka GmbH, Linz, Austria

The interplay between the local film morphology and the organic solar cell efficiency is systematically investigated by apertureless near-field scanning optical microscopy (SNOM). A home-built parabolic mirror assisted SNOM is used to collect both the topography and optical (Raman and photoluminescence (PL)) information from the Poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61 butyric acid methyl ester (PCBM) blend film. Molecular domains composed of either PCBM or P3HT at nanometer scale are successfully determined by their corresponding Raman fingerprint information and PL information. The regularity of P3HT polymer influenced by the clustering of PCBM during thermal annealing is compared considering the FWHM broadening of the C=C vibration Raman peak. The influences of the local

film morphology and the local distribution of P3HT/PCBM on the solar cell efficiency are discussed based on the different PL quenching levels induced by the exciton dissociation and electron transfer at P3HT/PCBM interfaces.

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**Ultrahigh time resolution nonlinear spectroscopy of polymer/fullerene blends** — ●SARAH MARIA FALKE<sup>1</sup>, DANIELE BRIDA<sup>2</sup>, GIULIO CERULLO<sup>2</sup>, and CHRISTOPH LIENAU<sup>1</sup> — <sup>1</sup>Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — <sup>2</sup>Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy

Blends of polymers and fullerene derivatives are important prototype structures for efficient photoinduced charge generation and transport in organic photovoltaic devices. It is well established that photoexcitation of polymer/fullerene blends can result in an efficient ultrafast charge transfer from the excited polymer to the electron accepting fullerene moiety. It is generally believed that this charge transfer occurs within 50-100 fs [1]. Here we study ultrafast nonlinear spectra of pristine polymers (poly(3-hexylthiophene-2,5-diyl, P3HT) and polymer/fullerene ([6,6]-phenyl-C<sub>61</sub> butyric acid methyl ester, PCBM) blends with a high time resolution of only 5 fs using a novel two-color pump-probe setup with broadband detection range. By comparing transient spectra of polymers and the polymer blend we observe an extremely rapid buildup of a band between 450 nm and 525 nm in the blend, occurring on a sub-10-fs time scale. Since the band is generally assigned to the stimulated emission from the indirectly excited fullerene moiety, our results indicate excitation transfer from the photoexcited polymer to the fullerene moiety on a sub-10-fs time scale, much faster than previously thought. The implications of these results for the microscopic charge generation processes in polymer/fullerene blends are discussed. [1] C.J. Brabec, Chem. Phys. Lett. **340**, 232 (2001).

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**A synthetic way towards rational design of discotic liquid crystals with high charge carrier mobilities** — ●DENIS ANDRIENKO<sup>1</sup>, XINLIANG FENG<sup>1</sup>, VALENTINA MARCON<sup>1</sup>, WOJCIECH PISULA<sup>1</sup>, JAMES KIRKPATRICK<sup>2</sup>, FERDINAND GROZEMA<sup>3</sup>, KURT KREMER<sup>1</sup>, and KLAUS MUELLEN<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>Imperial College London, UK — <sup>3</sup>Delft University of Technology, The Netherlands

Conjugated materials offer the revolutionary prospect of producing semiconductor devices at low cost. The best to date discotics are built around the coronene unit and possess six fold symmetry. In the discotic phase six fold symmetric molecules stack with an average azimuthal twist of 30 deg, whereas the angle which would lead to the greatest electronic coupling and hence highest charge mobility is 60 deg. Here, a molecule with three fold symmetry and alternating hydrophilic/hydrophobic side chains is synthesized and X-ray scattering is used to prove the formation of the desired helical microstructure. Pulse radiolysis time resolved microwave conductivity measurements show that the material has indeed a very high mobility in the plastic crystalline phase, in the range of 0.1 – 0.2 cm<sup>2</sup>/Vs. The physical structure of the assemblies of molecules are simulated using molecular dynamics. This, together with quantum chemical techniques, allows the computation of charge mobilities without fitting parameters. The calculations prove that mobility is still limited by structural defects and that a defect free assembly would lead to mobilities in excess of 10 cm<sup>2</sup>/Vs.

CPP 33.6 Thu 15:15 ZEU 222

**Absorption enhancement in excitonic solar cells by a photonic crystal top layer** — ●STEFAN GULDIN<sup>1</sup>, NICOLAS TETREAU<sup>1,3</sup>, MATHIAS KOLLE<sup>1</sup>, SVEN HÜTTNER<sup>1</sup>, MARK WELLAND<sup>2</sup>, PETER MÜLLER-BUSCHBAUM<sup>4</sup>, RICHARD FRIEND<sup>1</sup>, and ULLRICH STEINER<sup>1</sup> — <sup>1</sup>Cavendish Laboratory, University of Cambridge, UK — <sup>2</sup>Nanoscience Center, University of Cambridge, UK — <sup>3</sup>LPI, Ecole Polytechnique Federale de Lausanne, CH — <sup>4</sup>Physik-Department, E13, TU München

Photonic crystal structures have been identified by theorists as a candidate to enhance the still relatively low response of excitonic photovoltaic cells in the near infrared. We present a new material route that enables the fabrication of a double layer dye-sensitized solar cell,

including a mesoporous TiO<sub>2</sub> underlayer with high surface area and an optically active TiO<sub>2</sub> photonic crystal layer. A diblock copolymer acts as a structural directing agent for the mesoporous TiO<sub>2</sub>, arranging the sol-gel-derived material into a highly ordered nanostructure. The hybrid underlayer is not porous in its unannealed state and thus allows the self-assembly and infiltration of a photonic crystal template. This approach represents, to our knowledge, the first successful method that couples a photonic crystal top layer into a functioning dye-sensitised solar cell with front illumination, opening up a vast parameter space for effective light management. In this first attempt an increase in normalised photon to electron conversion of 20.4% was observed in the range from 520 nm to 725 nm (at the tail of the dye absorption spectrum).

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**Investigation of ageing processes in bulk-heterojunction P3HT:PCBM organic solar cells by means of impedance spectroscopy** — ●ULI WÜRFEL<sup>1,3</sup>, BAS V. D. WIEL<sup>2</sup>, BIRGER ZIMMERMANN<sup>1,3</sup>, and MICHAEL NIGGEMANN<sup>3</sup> — <sup>1</sup>Freiburg Materials Research Centre, Freiburg, Germany — <sup>2</sup>Universiteit Utrecht, Netherlands — <sup>3</sup>Fraunhofer Institute for Solar Energy Systems, Freiburg, Germany

The improvement of the long term stability is one important task in the development of organic photovoltaic (OPV) devices. Although promising device stabilities in the order of years can be expected the degradation mechanisms are not understood completely. They have to be identified to define conditions for accelerated degradation experiments to predict the lifetime of a device. Oxygen and water are well known as most harmful chemical species for OPV devices. We

will present results of accelerated ageing experiments done on bulk-heterojunction P3HT:PCBM solar cells. The cells were placed in a gas tight flow cell and exposed either to ambient air, pure dry oxygen or nitrogen saturated with water vapour. They were repeatedly measured by recording dark and illuminated current-voltage characteristics and a series of impedance spectra for different applied bias voltages. By means of the impedance spectra it is possible to distinguish between different degradation phenomena - like e.g. doping and interface degradation - and gain a deeper understanding of the underlying processes. Finally, simulations were carried out to model the change in the physical properties of the organic semiconductor and its impact on the device performance.

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**Influence of polymer solar cell geometry on device parameters** — BURHAN MUHSIN<sup>1</sup>, JOACHIM RENZ<sup>1</sup>, KARL-HEINZ DRÜE<sup>2</sup>, GERHARD GOBSCH<sup>1</sup>, and ●HARALD HOPPE<sup>1</sup> — <sup>1</sup>Institute of Physics, Ilmenau Technical University, Weimarer Str. 32, 98693 Ilmenau, Germany — <sup>2</sup>Electronic Technology, Ilmenau Technical University, Gustav-Kirchhoff-Str. 7, 98693 Ilmenau, Germany

In order to study the influence of the device shape on the solar cell device parameters, we systematically varied its geometry. By determining all sheet and contact resistances in the device, we were able to correlate the series resistance with the geometry of the device using a simple model for its calculation. As a result, rules for optimal design of solar modules were derived. However, further refinement of the calculation is required in order to minimize the deviation between calculus and experiment.