

CPP 41: Organic Electronics and Photovoltaics IV: OPV (joint session CPP/DS/HL, organized by CPP)

Time: Wednesday 15:00–18:30

Location: ZEU 260

Invited Talk CPP 41.1 Wed 15:00 ZEU 260
The role of incoherent hopping in the photogeneration of charges in organic semiconductors — ●ANNA KÖHLER — University of Bayreuth, 95400 Bayreuth, Germany

We demonstrate that efficient and nearly field-independent charge separation in organic planar heterojunction solar cells can be described by an incoherent hopping mechanism that can be modelled by kinetic Monte Carlo simulations that include the effect of on-chain delocalization. We address, first, the issue of differentiating between geminate and nongeminate recombination in solar cells. (Adv. Funct. Mater. 2016, DOI: 10.1002/adfm.201604906) We show that a reduced fill factor and the appearance of an s-shaped I-V curve even at low light intensities results from geminate recombination due to the back diffusion of holes toward their siblings at the donor-acceptor interface rather than to charge accumulation at the donor-acceptor interface. Second, we consider how optical excitation of C60 and PCBM contribute to the photogeneration of charge carriers. (J. Phys. Chem. C 2016 DOI: 10.1021/acs.jpcc.6b0847). We find that intrinsic photogeneration starts at a photon energy of about 2.25 eV, i.e., about 0.4 eV above S1. It originates from charge transfer type states that can autoionize incoherently via thermalization before relaxing to S1 state, in the spirit of Onsager's 1938 theory.

CPP 41.2 Wed 15:30 ZEU 260
Charge separation and recombination in PBTT-T/fullerene blends and solar devices — ●ELISA COLLADO FREGOSO¹, JONA KURPIERS¹, SAMANTHA HOOD², IVAN KASAL², JAMES DURRANT³, and DIETER NEHER¹ — ¹Institut für Physik und Astronomie, Potsdam University, Potsdam-Golm, Germany — ²Centre for Quantum Computation and Communication Technology, The University of Queensland, Brisbane, Australia — ³Centre for Plastic Electronics, Department of Chemistry, Imperial College London, UK

Organic solar cells, particularly polymer/fullerene solar cells, are an important area of scientific research on the generation of sustainable and renewable energy. However, further optimization of solar device efficiency is still needed to reach commercialization.

In this talk, the relationship between active layer nanostructure and charge separation and recombination kinetics in thin films and solar devices fabricated with mixtures of PBTT-T/fullerene will be established. Via a combined theoretical and experimental kinetic study using Transient absorption spectroscopy (TAS) and Time-delayed collection field (TDCF) we clearly establish the effect of an intermixed versus a more flat interface towards the separation of bound charges and charge recombination regimes. This is further correlated with device performance, thus showing the importance of careful blend nanostructure control.

CPP 41.3 Wed 15:45 ZEU 260
Electron Affinity and Charge Trapping in Ternary Fullerene-based Donor:Acceptor Films for Organic Photovoltaics — ●MICHAEL AUTH¹, MICHAEL BRENDEL¹, ANDREAS SPERLICH¹, STEPHAN VÄTH¹, JENS PFLAUM^{1,2}, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Fullerene materials for organic photovoltaics (OPV) are highly expensive, due to their elaborate purification. To determine if this step is necessary to a high degree, we investigate the influence of fullerene mixtures, i.e. unpurified fullerenes, in ternary OPV materials. As the molecule's electron affinity determines where charge carriers reside, it also determines if unintentional molecules act as trap sites. Since electron paramagnetic resonance (EPR) addresses localised charges, we investigate photo-induced charge transfer via EPR in correlation with solar cell parameters (V_{OC} , J_{SC} , PCE). For polymer-fullerene blends we used the conjugated polymers P3HT or PTB7, together with the soluble fullerene derivatives PC₇₀BM, PC₆₀BM and IC₆₀BA. As comparison, we furthermore investigated solar cell absorbers made of various vacuum deposited mixtures of C₇₀ and C₆₀ fullerenes on top of Diindenoperylene (DIP). For all configurations we compare the redistribution of electrons in the fullerene phase with the corresponding stoichiometry to determine electron affinity differences. In conjunction

with solar cell parameters we are then able to determine the influence of unpurified fullerenes upon OPV.

CPP 41.4 Wed 16:00 ZEU 260
Role of trapped and free charges on the recombination in a low band-gap organic solar cell — ●STEFFEN ROLAND¹, ANTONIO FACCHETTI², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — ²Northwestern University, Department of Chemistry, Evanston, IL-USA

While the role of traps on the transport of photogenerated charges has been analyzed in detail in the literature, the effect of energetic disorder on the rate of non-geminate recombination is yet not very clear. In this talk a new comprehensive approach of how to treat recombination in energetically disordered organic solar cells is proposed. Charge extraction techniques are used to examine the recombination dynamics of a typical organic solar cell (PMDPP3T:PCBM) in detail. While temperature dependent steady-state charge extraction experiments predict a significant amount of trapped charges, it is found that the recombination current (J_R) is dominated by a bimolecular process. A model is introduced in which free charges (outside the Fermi-gap) that contribute to J_R are discriminated from trapped charges (inside the Fermi-gap), which do not contribute to J_R . The free charge carrier recombination coefficient is determined by time delayed collection field measurements and used to accurately fit the measured JV-characteristics over a wide range of light intensities. These results prove that in this system, although charges undergo trapping, the recombination current is dominated by free bimolecular carrier recombination. This work sheds new light on the influence of trapped charges on the recombination process, a topic that has yet remained controversial within the field.

CPP 41.5 Wed 16:15 ZEU 260
Recombination Dynamics and the Role of Space Charge Effects in Organic Photovoltaics — ●MARTIN STOLTERFOHT¹, ARDALAN ARMIN², SAFA SHOAEI¹, BRONSON PHILIPPA³, PAUL MEREDITH², and DIETER NEHER¹ — ¹University of Potsdam, Potsdam-Golm, Germany — ²The University of Queensland, Brisbane, Australia — ³James Cook University, Cairns, Australia

The origin of photocurrent losses in the power-generating regime of organic solar cells (OSCs) remains a controversial topic, although recent literature suggests the importance of bimolecular recombination in determining the bias dependence of the photocurrent. Here we studied the steady-state recombination dynamics in OSCs with different hole mobilities from short-circuit to maximum power point (Adv. Energy Mater. DOI: 10.1002/aenm.201601379). We show that in this bias regime, first-order recombination outweighs bimolecular recombination of free charges. We demonstrate that the first-order losses increase with decreasing slower carrier mobility and attribute them to recombination of photogenerated and injected charges and/or geminate recombination. We also present how the competition between bimolecular recombination and extraction can be described using a simple figure of merit under consideration of space charge effects (J. Phys. Chem. Lett. DOI: 10.1021/acs.jpcclett.6b02106). The experimental results obtained on 25 different OSCs represent a conclusive understanding of bimolecular recombination and allow to minimize these losses for given device parameters. Nevertheless, more work is necessary to understand the recombination losses in the power-generating regime in full generality.

CPP 41.6 Wed 16:30 ZEU 260
Experimental and simulated illumination dependent conductivity changes in organic bulk hetero junction solar cells — ●ARNE MÜLLER, VLADISLAV JOVANOVIĆ, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28579 Bremen, Deutschland

The usage of organic solar cells for indoor application or for wearable electronics requires a good functionality for a wide range of irradiated light intensities. Therefore the IV behaviour of bulk hetero junction solar cells is analysed for a large variety of illumination intensities. We find that the IV-characteristic differs from the predictions of the Shockley-model, which is attributed to the low mobility of the charge carriers. The results are compared to drift-diffusion device simulations and with a simplified device model based on the Fermi-level spitting

behaviour inside the semiconductor. In addition JscVoc experiments were performed to gain an insight into the series-resistance properties at different light intensities. As expected we found that the conductivity of the device is changed due to the light created charge carriers. The findings of the JscVoc analysis are then compared to our improved device model.

15 min break

CPP 41.7 Wed 17:00 ZEU 260

Design and Application of NIR Absorbing Donor Materials for Efficient Organic Solar Cells — ●SEBASTIAN SCHELLHAMMER^{1,2,3}, FRANK ORTMANN^{1,2}, and GIANAURELIO CUNIBERTI^{1,2,3} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — ²Dresden Center for Computational Materials Science, TU Dresden — ³Center for Advancing Electronics Dresden, TU Dresden

Recently, fluorene-functionalized aza-BODIPYs have been successfully applied as donor material in organic solar cells.[1] Optimized bulk heterojunction solar cells with C60 have yield power conversion efficiencies up to 4.5 %, rendering the compounds highly competitive among other NIR-absorbing small-molecule donor materials. Based on an analysis of electronic properties, internal reorganization energies, and the optical properties of more than 100 aza-BODIPYs we give guidelines for the design of further optimized materials for solar cell applications. The observed independence of most of the functionalization strategies makes them an ideal material class for tailor-made donor materials that can cover a broad range of absorption, charge transport, and energetic regimes.

[1] M. Lorenz-Rothe, K. S. Schellhammer et al. Adv. Electron. Mater. 2, 1600152 (2016).

CPP 41.8 Wed 17:15 ZEU 260

Manipulating the morphology in printed organic solar cells — ●STEPHAN PRÖLLER¹, DANIEL MOSEGUÍ GONZÁLES², CHENHUI ZHU³, ALEXANDER HEXEMER³, PETER MÜLLER-BUSCHBAUM², and EVA M. HERZIG¹ — ¹TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — ²TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ³Lawrence Berkeley National Laboratory, Advanced Light Source, Berkeley, USA

The nanomorphology can strongly influence the physical properties of organic thin films. For example, polymer:fullerene blends used in organic photovoltaics vary significantly in performance depending on the inner film morphology. To allow large-scale production of these devices, control of the nanostructure during the processing of the active layer is important. This firstly needs an understanding of the processes involved during the drying of the film. Using an industrial slot-die coater implemented into a synchrotron beamline we have successfully characterized the solidification process of an active layer using grazing incidence small and wide angle X-ray scattering (GISAXS/GIWAXS). We use the gained knowledge to further manipulate the structure of printed organic thin films by external intervention while printing. With this manipulation, we are able to positively influence the morphological evolution and thus the performance of the produced devices.

CPP 41.9 Wed 17:30 ZEU 260

On the Role of Triplet Excitons in Organic Solar Cells — ●ANDREAS SPERLICH¹, STEFAN VÄTH¹, HANNES KRAUS¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

A strategy for increasing the conversion efficiency of organic photovoltaics has been to increase V_{OC} by tuning the energy levels of donor and acceptor components. However, this opens up a new loss pathway from an interfacial charge transfer state (CTS) to a donor triplet exciton (TE) state called electron back transfer (EBT), which is detrimental to device performance. To test this hypothesis, we study triplet formation in high performing blends of the fullerene PC₇₀BM with either the polymer PTB7 [1] or the soluble small molecule p-DTS(FBTTh₂)₂ [2] and determine the impact of the morphology-optimizing additive 1,8-diiodooctane (DIO). Using photoluminescence and spin-sensitive optically and electrically detected magnetic resonance (ODMR, EDMR) measurements we find that TE formation does not only depend on the

materials' energetics, but also on temperature and nano-morphology. Furthermore, we observe TEs in real devices under realistic working conditions even for the most efficient solar cells, which has implications not only for efficiency, but also for devices stability.

[1] H. Kraus, et al., Sci. Repts. 6, 29158 (2016)

[2] S. Vãth, et al., Adv. Energy Mater., doi: 10.1002/aenm.201602016 (2016)

CPP 41.10 Wed 17:45 ZEU 260

Watching Paint Dry: The Impact of Diiodooctane on the Kinetics of Aggregate Formation in Thin Films of Poly(3-hexylthiophene) — ●MARKUS REICHENBERGER¹, SEBASTIAN BADERSCHNEIDER², DANIEL KROH¹, STEFFEN GRAUF¹, JUERGEN KOEHLER^{2,3}, RICHARD HILDNER², and ANNA KOEHLER^{1,3} — ¹Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — ²Experimental Physics IV, University of Bayreuth, 95440 Bayreuth, Germany — ³Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, 95440 Bayreuth, Germany

We have investigated how the addition of 1,8-diiodooctane (DIO) alters the formation of disordered and ordered phases in a film of poly(3-hexylthiophene-2,5-diyl) (P3HT). By combining in situ time-resolved absorption spectroscopy with 60 ms time resolution, optical and transmission electron microscopy and spatially resolved photoluminescence spectroscopy, we show that, in addition to the excitonic coupling, the film formation process during spin-coating as well as the subsequent long-time film drying process differ significantly when DIO is added to a solution of P3HT. During spin-coating, the addition of DIO reduces the actual time for transformation from disordered to ordered phase, even though it increases the time until the disorder-order transition sets in. In place of a solidification front, we observe an all-over solidification throughout the entire film. The phase separation between nonaggregated and aggregated phase increases when using DIO, with compositional variation in the content of aggregated phase on a micrometer scale.

CPP 41.11 Wed 18:00 ZEU 260

Bicontinuous Morphologies in Ternary Blends of Molecular Glasses — ●MICHAEL GRIMANN, EVGENY TATAROV, and THOMAS FUHRMANN-LIEKER — University of Kassel, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, 34109 Kassel, Germany

We demonstrate nanoscale phase separated morphologies in organic functional materials. These glassy compounds comprise structural motifs known from OLED or organic laser materials like oligophenyls and triarylaminas as electron donors. We developed electron acceptors containing perfluorinated aromatic moieties which lead to a miscibility gap with the respective donors. Binary blends thereof undergo phase separation via spinodal decomposition in eutchoric compositions. Kinetics of this demixing process can be significantly slowed by addition of especially designed surfactant-like bipolar materials. The resulting bicontinuous morphologies of tuneable scale are useful for future random lasing and photovoltaic applications.

CPP 41.12 Wed 18:15 ZEU 260

Controlling the aggregation of native polythiophene during in situ polymerization — ●JENNY LEBERT, EVA M. KRATZER, MICHAEL CORIC, SALMA MANSI, and EVA M. HERZIG — TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany

Native polythiophene belongs to the class of conjugated, semiconducting polymers which become conductive upon doping and therefore offer a broad range of potential applications in organic electronics. While polythiophene itself is insoluble, it is possible to obtain solution processed thin films by employing an in situ polymerization technique. This way, the soluble monomers are deposited to the substrate and chemically linked afterwards. Since it is well known, that the performance of polymeric electronic devices depends strongly on the molecular interactions within the thin films, understanding and controlling the crystallization and film morphology are of crucial importance.

Here, we would like to present the possibilities of influencing the aggregation of the polythiophene chains in the film formation process by varying easily changeable synthetic parameters. The synthesized polymer films are analyzed regarding their optic and electronic properties as well as their morphology to show a clear dependence of the chosen synthetic path on the final film characteristics.