

CPP 39: Organic Electronics and Photovoltaics IV (joint session CPP/HL/O/DS)

Time: Thursday 9:30–13:00

Location: H34

Invited Talk

CPP 39.1 Thu 9:30 H34

Influence of morphology on organic solar cell performance comparing crystalline diindenoperylene (DIP) and its amorphous derivative tetraphenylidibenzoperiflanthene (DBP) — STEFAN GROB, MARK GRUBER, ULRICH HÖRMANN, and WOLFGANG BRÜTTING — Institute of Physics, 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, the four 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. In contrast, the structural disorder in DBP combined with a little smaller optical gap leads to light absorption which is about eight times higher than in DIP, whereby the short-circuit current density almost doubles in corresponding solar cell devices. Moreover, open circuit voltages are high and - due to similar energy level alignments - comparable, by using the materials both as donor with C60 (0.9 V) and as acceptor with 6T (1.2 V). Based on these results, we discuss the influence of different film structure and morphology on electrical transport and device performance.

CPP 39.2 Thu 10:00 H34

Influence of fluorine content in manipulating the nanomorphology of PTB7:PC70BM bulk heterojunction systems — SHUAI GUO¹, JING NING¹, VOLKER KÖRSTGENS¹, YUAN YAO¹, CHEN LIN¹, STEPHAN ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany

Polymer-based photovoltaics have drawn tremendous attention in both basic research and application fields during the last decade. Here, the up-to-date highest efficient bulk heterojunction system PTB7 with varied fluorine content and the fullerene derivative PC70BM are thoroughly investigated. It is known that the amount of fluorine along the polymer chain strongly influences the film formation and therefore the solar cell performance. Additionally, it is of great interest to explore the effect of solvent additive 1,8-diiodooctane (DIO) on differently fluorinated films. To address the relation between the morphology and efficiency completely, a series of measurements have been done. The film surface structure is investigated by optical microscopy and AFM. The inner film structures, crystal orientation as well as the crystallinity are probed by advanced scattering techniques such as XRR, GISAXS and GIWAXS. By integrating all data, the three-dimensional morphology of the active layer is detected. Consequently, the different morphologies introduced by varying the fluorine content and the addition of DIO are determined and compared with the corresponding performance of these systems.

CPP 39.3 Thu 10:15 H34

Influence of nanostructural changes on the charge carrier dynamics in PTB7 based solar cells — ANDREAS ZUSAN¹, ANDREAS BAUMANN², JENS LORRMANN¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

For organic bulk heterojunction solar cells, the blend morphology is one of the most crucial parameters influencing the device performance. Inducing nanostructural changes by means of the use of processing additives is a common practice to increase the power conversion efficiency. Hence, understanding the effect of modified structural properties of organic layers on the charge carrier transport and lifetime is a key issue for further progress in organic photovoltaics. In this context, we applied our novel charge extraction technique OTRACE (Open Circuit Corrected Transient Charge Extraction) to high efficiency solar cells made from the low-bandgap polymer PTB7 in combination with PC70BM using the solvent additive diiodooctane (DIO). The results

show two different nongeminate decay regimes identified as a fast direct recombination of free polarons and a trap assisted decay. We find that the DIO induced alteration of the morphology significantly reduces the recombination order of the first regime, whereas it has no influence on the second part arising from the delayed emission of trapped charges. Our explanation based on a multiple-trapping-and-release approach clarifies the large impact of phase separation on charge carrier dynamics.

CPP 39.4 Thu 10:30 H34

Diffusion limited charge generation from fullerene excitons in low bandgap polymer solar cells — CLARE DYER-SMITH, IAN HOWARD, and FRÉDÉRIC LAQUAI — Max Planck Institut für Polymerforschung, Mainz, Germany

Organic solar cells with high power conversion efficiencies have been realised in recent years by the use of low bandgap polymers in combination with C70-based electron acceptors to provide good absorption coverage across the entire solar emission spectrum. Diffusion-limited charge generation from fullerene excitons has been observed in such blends, including the high-performance PTB7:PC70BM blend system which is the subject of the present study. We characterise the diffusion-limited charge generation from fullerene excitons in this system using transient absorption and photoluminescence spectroscopy. Fitting to a simple exciton quenching model allows us to determine the size of fullerene domains in the blend, showing quantitatively how blend morphology limits device performance, and allowing us to identify selection criteria for the optimum blend morphology in devices based upon light-absorbing fullerene acceptors.

CPP 39.5 Thu 10:45 H34

Impact of molecular weight on the intrinsic charge carrier mobility of Si-PCPDTBT:[C70]PCBM thin films — ANDREAS FRITZE¹, ANDREAS SPERLICH¹, ANDREAS ZUSAN¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

We investigated the influence of the molecular weight on the performance of solar cells from solution processed Si-PCPDTBT:[C70]PCBM blends. A significant increase in the short circuit current density j_{SC} was found with increasing molecular weight of the polymer. To explain this behavior, we performed transient microwave conductivity (TRMC) experiments and found much higher intrinsic mobilities in thin films based on the higher molecular weight donor. In order to distinguish between the influence of intra- and intermolecular charge transport on the obtained intrinsic TRMC mobility, we used two different solvents to influence the molecular environment in the film. We discuss our findings in view of the impact of the local order, influenced by the molecular weight on the performance of organic solar cells.

CPP 39.6 Thu 11:00 H34

Charge generation and recombination in PCPDTBT:PCBM and PSBTBT:PCBM bulk heterojunction photovoltaic blends — FABIAN ETZOLD, IAN HOWARD, MICHAEL MEISTER, and FRÉDÉRIC LAQUAI — Max Planck Research Group for Organic Optoelectronics, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present a comparative study of the photophysical processes leading to photocurrent generation and photocurrent loss in photovoltaic blends of the low-bandgap polymer PCPDTBT with PCBM and its silicon-substituted analogue PSBTBT with PCBM studied by Vis-NIR transient absorption pump-probe spectroscopy and variable time-delay double-pump photocurrent extraction experiments. Our experiments demonstrate that the power conversion efficiency of PCPDTBT:PCBM blends is largely limited by sub-nanosecond geminate recombination of interfacial charge-transfer states plus fast non-geminate recombination of free charges competing efficiently with charge extraction. In comparison photovoltaic blends of the silicon-substituted polymer PSBTBT with PCBM exhibit significantly less geminate recombination in conjunction with much slower non-geminate recombination of free charges leading in turn to substantially higher photocurrents and fill factors and thus overall increased photovoltaic performance. We also observed a pronounced excitation wavelength dependence of the pho-

tophysical processes occurring after excitation of either the polymer or the fullerene component of the blend at different photon energies. [1] F. Etzold et al., *J. Am. Chem. Soc.* 2012, 134 (25), 10569-10583.

15 min. break

CPP 39.7 Thu 11:30 H34

Charge Generation in PBDTPD:PCBM and Si-PCPDTBT:PCBM Solar Cells: The Influence of Excess Photon Energy and Electronic Energy Level Offsets — ●STEVE ALBRECHT¹, KOEN VANDEWAL², ALBERTO SALLES², and DIETER NEHER¹ — ¹University of Potsdam, Soft Matter Physics, Potsdam, Germany — ²Stanford University, Department of Materials Science and Engineering, Stanford, USA

In the last years a dramatic increase in organic solar cell efficiency has been reported with polymers and fullerene derivatives processed from solution. However, the fundamental process involved in the conversion of absorbed photons to free charges is still not fully understood. In this work, we use time delayed collection field (TDCF) [1] with variable excitation wavelength to gain insight into the effect of the excess photon energy on the quantum efficiency and field-dependence of free charge carrier generation. With two high efficiency model systems showing either field independent CT-state splitting (PBDTPD:PCBM) or a weak field-dependence of free charge formation (Si-PCPDTBT:PCBM), we show how the field-dependence changes with direct CT state excitation in the absorption region below the band-gap. Additionally, we show how generation and bimolecular recombination is affected when the fullerene derivative PCBM is exchanged by higher LUMO adducts ICMA, ICBA or ICTA with reduced driving force for CT-state splitting.

[1] Albrecht, S.; Janietz, S.; Schindler, W.; Frisch, J.; Neher, D., *Journal of the American Chemical Society* 134 (36), 14932 (2012).

CPP 39.8 Thu 11:45 H34

Sub-Bandgap Absorption in Polythiophene–Fullerene Heterojunctions: Experiment and Theory — ●WICHARD BEENKEN, FELIX HERRMANN, MARTIN PRESSELT, HARALD HOPPE, SVIATOSLAV SHOKHOVETS, GERHARD GOBSCH, and ERICH RUNGE — Technische Universität Ilmenau, Institut für Physik and Institut für Mikro- und Nanotechnologien, 98693 Ilmenau, Germany

Most high-performance organic solar cells base on P3HT/PCBM bulk-heterojunctions. Spectroscopy of the sub-bandgap region, i.e., below the bulk absorption of the individual components, provides unique opportunities to study interface-related properties. In order to characterize some of the unsettled spectral features, we applied quantum-chemical calculations of a oligothiophene–fullerene model complex, which in particular allow us to identify spectral signatures of charge-transfer excitons in the sub-bandgap absorption and external quantum efficiency.

CPP 39.9 Thu 12:00 H34

A new multiscale modeling method for simulating the loss processes in polymer solar cell nanodevices — ●ANTON PERSHIN, SERGI DONETS, and STEPHAN A. BAEURLE — Institute of Physical and Theoretical Chemistry, University of Regensburg, D-93040 Regensburg, Germany

The photoelectric power conversion efficiency of polymer solar cells is till now, compared to conventional inorganic solar cells, relatively low with maximum values ranging from 7% to 8%. This essentially relates to the existence of exciton and charge carrier loss phenomena, significantly reducing the performance of polymer solar cells. Here, we introduce a new computer simulation technique [1], which permits to explore the causes for the occurrence of such phenomena at the nanoscale and to design new photovoltaic materials with optimized opto-electronic properties. Using our approach, we find that the disjunction of continuous percolation paths leads to the creation of dead ends, resulting in charge carrier losses through charge recom-

bination. Moreover, we observe that defects are characterized by a low exciton dissociation efficiency due to a high charge accumulation, counteracting the charge generation process. Finally, by analyzing the photovoltaic behavior of the nanostructures under different circuit conditions, we demonstrate that charge injection at the electrodes determines the impact of the defects on the solar cell performance. [1] A. Pershin, S. Donets, S.A. Baeurle, *J. Chem. Phys.* 136, 194102 (2012).

CPP 39.10 Thu 12:15 H34

Morphology and Charge Transport in Polythiophene/PCBM Blends: Insight from Molecular Simulations — ●OLGA GUSKOVA¹, JULIA ROMANOVA², ANDREAS JOHN¹, PETER FRIEDEL¹, and JENS-UWE SOMMER^{1,3} — ¹Leibniz Institute of Polymer Research, Dresden, Germany — ²University of Namur, Namur, Belgium — ³TU Dresden, Dresden, Germany

Combined structural-computational approach to study the organic photovoltaic materials, namely mixtures of polythiophenes (donor, D) and [6,6]phenyl-C61-butyric acid methyl ester (acceptor, A) was applied. The quantum mechanical computational level was used (1) to improve the force field for subsequent molecular dynamics (MD) modeling, (2) to calculate the ionization energies, electron affinities, HOMO/LUMO energies and charge transfer characteristics of D/A pair. We have performed a large-scale all-atomistic MD simulation to investigate both the geometry of D/A interface between two crystals and the D/A blend morphology in self-organized systems (the ordering and molecular orientation, the formation of polythiophene paracrystals and PCBM-rich phases in amorphous regions of polythiophene).

CPP 39.11 Thu 12:30 H34

Electroabsorption spectroscopy on organic pin solar cells — ●ELLEN SIEBERT-HENZE, VADIM G. LYSSENKO, JANINE FISCHER, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photo-physik, George-Bähr-Str. 1, Dresden, Germany

The built-in voltage has a significant impact on the solar cell performance, but its origins are controversially discussed. In our work we determine the built-in voltage of small molecule organic solar cells based on the pin concept by electroabsorption spectroscopy (EA).

EA detects the change in absorption caused by an electrical field (Stark effect). A change in DC bias on the device results in a variation of the Stark signal. It is probed adding an AC voltage on top of the DC bias enabling the detection using a lock-in amplifier. Thus, the information about the built-in voltage can be evaluated.

As a model system, flat heterojunction solar cells containing C₆₀ as acceptor and MeO-TPD as donor material are investigated. The doping concentration of both the hole and the electron transport layer is modified and it is shown that there is an influence of the consequential change of their work functions on the built-in voltage. Both the short-circuit current as well as the fill factor increase for larger built-in voltages.

CPP 39.12 Thu 12:45 H34

First-principles calculations of the TCO–Organic interface in an OLED — ●ARNO FEY¹, PAUL ERHART², and KARSTEN ALBE¹ — ¹Fachbereich Material- und Geowissenschaften, Technische Universität Darmstadt, Darmstadt, Germany — ²Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

The ongoing development in the field of organic light emitting diode (OLED) technology and the continuously improvement towards higher efficiencies has created a need to understand the interaction between the different layers in an OLED. In this contribution we focus on the interface of the transparent conductive oxide (TCO) and the organic molecule. The interaction between the polar and hydrophilic oxide surface on the one side and the organic and non-polar thin film on the other side determines the growing of the organic film and therefore directly influences the conductivity. The calculations based on the density functional theory (DFT) were carried out using the Vienna ab initio simulation Package (VASP) with Generalized Gradient Approximations (GGA).