

DS 24: Organic Electronics and Photovoltaics CPP-II (jointly with CPP, HL, and O)

Time: Tuesday 10:30–13:00

Location: ZEU 222

Topical Talk

DS 24.1 Tue 10:30 ZEU 222

Modelling charge transport in organic semiconductors —

•DENIS ANDRIENKO — MPI for Polymer Research, Mainz, Germany

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes,¹ perylenediimides,² tri-angulantly shaped polyaromatic hydrocarbons,³ Alq3,⁴ polypyrrole and a variety of organic crystals. Simulations are performed using a package developed by Imperial College, London and MPI for Polymer Research, Mainz (www.votca.org⁵). This package combines: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1]. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, *Phys. Rev. Lett.*, 98, 227402, 2007[2]. V. Marcon, W. Pisula, J. Dahl, D. W. Breiby, J. Kirkpatrick, S. Patwardhan, F. Grozema, D. Andrienko, *J. Am. Chem. Soc.*, 131, 11426, 2009[3]. X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, and K. Müllen, *Nature Materials* 8, 421, 2009[4]. A. Lukyanov, D. Andrienko, *Phys. Rev. B*, 82, 193202, 2010[5]. V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, *J. Chem. Theor. Comp.* 5, 3211, 2009

DS 24.2 Tue 11:00 ZEU 222

Performance of density functional theory for donor-acceptor systems: a case study for TTF and TCNQ molecules —•VIKTOR ATALLA¹, MINA YOON^{1,2}, and MATTHIAS SCHEFFLER¹ — ¹Fritz-Haber-Institut der MPG, Berlin, Germany — ²Oak Ridge National Laboratory, USA

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing properties. However, from a theoretical point of view these materials are challenging because they are often composed of donor-acceptor systems, for which density-functional theory (DFT) with state-of-the-art exchange-correlation (XC) functionals is often suspected to fail. Here we study the performance of DFT in describing electron affinities, ionization potentials, and charge transfer for clusters of the prototypical electron donor molecule TTF and acceptor molecule TCNQ.

For the individual molecules we calculate the dependence of the HOMO and LUMO levels on the fraction of exact exchange and the screening length [1]. We find that conventional semilocal and hybrid XC functionals severely underestimate HOMO-LUMO gaps. For weakly bound TTF-TCNQ dimers all investigated XC functionals consistently give charge transfer from the donor to the acceptor, however the amount of transferred charge is strongly functional dependent - in particular all semilocal functionals have significant artificial charge transfer in the asymptotic limit.

[1] A. Krukau *et al.*, *J. Chem. Phys.* **125**, 2006

DS 24.3 Tue 11:15 ZEU 222

Sub-Bandgap Absorption in Polymer-Fullerene Solar Cells —•MARTIN PRESSELT¹, FELIX HERRMANN¹, MARCO SEELAND¹, MAIK BÄRENKLAU¹, ROLAND RÖSCH¹, WICHARD J. D. BEENKEN², ERICH RUNGE², SVIATOSLAV SHOKHOVETS¹, HARALD HOPP¹, and GERHARD GOBSCH¹ — ¹Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — ²Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

We present external quantum efficiency (EQE) studies of P3HT:PCBM based bulk heterojunction polymer solar cells with improved intensity resolution in the sub-bandgap (SBG) region, i.e. the energy range below the optical bandgaps of the pristine materials. Varying the P3HT:PCBM blending ratio, we find that in addition to a Gaussian profile an exponential tail is needed for a quantitative description of the SBG EQE spectra. To gain insights into the origin of the single contributions, absorption and emission spectra covering several decades of intensity and SBG EQE signals are discussed in detail.

DS 24.4 Tue 11:30 ZEU 222

Quantitative analysis of optical spectra and solar cell performance of P3HT:PCBM blends —

•SARAH T. TURNER, PATRICK PINGEL, ROBERT STEYRLLEUTHNER, and DIETER NEHER — Institute of Physics and Astronomy, University of Potsdam, Germany

The properties of solar cells made from a blend of regioregular poly(3-hexylthiophene) (P3HT) with [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM) are known to depend largely on the layer morphology. Here, we present the results of optical studies on P3HT:PCBM blends coated from chloroform and dichlorobenzene with subsequent thermal annealing. A recently established analytical model developed by Spano for the absorption of weakly interacting H-aggregates was used to obtain information about the fraction of crystallized chains, the width of the aggregates, and the energetic disorder in the P3HT phase [1]. In terms of an increased aggregate width and a decreased energetic disorder in the P3HT phase, thermal annealing was found to have little effect on the films prepared from dichlorobenzene and an appreciable effect on the films prepared from chloroform. The results from the model were compared with the performance of solar cell devices and single-carrier devices with the same active layer. Most importantly, the initial increase in P3HT aggregate size upon thermal annealing showed a good correlation with an increase in hole mobility. Further increases in solar cell device performance at higher annealing temperatures were correlated with a decrease in P3HT energetic disorder and an increase in PCBM aggregation.

[1] F.C. Spano, *J. Chem. Phys.* 2005, 122, 234701.

DS 24.5 Tue 11:45 ZEU 222

Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells —•ANDREAS BAUMANN¹, TOM J. SAVENIJE³, DHARMAPURA H. K. MURTHY³, MARTIN J. HEENEY⁴, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — ³Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, 2628 BL Delft, The Netherlands — ⁴Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

The morphology of a bulk heterojunction solar cell plays an important role in the dynamics of charge carriers, whereas the donor-acceptor ratio have a great impact on the extent of phase segregation. A fine phase intermixing is believed to be beneficial for an efficient photogeneration. However, the charge transport is strongly related to percolated pathways to the electrodes. We studied the influence of phase segregation on the dynamics in the blend system poly(2,5-bis(3-dodecyl thiophen-2-yl) thieno[2,3-b]thiophene) (pBTCT) mixed with [6,6]-phenyl-C₆₁-butyric acid methyl ester. We used the technique of charge extraction by linearly increasing voltage and transient microwave conductivity to study the macroscopic and microscopic transport properties, respectively. We found an enhanced geminate recombination in the 1:1 ratio blends due to fine phase intermixing, whereas extensive phase segregation in the 1:4 ratio led to an efficient polaron pair dissociation.

DS 24.6 Tue 12:00 ZEU 222

Charge separation at molecular donor-acceptor interfaces: correlation between interface morphology and solar cell performance —

•ANDREAS OPITZ, JULIA WAGNER, MARK GRUBER, ULRICH HÖRMANN, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combinations of organic electron and hole conductive materials are widely used for ambipolar charge carrier transport and donor/acceptor photovoltaic cells. Thereby the efficiency of these excitonic solar cells is correlated to the morphology of the interface between the donor and the acceptor materials.

In this contribution we show the effect of crystallization behaviour on molecular bulk and planar heterojunction solar cells [1]. Different donor (copper phthalocyanine – CuPc, diindenoperylene – DIP) and acceptor (Fullerene – C₆₀, per-fluorinated copper phthalocyanine – F₁₆CuPc) materials are analysed for their growth morphology in planar and mixed films as well as for their performance in photovoltaic cells. The morphology of the blended layer ranges from molecularly

mixed films in the case of the two phthalocyanines to phase-separated films when mixing CuPc or DIP with C₆₀. A corrugated interface is found for bilayered structure of DIP/C₆₀ [2]. Additionally a good crystallization behaviour of DIP improves the solar cell performance even for its lower absorption in comparison to CuPc.

[1] A. Opitz et al., IEEE J. Sel. Top. Quant. (2010), early view.

[2] J. Wagner et al. Adv. Func. Mater. (2010), early view.

DS 24.7 Tue 12:15 ZEU 222

Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — ●CHETAN RAJ SINGH¹, MICHAEL SOMMER^{2,3}, MARCEL HIMMERLICH¹, ANDRÉ WICKLEIN³, STEFAN KRISCHOK¹, MUKUNDAN THELAKKAT³, and HARALD HOPPE¹ — ¹Institute of Physics, Ilmenau University of Technology, Germany — ²Department of Chemistry, University of Cambridge, United Kingdom — ³Applied Functional Polymers, University of Bayreuth, Germany

We present the thorough optimization of block copolymer (BCP) based polymer solar cells utilizing a blend of a self-assembling P3HT-bPPerAcr BCP and an PPerAcr acceptor homopolymer. As an effect of increasing acceptor content in the block copolymer/homopolymer blend, we observe a continuous rise in the open circuit voltage (Voc) and the short circuit current (Isc) leading to an overall improved photovoltaic performance. The improved performance with increasing acceptor content is attributed to (a) an increase of the acceptor domain size leading to improved charge transport and to (b) a reduced recombination of charge carriers at the cathode interface due to the surface segregation of the acceptor. The surface segregation of the acceptor is identified by atomic force microscopy and X-ray photoelectron spectroscopy. Furthermore we show that by deliberately introducing an acceptor buffer layer at the cathode interface, we are able to control Voc at relatively high values (~ 640 mV), independently of the bulk heterojunction morphology underneath.

DS 24.8 Tue 12:30 ZEU 222

Triplet Excitons and Cations in dicyanovinyl end-capped quaterthiophenes with varying side chain length — ●CHRISTIAN KOERNER¹, HANNAH ZIEHLKE¹, ROLAND FITZNER², EGON REINOLD², PETER BÄUERLE², KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden — ²Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Dicyanovinyl end-capped oligothiophenes (DCV-nT) are highly suitable for systematical investigations of energy and charge transfer processes in donor-acceptor blends because of the tunability of electronic

and morphological properties by varying e.g. length of backbone or side chains. Moreover, it has been shown to work well as absorber in small molecule organic solar cells (OSC) achieving up to 5.2% power conversion efficiency (PCE) for DCV-5T in a bulk heterojunction (BHJ) device¹.

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (μ s-ms) excited states (triplet excitons, cations) after photoexcitation of DCV-nT:C₆₀ blends. With PIA, their generation and recombination behaviour can be investigated. Here, we report our results obtained on a series of DCV-4Ts with varying side chains from none to methyl side chains which supposedly mainly influences the morphology of the thin film. We complement our studies by exploring the potential of these materials as absorber layer in planar and BHJ solar cells. For example, DCV-4T without side chains gives an open circuit voltage of 1V and PCEs of 1.9% in a BHJ solar cell with C₆₀.

¹ Fitzner et al., Adv. Func. Mat., accepted

DS 24.9 Tue 12:45 ZEU 222

Surface structure of organic heterojunction solar cells — ●M. ZERSON¹, E.-C. SPITZNER¹, C. RIESCH¹, A. SPERLICH², H. KRAUS², A. FÖRTIG², C. DEIBEL², V. DYAKONOV², R. LOHWASSER³, M. THELAKKAT³, and R. MAGERLE¹ — ¹Chemische Physik, TU Chemnitz — ²Experimental Physics VI, Julius-Maximilians-University of Würzburg — ³Makromolekulare Chemie I, Univ. Bayreuth

In organic heterojunction solar cells based on P3HT and PCBM, the charge transfer within the active layer as well as the charge transport towards the electrodes are determined by the electronic properties of the interfaces and their microstructure. The surface of semicrystalline polypropylene has been shown to be covered by a thin layer of amorphous material. We aim at investigating potential similarities between organic semiconductors for photovoltaics. We report on 3D depth profiling of the surface structure of different types of P3HT and blends of P3HT with PCBM using amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance curves, the tip indentation into the soft (compliant) amorphous surface layer is measured. This spatial information serves as depth coordinate for reconstructing high resolution cross sections and 3D depth profiles of the top 10 nm of the specimen. Furthermore, the shape of the unperturbed (true) surface and the thickness of the amorphous top layer are determined. The latter is found to be between 4 and 10 nm thick, depending on the type of material and the sample preparation conditions (thermal and solvent annealing). We discuss the impact of the thickness of the amorphous top layer on the efficiency of organic solar cells.