

CPP 2: Organic Electronics and Photovoltaics (joint session with DS/HL/O) I

small molecules, hybrid materials

Time: Monday 9:30–12:15

Location: ZEU 222

Invited Talk

CPP 2.1 Mon 9:30 ZEU 222

Structure-property relations in perylene bisimides: Charge mobility, exciton diffusion and singlet exciton fission — ●FERDINAND GROZEMA — Delft University of Technology, Department of Chemical Engineering, Delft, The Netherlands

Perylene diimides (PDIs) represent a class of materials that is promising for application as the active layer in field effect transistors and as an electron accepting material in organic photovoltaic cells. The electronic properties of PDI-based materials strongly depend on the supramolecular order in the material. Therefore, a thorough understanding of the relation between the electronic properties and the organization on the molecular scale can result in design rules for the synthesis of new π -conjugated organic molecules.

To achieve this we have performed a combined experimental and theoretical study of the electronic properties of a large library of PDI derivatives that differ in the side chains, resulting in subtle differences in the crystal structure. By time-resolved microwave conductivity measurements we show a strong correlation between the supramolecular organization and the charge carrier mobility, with a maximum mobility of 0.41 cm²/Vs. Singlet exciton fission, a process in which a singlet excited state is efficiently converted into two triplets, is also found to be strongly dependent on the supramolecular organization.

This comprehensive study shows that the engineering of the supramolecular organization in PDIs and conjugated molecules in general is a viable approach to tailor a variety of electronic properties of such materials over a wide range.

CPP 2.2 Mon 10:00 ZEU 222

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenylidibenzoperiflanthene (DBP) — ●STEFAN GROB, MARK GRUBER, ULRICH HÖRMANN, THERESA LINDERL, and WOLFGANG BRÜTTING — University of Augsburg, Germany

The DIP molecule, consisting of seven benzene and two cyclopentadiene rings, forms the backbone of the DBP molecule, which has two further benzene rings and four additional, rotatable phenyl groups. Compared to the planar arrangement of DIP, these phenyl groups give DBP a more three-dimensional shape, changing the growth behavior in thin films completely. While we observe crystalline domains of almost upright standing DIP, layers of DBP exhibit an amorphous character and therefore a relatively small exciton diffusion length, being about ten times shorter than that of its crystalline counterpart. However, the drawback of the upright standing arrangement of DIP molecules is the unfavorable orientation of the transition dipole moment resulting in a low absorption coefficient and thus a smaller short-circuit current density. The difference in morphology also leads to different coupling between donor and acceptor molecules at the interface. As a consequence there is an appreciable distinction in the recombination processes occurring within the solar cell. We investigate this phenomenon by temperature-dependent *j*-*V*-measurements, electroluminescence and photothermal deflection spectroscopy. Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

CPP 2.3 Mon 10:15 ZEU 222

Spray deposition of zinc oxide nanostructured films for applications in dye-sensitized solar cells — ●KUHU SARKAR¹, ERIK V. BRADEN¹, STEFAN POGORZALEK¹, SHUN YU², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²DESY, Notkestr. 85, 22607 Hamburg

Zinc oxide (ZnO) has emerged as a suitable alternative to titania (TiO₂) in the recent years in the field of dye-sensitized solar cells (DSSCs). The inorganic metal oxide films for DSSCs are highly desirable to have an increased surface for enhanced adsorption of a photosensitizer. Hence, nanostructured films of ZnO are synthesized from a solution based approach. Different deposition techniques are investigated to have a significant film thickness for a considerable amount of light absorption. In this respect, spray deposition is shown to be a highly efficient and scalable technique to produce films matching the

above-mentioned criteria. Surface as well as bulk morphology of the films have been studied using SEM and GISAXS. These ZnO films are successfully shown to provide good performance in a dye-sensitized solar cell with the highest short circuit current density reported so far.

CPP 2.4 Mon 10:30 ZEU 222

Extremely Thin Absorber Solar Cells based on Sb₂S₃ — ●EUGEN ZIMMERMANN, JONAS WEICKERT, THOMAS PFADLER, JAMES DORMAN, and LUKAS SCHMIDT-MENDE — Universität Konstanz

The introduction of nanostructured metal oxides as electron acceptor resulted in the concept of extremely thin absorber solar cells. Thus, low cost fabricated inorganic semiconductors like Sb₂S₃ can be utilized as sensitizer, which typically possess promising properties, such as a tunable band gap and high extinction coefficient. However, optimization of the fabrication process and a detailed characterization of intrinsic properties is unavoidable in order to find the best device architecture and suitable material combinations for highly efficient solar cells. For this purpose, chemical bath deposition conditions and parameters have been examined and resulted in a detailed recipe for fabrication of high quality Sb₂S₃ coatings. In combination with optimized layer thicknesses of P3HT, efficiencies of up to 3.2% could be achieved in flat heterojunction architecture. In order to identify intrinsic limitations, comparative measurements with P3HT:PCBM cells have been, revealing monomolecular recombination processes of excitons, a potential dependency of charge separation, and long charge carrier pathways as main loss mechanisms of fabricated flat heterojunction cells. In addition, investigation of several hole transport materials (HTM) revealed a disadvantageous influence on charge generation due to the parasitic absorption of light by the HTM. Based on these results, the use of nanostructured metal oxides in combination with transparent HTMs is proposed to possibly overcome some of the found limitations.

CPP 2.5 Mon 10:45 ZEU 222

Towards low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics — MARTIN A. NIEDERMEIER¹, MONIKA RAWOLLE¹, ERIK V. BRADEN¹, KUHU SARKAR¹, EVA M. HERZIG², VOLKER KÖRSTGENS¹, and ●PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²TU München, Munich School of Engineering, James-Frank-Str. 1, 85748 Garching

In a hybrid solar cell an inorganic matrix, such as titania, is combined with a hole-conducting polymer to form a so-called bulk heterojunction. The functionality of such a system depends strongly on the quality of the polymer/semiconductor interface. A very common approach to fabricate that interface is the so-called backfilling of the existing inorganic matrix with the conducting polymer. This approach is generally a two-step process, as the fabrication of the inorganic matrix usually involves high temperatures, which destroy all organic material present in the system. To date the subsequent backfilling of that matrix remains challenging, since a lot of problems have to be overcome. A workaround to these problems is promised by a low-temperature sol-gel process, in which the polymer and the inorganic semiconductor network are fabricated simultaneously. Approaches towards such low-temperature synthesis of polymer/titania hybrid films for application in photovoltaics are presented. These novel routes make use of special tailored block copolymers as structure directing agent. Film morphology and device function are investigated.

15 min break

CPP 2.6 Mon 11:15 ZEU 222

Photoinduced charge transfer in CuInS₂ nanocrystal/polymer composites — ●RANY MIRANTI¹, YULIAR FIRDAUS², CHRISTOPHER KRAUSE¹, MARK VAN DER AUWERAER², HOLGER BORCHERT¹, and JÜRGEN PARISI¹ — ¹Univ. of Oldenburg, Dept. of Physics, Energy and Semiconductor Research Laboratory, 26129 Oldenburg, Germany — ²Lab. for Photochemistry & Spectroscopy, Div. of Mol. Imaging & Photonics, Chemistry Dept., Katholieke Universiteit Leuven, Celestijnenlaan 200 F B-3001 Heverlee, Belgium.

The photoinduced excited states and the effects properties of charge transfer in CuInS₂ (CIS) nanocrystal/polymer composites were studied by applying quasi steady-state photoinduced absorption (PIA) and steady state photoluminescence as well as time-resolved photoluminescence. The time-resolved properties and excited state dynamics of our systems were studied using the time-correlated single photon counting (TCSPC) technique. We used two different systems of composites with two different kind of polymer, i.e. poly(3-hexylthiophene) (P3HT) and poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT). Optical absorption and emission spectra of thin films of CIS nanocrystal/polymer composites exhibit several interesting features such as luminescence quenching and polaronic photoinduced absorption (PIA) indicating photoinduced charge transfer. The effect of different organic ligands surrounding the CIS nanocrystals on the charge separation process in CIS nanocrystal/ polymer composites will be presented as well.

CPP 2.7 Mon 11:30 ZEU 222

Structured growth of ZnO for light trapping enhancement in organic solar cells — ●NIVEDITA YUMNAM and VEIT WAGNER — Jacobs University, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area and low-cost production of solar cells. However, their performance is limited due to the short diffusion length of excitons and low absorption in the active semiconductor layer. The absorption of light can be enhanced by incorporating ZnO nanostructures, which act as scattering centres and hence, they increase the optical path length of light. Our work focuses on the investigation of light trapping mechanism of solar cells based on electrochemically grown ZnO nanorod and active layer of conjugated polymer P3HT and PCBM. The size and the structure of the ZnO nanorods are varied by changing the parameters of electrochemical deposition. Angle resolved scattering measurements are employed to investigate the amount of light scattered by the nanorods. These results are correlated to the performance of the solar cell determined from electrical measurements.

CPP 2.8 Mon 11:45 ZEU 222

Temperature-dependent molecular orientation of the organic semiconductor PTCDI-C₈: Optical and structural properties — ●SEBASTIAN BOMMEL^{1,2}, LINUS PITHAN², CHRISTOPHER WEBER², ANTON ZYKOV², GONZALO SANTORO¹, STEPHAN V. ROTH¹, JÖRG MEGOW², and STEFAN KOWARIK² — ¹Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Optical and structural properties of molecular materials are not only essential for the rational design of opto-electrical devices, but also for the understanding of intermolecular interactions. Here, we report on the structural and optical properties of the organic semiconductor PTCDI-C₈ investigated by temperature-dependent Grazing Incidence X-ray Diffraction (GIXD) and photoluminescence (PL) measurements. Our *in situ* studies yield a large impact of temperature on unit cell parameters and optical transitions. The energy of the optical transition E₁₀-E₀₁ in the PL spectra shifts from 1.80 eV for 273 K to 1.85 eV for 413 K. Furthermore, a rearrangement of the molecular ensemble was found, indicated by a large change of the beta-angle of the PTCDI-C₈ unit cell from 107° (273 K) to 102° (413 K). The influence of these structural changes, which are an indication for a change of molecular orientation with temperature, on the optical properties will be discussed in detail. Additionally, the structural and optical properties are supported by temperature-dependent molecular dynamics (MD) simulation based calculations.

CPP 2.9 Mon 12:00 ZEU 222

Highly Efficient Silicon/Polythiophene Hybrid Solar Cell Devices — ●MATTHIAS ZELLMIEER¹, JOHANNES FRISCH², SILVIA JANIEZ³, NORBERT KOCH², JÖRG RAPPICH¹, and NORBERT NICKEL¹ — ¹Helmholtz-Zentrum Berlin, Institut für Silizium Photovoltaik, Kekuléstr. 5, D-12489 Berlin — ²Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin — ³Fraunhofer-Institut für Angewandte Polymerforschung IAP, Abteilung Polymere und Elektronik, Geiselbergstr. 9, D-14476 Potsdam

Highly efficient hybrid solar cell devices based on crystalline silicon with three different solution processed polymer emitter layers are realized. The inorganic part of the device is optimized with a hole-selective back contact (BSF) and a low defect density hot water oxide ($D_{it}=2 \times 10^{-12} \text{ eV}^{-1} \text{ cm}^{-2}$), which provides the necessary wetting properties for the solution processed emitter layers. The applied polymer materials, e.g. poly(3-hexylthiophene-2,5-diyl) (P3HT), poly(3-[3,6-dioxahexyl]-thiophene) (P3DOT), and poly(3-[2,5,8-trioxanonyl]-thiophene) (P3TOT), differ mainly in the oxygen content in the side groups. Substituting the alkyl chains attached to the thiophene rings with ether groups leads to a modified layer formation during spin coating. The results of the optical, electrical and structural characterization of the polymer layers is correlated to the key figures in the final devices. The open circuit voltage V_{OC} increases from 0.3 V to 0.5 V and the short circuit current j_{SC} increases from 15.2 mA cm⁻² up to 28.3 mA cm⁻² in the sequence P3HT, P3DOT, P3TOT and results in a power conversion efficiency close to 10 % for a planar Si/P3TOT device.