HL 35.2 Tue 11:00 ZEU 222
Performance of density functional theory for donor-acceptor systems: a case study for TTF and TCNQ molecules —

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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 bonded clusters (dimers and trimers) we 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.


HL 35.3 Tue 11:15 ZEU 222
Sub-Bandgap Absorption in Polymer-Fullerene Solar Cells —

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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.

HL 35.4 Tue 11:30 ZEU 222
Quantitative analysis of optical spectra and solar cell performance of P3HT:PCBM blends —

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The properties of solar cells made from a blend of regiorregular 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 chlorobenzene and chloroform 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 chlorobenzene 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.


HL 35.5 Tue 11:45 ZEU 222
Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells —

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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 gemicate 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.

HL 35.6 Tue 12:00 ZEU 222
Charge separation at molecular donor-acceptor interfaces: correlation between interface morphology and solar cell performance —

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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 F3CuPc) 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.


HL 35.7 Tue 12:15 ZEU 222
Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — •Chetan R. Singer1, Michael Sommer2,4, Marcel Himmerlich1, André Wücklen3, Stefan Krischok1, Mukundan Thelakkat4, and Harald Hoppe3 — 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-b-PPerAc BCP and an PPerAc 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.

HL 35.8 Tue 12:30 ZEU 222
Triplet Excitons and Cations in dicyanovinyl end-capped quaarterthiophenes with varying side chain length — •Christian Koerner1, Hannah Ziehlke1, Roland Fitzner2, Egon Reinold2, Peter Bauerle2, 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) device.

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (µs-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-4T 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 1 V and PCEs of 1.9% in a BHJ solar cell with C60.

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

HL 35.9 Tue 12:45 ZEU 222
Surface structure of organic heterojunction solar cells — •M. Zerön1, E.-C. Spitzner1, C. Riesch1, A. Spierlich2, H. Kraus2, A. Förtig2, C. Deibel3, V. Dyakonov2, R. Lohwasser3, M. Thelakkat3, and R. Magele3 — 1Chemische Physik, TU Chemnitz — 2Experimental Physik 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 unper-