HL 61: Organic electronics and photovoltaics III (organized by CPP)

Polymers, Solar Cells, OFETs, OLEDs, Spectroscopy

Time: Wednesday 9:30–12:45 Location: ZEU 260

HL 61.1 Wed 9:30 ZEU 260

Structural Degradation of Polymer Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Jendrzejewski[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department - LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

A major challenge in organic photovoltaics (OPV) is to elongate their lifetimes. Several mechanisms of organic solar cell degradation have been proposed in literature within the last years. However, insufficient research has been done on determining the role of transitions in the nanomorphology of the active layer of bulk-heterojunction (BHJ) polymer solar cells as an aspect of degradation. These transitions would strongly affect the properties of solar cells since the active layer morphology plays a crucial role in the energy conversion process.

We present a direct evidence of morphological degradation on a nanometer scale in polymeric solar cells by simultaneous in-situ GISAXS and current-voltage tracking on a running P3HT:PCBM solar cell. The loss of short-circuit current with time is fully modeled by the observed morphological transitions [1].

[1] C. J. Schaffer et al., *Adv. Mater.* **2013**, DOI: 10.1002/adma.201302854

HL 61.2 Wed 9:45 ZEU 260

Controlling nanomorphology in bulk heterojunction solar cells via addition of third component — •Eva M. Herzig[1], Ammara R. Akhtar[2], Anna Naumann[2], Shuai Guo[2], Gregory Tainter[2], Jianqi Zhan[2], Jan Perlich[3], Stephan V. Roth[3], Christine M. Papadakis[2], and Peter Müller-Buschbaum[2] — [1]TU München, MSE, Lichtenbergstr. 4, 85748 Garching — [2]TU München, Physik-Department,, James-Franck-Str. 1, 85748 Garching — [3]DESY, Notkestr. 85, 22603 Hamburg

Nanomorphology and effciency of organic solar cells are closely linked. It is therefore desirable to have control over the self-assembly process responsible for the morpholgy formation of the active material. Employing grazing incidence small and wide angle x-ray scattering(GISAXS & GIWAXS) as well as spectroscopy and microscopy methods allows us to characterize organic thin films on the nanoscale with high statistical relevance. Using these methods we thoroughly investigate the morphological changes upon the addition of a third polymeric component showing that the self-assembly process is altered. We find that the amount of the third component controls the phase separation in the bulk heterojunction active layer. Adjusting the preparation route to support crystallization of the active material leads to an increased solar cell performance for a tuned ternary solar cell system.

HL 61.3 Wed 10:00 ZEU 260

Layer by layer solution processing of nanostructured all-polymer solar cells — •Thomas Pfadler, Mihael Coric, Jonas Weickert, Karl-Philipp Strunk, and Lukas Schmidt-Mende — University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is focusing on nanoimprint lithography (NIL), a low-cost lithographic method for high-throughput patterning applicable to organic semiconductors. This technique can be used to tailor an organic solar cells active material on a nanometer scale. A promising application of NIL aims to control the nanostructure of a donor-acceptor interface in an organic all-polymer device. The electron accepting polymer is structured. A stiff polymer network featuring a nanostructured topography is developed by the usage of a photoactivable crosslinker molecule (sFPA). The crosslinked polymer matrix is not dissolved during spin-coating the donor polymer allowing fully solution processed device fabrication with controlled nanostructured donor-acceptor interfaces. Target of this approach is to investigate nanostructured bi-layer devices with controlled interfaces to finally enhance the overall efficiency by maximizing the interfacial area, increasing the exciton separation yield and ensuring direct pathways to the electrodes.

HL 61.4 Wed 10:15 ZEU 260

The role of processing additives in Organic Solar Cells after the preparation process — •Stefan Väth[1], Andreas Baumann[1], Andreas Sperlich[1], Carsten Deibel[1], Milutin Ivanovic[2], Heiko Peisert[2], Thomas Chassé[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Eberhard Karls University Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Processing additives are widely used in the preparation of new high performance bulk heterojunction organic solar cells to improve the power conversion efficiency (PCE) significantly. They act as selective solvent for fullerenes and are therefore improving the morphology of the active area. Nevertheless the question wether or not these co-solvents remain in the organic solar cells after the preparation process occurs. This question could be solved by investigating blends consisting of the material system PTB7:PC$_{60}$BM processed with the additives diiodooctane (DIO), octanedithiol (ODT) and without additives as reference. We used the spin sensitive measurement technique light induced Electron Paramagnetic Resonance (LESR) to distinguish between positive polarons on the polymer and negative charges on the fullerene by their different g-factors. Together with Photoelectron Spectroscopy (PES) measurements we could show that the additive DIO remains partly inside the active layer of organic solar cells even after a high vacuum preparation step. We propose that they do not only lead to an improved morphology, but also to a doping effect.

HL 61.5 Wed 10:30 ZEU 260

Radiative and non-radiative recombination in organic solar cells — •Kristofer Tvingstedt, Philip Pelchmann, Vladimir Dyakonov, and Carsten Deibel — Experimental Physics VI Julius Maximilian University of Würzburg 97074 Würzburg

Although several organic solar cells has reached close to unity internal quantum efficiency at short circuit conditions, the open circuit voltage is still very far from its potential upper limit due to substantial charge recombination of various types, which remains to be accurately determined. In this work we evaluate the limiting mechanisms in OPVs by employing complementary steady state measurements of recombination as a function of charge carrier density by thoroughly evaluating the diode ideality factor. The diode ideality is directly related to the order of recombination and we first assess it via light intensity dependent open circuit voltage characterization under the influence of a varying temperature. We focus our study on the ratio between radiative and non-radiative recombination via the interfacial charge transfer state as determined by absolute CT electroluminescence efficiency measurements, also as a function of temperature. The charge transfer state governs the radiative recombination in OPV bulk heterojunctions and is therefore crucial to evaluate in this context. Improving the radiative efficiency of OPVs will substantially increase the open circuit voltage and eventually put these promising photovoltaic converters in efficiency parity with their inorganic counterparts.

HL 61.6 Wed 10:45 ZEU 260

Electronic Structure of Fullerene Heterodimer in Bulk-Heterojunction Blends — •Andreas Sperlich[1], Oleg G. Poluektov[2], Jens Niklas[2], Kristy L. Mardis[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg and ZAE Bayern, 97074 Würzburg — [2]Chemical Sciences and Engineering Division, ANL, Argonne, Illinois 60439, USA — [3]Department of Chemistry and Physics, Chicago State University, Chicago, Illinois 60628, USA

To increase performance of organic solar cells, the optimization of the electron-accepting fullerenes has received less attention. Here, we report an electronic structure study of a novel covalently linked C$_{60}$-C$_{70}$-heterodimer in blend with the polymer PCDTBT. Upon optical excitation of polymer:heterodimer solid films, the electron is shared between both C$_{60}$ and C$_{70}$ cages. In contrast, in the solution the electron is localized on one half of the dimer. Electronic structure calculations reveal that for the heterodimer two nearly iso-energetic minima exist, essentially the cis and trans conformers. These conformers have different edge-to-edge distance between the two cages and therefor the electron is either shared between two dimer halves (cis) or localized on one half of the heterodimer (trans). By comparison with the experimental data, we conclude that the cis conformation is preferable in films, and the trans conformation in solution. These findings demonstrate how electronic coupling of the fullerene acceptor molecules is influenced by their packing in blends, which may have an impact on the charge carrier generation efficiency in solar cells.

15 min. break

HL 61.7 Wed 11:15 ZEU 260

Cyclic potential growth mechanism for electropolymerized polythiophenes as anode buffer layers in P3HT-PCBM solar cells — •Sidhant Bom, Marlis Ortel, and Veit Wagner — Research Center for Functional Materials and Nanomolecular Science, Jacobs University, Bremen, Germany

A new method for electro-polymerization of polythiophenes as anode buffer layer (ABL) is presented. The ABL is used in a bulk-heterojunction solar cell with P3HT-PCBM as active material. Electro-polymerized thiophenes (ePT) are grown electrochemically with a standard three electrodes system on conductive contacts. We find a distinct impact of the time variation of the growth potential on the obtained layer properties. A new time dependent cyclic potential electro-polymerization method is systematically compared to a standard constant potential method. AFM topography reveals that a uniform homogeneous film of ePT is obtained by the time dependent cyclic potential growth method. The devices were fabricated with a 10 nm ePT between the active layer and PEDOT:PSS with aluminum as cathode. With a cyclic potential method, about 20% enhancement in short circuit current was observed in contrast to 10% enhancement with constant potential method. Improvements by the ePT layer are attributed to better band alignment of the HOMO levels and a LUMO offset of 0.2eV which gives its electron blocking characteristics. In summary, the cyclic potential method results in a better quality of ePT layers with good homogeneity and area coverage leading to further improvements in device performance.

HL 61.8 Wed 11:30 ZEU 260

Intrinsic charge carrier mobility in PCDTBT:PC$_{71}$BM blend thin films investigated by simultaneous transient absorption and transient microwave conductivity measurements — •Andreas Fritze[1], Jeremias Weinrich[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

PCDTBT is a promising low-bandgap polymer for photovoltaic applications that has demonstrated unique recombination dynamics compared to the model P3HT system. Usually, the recombination dynamics in organics blends is expected to be proportional to the macroscopic charge carrier mobility, which is influenced by trapping and therefore potentially depends on the charge carrier concentration. For PCDTBT blends, we want to determine if the recombination dynamics are indeed governed exclusively by the low macroscopic mobility or if it is dominated by the, high local mobility. Therefor, we performed simultaneous measurements of transient absorption (TAS) and transient microwave conductivity on PCDTBT:PC$_{71}$BM thin films on a 10 ns to 1 ms time scale. TAS probes the charge carrier density, whereas the microwave experiment is sensitive to the intrinsic, high frequency conductivity. By investigating the charge carrier dynamics and conductivity at different laser pump intensities and temperatures, we can separate the effects of mobility relaxation from carrier concentration dependent mobility in order to understand the dominant loss mechanism in organic solar cells.

HL 61.9 Wed 11:45 ZEU 260

On the role of the effectiv mass, ground state complexes and interfacial dipoles on exciton dissocitation in organic donor-acceptor systems — •Anna Köhler — University of Bayreuth, Bayreuth, Germany

Efficient exciton dissociation at a donor-acceptor interface is a necessary condition for obtaining high efficiency polymeric solar cells. Despite its importance, this step is still not fully understood. A central question is how and why, after photoexcitation of the donor and transfer of an electron onto the acceptor, the the e-h pair can overcome their considerable mutual Coulomb potential. Possibilities that are currently discussed include the degree of delocalization of both an exciton and a charge in a conjugated polymer, ground state charge transfer complexes as well as interfacial dipoles that may exist at the donor-acceptor interface in the ground state, and the degree of energetic and structural order/disorder. In this talk I will show how we combine insight gained from ultrafast pump-probe spectroscopy, field dependent photocurrent measurements, photoemission measurements and modeling to assess which factors control the dissociation process.

HL 61.10 Wed 12:00 ZEU 260

Non-photochemical self-quenching mechanism in conjugated polymers revealed by control of chain length and morphology — •Florian Steiner, Jan Vogelsang, and John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D- 93040 Regensburg

Unraveling the complex photophysics of multichromophoric systems like conjugated polymers (CPs) is an ongoing interdisciplinary task. Some of the pressing questions in CP photophysics are: (i) what unit absorbs and emits the light in a CP? (ii) What processes take place between the absorption and emission event? And (iii) what is the interplay between excitation energy transfer between chromophores and non-radiative fluorescence decay? Answering these questions will lead to a fundamental understanding of the photophysics of CPs, which in turn can highlight important loss mechanisms regarding the efficiency in CP-based devices, such as self-quenching.

We illustrate that control of size and morphology in combination with several single-molecule techniques leads to a universal picture of the self-quenching mechanism in CPs by addressing these questions. As a model system we chose the device-relevant prototypical CP poly(3-hexylthiophene). Morphological control, combined with well-defined sub-populations of different sizes, enabled us to correlate a diverse set of photophysical observables (brightness, emission polarization, emission spectra, photon antibunching) with each other and the size. Finally, the increasing fluorescence self-quenching with size and morphological order is rationalized with a comprehensive photophysical model.

HL 61.11 Wed 12:15 ZEU 260

Conformations and electronic structure of Oligo-PPEs Investigated by Pulsed Electron Paramagnetic Resonance Spectroscopy — Patrick Korf, Friederike Schütze, Christian Hintze, Stefan Mecking, and •Malte Drescher — Department of Chemistry, University of Konstanz, Germany

Poly(para-phenyleneethynylene)s (PPE) are versatile polymers that are synthetically easily accessible.

Owing to their application in organic electronics and cell microscopy their microscopic and electronic properties are of high interest.

Herein we report the investigation of the electronic structure including the photo-excited triplet state of rod-like Oligo-PPEs. The lifetime, relaxation rates and populations of the triplet sublevels are quantitatively analyzed at cryogenic temperatures in a glassy toluene matrix via time-resolved EPR with synchronized UV laser flash excitation. The photo-physical properties are studied depending on the size of the delocalized π-electron system by varying the number of repeat units in the Oligo-PPEs.

In addition, their microscopic material properties are studied in particles with confined size constituted by block coplymers of PEGylated Oligo-PPEs. The molecular conformation is investigated by EPR distance measurements in solution, in bulk material as well as in particles. The data suggest that the rod-like Oligo-PPEs are present in a collapsed state in the particles.

HL 61.12 Wed 12:30 ZEU 260

Structural and electrical characterization of Hex-5T-Hex oligothiophene thin films during film formation — •Eduard Mikayelyan[1], Linda Grodd[1], Ullrich Pietsch[1], Artem. V. Bakirov[2], Maxim. A. Shcherbina[2], Sergei N. Chvalun[2], and Souren Grigorian[1] — [1]University of Siegen — [2]Enikolopov Institute of Synthetic Polymeric Materials of Russian Academy of Sciences

Organic semiconductors are attractive for electronics due to the low cost processing methods and their high electrical conductivity. Thiophene based polymers and oligomers are demonstrating relatively high mobility, excellent luminescence properties which used for application in solar cells, radio-frequency identification, etc. [1, 2]. We have investigated the thiophene based oligomer Hex-5T-Hex. Structural characterization has been performed by grazing incidence x-ray diffraction (GIXD)method, in particular we probed the crystallite orientations in prefabricated thin films. The 3D structure of Hex-5T-Hex oligomer evaluated from the in-plane (010), (020) and (021) reflections is consistent with 2D structure suggested from 5T based oligomer self-assembled monolayer (SAM) [3]. Additionally, we found the (100) and (100)' reflections in out-of-plane direction characterizing two different stacking along thiophene backbone axis. In order to correlate the structural properties of oligothiophene thin films with the electrical characteristics both properties were probed simultaneous during film formation. This work was supported by BMBF, project number 05K10PSC.