

CPP 23: Organic Photovoltaics I

Time: Tuesday 9:30–13:00

Location: C 243

Invited Talk

CPP 23.1 Tue 9:30 C 243

Non-fullerene acceptors for commercially viable organic photovoltaics — ●DERYA BARAN — King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

The commercialization of OPV requires the availability of inexpensive materials in large quantities, such as poly(3-hexylthiophene) (P3HT). P3HT is readily scalable via flow or micro-reactor synthesis, even using green solvents, whilst retaining a high degree of control over molecular weight and regio-regularity. However, it has a limited open-circuit voltage (Voc), short-circuit current (Jsc) and stability in photovoltaic devices when fullerene derivatives are used as acceptors. This talk will focus on the alternative small molecule non-fullerene acceptors that lead to the highest power conversion efficiencies with P3HT donor. The devices show excellent stability in air and are promising for commercializing OPV in the near future.

CPP 23.2 Tue 10:00 C 243

Developing design criteria for organic solar cells using well-absorbing non-fullerene acceptors — ●LISA KRÜCKEMEIER¹, PASCAL KAIENBURG¹, and THOMAS KIRCHARTZ^{1,2} — ¹IEK5 Photovoltaics, Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — ²Faculty of Engineering and CENIDE, University of Duisburg-Essen, Carl-Benz-Str. 199, 47057 Duisburg, Germany

In recent years, a variety of promising, well-absorbing non-fullerene acceptor molecules (NFAs) for bulk heterojunction OPV has been developed, which often achieve higher efficiencies than their fullerene-based counterparts. Unlike fullerene acceptors, these various NFAs have their respective absorption peak at different positions of the visible spectrum, allowing the absorption behavior of the blend to be flexibly adjusted by changing its composition. Thus, the fundamental question arises, how to adjust these two absorption spectra of the acceptor and donor to each other in order to best exploit the incident power of the sun and get high solar cell efficiencies. A series of parameters, such as layer thickness, electronic quality and the amount of non-radiative voltage losses affects this optimum. By using numerical simulations, we have developed design criteria for organic solar cells with well-absorbing non-fullerene acceptors that take these influences into account. Only when the electronic quality of the layer still allows a sufficient charge carrier collection for layer thicknesses around the second interference maximum, a combination of complementary absorbing molecules is more efficient. For smaller thicknesses, a blend of molecules with the same absorption onset achieves higher efficiencies.

CPP 23.3 Tue 10:15 C 243

Photovoltaic Performance of Non-Fullerene Acceptors with Anthracene-Containing PPE-PPV — SHAHIDUL ALAM^{1,2}, RICO MEITZNER^{1,2}, CHRISTIAN FRIEBE^{1,2}, JONATHAN CANN⁴, JOHANNES AHNER², CHRISTOPH ULBRICHT³, ZHIPENG KAN⁵, STEPHANIE HOEPPENER², MARTIN D. HAGER^{1,2}, DANIEL A. M. EGBE³, GREGOR C. WELCH⁴, FRÉDÉRIC LAQUAI⁵, ULRICH S. SCHUBERT^{1,2}, and ●HARALD HOPPE^{1,2} — ¹CEEC, Friedrich Schiller University Jena — ²IOMC, Friedrich Schiller University Jena — ³Institute of Polymeric Materials and Testing, Johannes Kepler University, Linz, Austria — ⁴Department of Chemistry, University of Calgary, Canada — ⁵KAUST, Kingdom of Saudi Arabia

Recently, non-fullerene acceptors (NFAs) have received increasing attention for use in polymer-based bulk-heterojunction organic solar cells, as they have demonstrated improved photovoltaic performances as compared to conventional polymer-fullerene blends. Polymer solar cells based on an anthracene-containing poly(p-phenylene ethynylene)-alt-poly(p-phenylene vinylene) (PPE*PPV) copolymer with statistical side chain configuration (AnE-PVstat) in combination with various electron accepting materials were prepared and studied. In contrast to blends with PCBM, the almost complete extinction of the polymer photoluminescence in these donor-acceptor blends indicated too fine-scaled intermixing. This seems to cause poor photovoltaic performance. Time-delayed collection-field (TDCF) measurements revealed that the photovoltaic effectiveness of these organic semiconductor blends was strongly limited by insufficient charge generation and extraction.

CPP 23.4 Tue 10:30 C 243

The Impact of Driving Force and Temperature on the Electron Transfer in Donor-Acceptor Blend Systems — T UNGER¹, ●S WEDLER¹, F-J KAHLER¹, U SCHERF³, H BÄSSLER², and A KÖHLER^{1,2} — ¹Experimental Physics II, Uni Bayreuth — ²BIMF, Uni Bayreuth — ³Makromolekulare Chemie, Uni Wuppertal

We discuss whether electron transfer from a photoexcited polymer donor to a fullerene acceptor in an organic solar cell is tractable in terms of Marcus theory, and whether the driving force ΔG_0 is crucial in this process (JPCC 2017, 121, 22739). Considering Marcus rates to be thermally activated, we measured the appearance time of the polaron signal between 12 and 295 K for the representative donor polymers PTB7, PCPDTBT and Me-LPPP blended with PCBM. In all cases, the dissociation process was faster than the temporal resolution of our experimental setup (220-400 fs), suggesting that the charge transfer is independent of ΔG_0 . We find that for the PCPDTBT:PCBM ($\Delta G_0=0.2$ eV) and PTB7:PCBM ($\Delta G_0=0.3$ eV) the data is mathematically consistent with Marcus theory, yet the condition of thermal equilibrium is not satisfied. For MeLPPP:PCBM in the Marcus inverted regime, the dissociation rate is inconsistent with Marcus theory but formally tractable using the Marcus-Levich-Jortner tunneling formalism which also requires thermal equilibrium. This is inconsistent with the short transfer times we observed and implies that coherent effects need to be considered. Our results imply that any dependence of the total photocurrent yield must be ascribed to the secondary escape of the initially generated CT-state from its Coulomb potential.

CPP 23.5 Tue 10:45 C 243

Charge photogeneration in organic solar cells composed of over 90% C60 — ●ELISA COLLADO-FREGOSO¹, JOHANNES BENDUHN², KOEN VANDEWAL², and DIETER NEHER¹ — ¹Institut für Physik und Astronomie, Potsdam University, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm, Germany — ²Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

The involvement of charge-transfer (CT) states in the processes of charge generation and recombination has been an important focus of study within the organic photovoltaic community. However, it has proved challenging to systematically address specific molecular properties without modifying the microstructure of the blend. In this work, we study the mechanism of charge generation in a series of solar cell devices with active layers composed mainly of vacuum deposited C60 and small amounts ($\sim 5\%$ mol) of organic molecular donors. This ensures a constant morphology dictated by the fullerene acceptor. Using time-delayed collection field measurements, we demonstrate that the short circuit current and fill factor in these devices are largely determined by the charge generation efficiency and its bias dependence, which is more pronounced with decreasing CT state energy. This finding challenges current views that the existence of fullerene aggregates is sufficient to ensure efficient CT dissociation, and questions the picture of a necessary driving energy for charge generation. We discuss the implications of these findings within the framework of the Onsager-Brown model and propose guidelines to improve charge generation.

15 min. break

CPP 23.6 Tue 11:15 C 243

Phonon-Induced Absorption Line Shapes in Organic Semiconductors — ●MICHEL PANHANS¹, JOHANNES BENDUHN², KARL SEBASTIAN SCHELLHAMMER¹, KOEN VANDEWAL², and FRANK ORTMANN¹ — ¹Center for Advancing Electronics Dresden, TU Dresden — ²Institute for Applied Photophysics, TU Dresden

Quantifying disorder is an important task in organic semiconductor research [1,2] because of its impact on the carrier mobility and device performance. We analyze models of amorphous and crystalline donor-acceptor systems regarding their response to optical excitations. [3] We study the excited-state density of states with varying electronic disorder and electron-phonon interaction and compare our results to absorption measurements on donor-acceptor blends.

[1] D. Venkateshvaran et al. Nature 515, 384 (2014).

[2] K. Vandewal et al. J. Am. Chem. Soc. 139, 1699 (2017).

[3] M. Panhans et al. (in preparation)

CPP 23.7 Tue 11:30 C 243

Investigation of degradation processes in low bandgap polymers for organic photovoltaics — ●FRANZISKA C. LÖHRER, CHRISTOPH SENFTER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic photovoltaics have experienced a drastic increase in research and are gaining impact as a feasible alternative to conventional solar cells. With their easy processability, high flexibility and tunable optical properties, organic materials such as photoactive polymers offer a wide range of potential applications. Recent efforts focus on identifying new materials in order to enhance the device performance. This has led to the development of low bandgap polymers such as PTB7 and its derivatives with reported efficiencies surpassing the 10 % limit. However, especially high-efficiency polymers are sensitive to various degradation processes, which strongly decrease their lifetime. We follow the chemical and physical changes occurring in low bandgap polymers during light-induced aging and test ways to eliminate typical degradation pathways. The thin film morphology is investigated using real-space imaging as well as X-ray scattering techniques. Optical and IR spectroscopy methods give insights into the chemical changes inside the polymer.

CPP 23.8 Tue 11:45 C 243

Charge Carrier Recombination Dynamics in Squaraine-Based Bulk-Heterojunction Solar Cells — ●DOROTHEA SCHEUNEMANN¹, OLIVER KOLLOGE¹, SEBASTIAN WILKEN¹, MAJGOR MACK¹, JÜRGEN PARISI¹, MATTHIAS SCHULZ², ARNE LÜTZEN², and MANUELA SCHIEK¹ — ¹University of Oldenburg, Institute of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg — ²University of Bonn, Kekulé Institute of Organic Chemistry and Biochemistry, 53121 Bonn

Squaraine (SQ) dyes receive increasing attention as donor materials in organic photovoltaics since they combine high absorption in the deep-red with a general environmental stability and non-toxicity. Together with common fullerene acceptors, SQ-based bulk-heterojunction devices have been demonstrated to deliver a high open-circuit voltage, but suffer from a comparatively low fill factor [1]. However, little effort has been made to develop a better understanding of the underlying loss mechanisms. In this work, we focus on transient optoelectronic characterization methods to study the loss mechanisms in photovoltaic devices of a benchmark squaraine (SQIB) blended with a fullerene (PC60BM). These devices show a gradual decrease of the fill factor when increasing the active layer thickness and incident light intensity. We show that the low fill factor is a consequence of slow charge carrier collection competing with bimolecular recombination.

[1] Scheunemann et al., Appl. Phys. Lett. 111 (2017) 183502.

CPP 23.9 Tue 12:00 C 243

Recombination in Organic Solar Cells: Are There Still Lessons to Learn from P3HT:PCBM? — ●SEBASTIAN WILKEN, DOROTHEA SCHEUNEMANN, and JÜRGEN PARISI — Institute of Physics, University of Oldenburg, Germany

The nature of the non-geminate recombination in organic bulk heterojunction solar cells remains controversial. In this talk, we present new data on an old hat: P3HT:PCBM. By tailoring the nanoscale morphology, we observed a novel kind of structure–property relationship in P3HT:PCBM devices that is at variance with current theoretical models. We discuss whether these findings provide new avenues for understanding the role of phase separation and interface states in the non-geminate recombination dynamics.

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Apparent Field Dependence of Charge Carrier Generation and Recombination Coefficient in Organic Solar Cells — ●ULI WÜRFEL and MORITZ UNMÜSSIG — Fraunhofer ISE, Heidenhofstr. 2, 79110 Freiburg, Germany

Charge carrier generation in organic solar cells is often reported to show an electric field dependence. However, it is not measured directly but is derived from transient charge carrier extraction experiments based on the time delayed collection field (TDCF) method. In this contribution, numerical simulations of TDCF experiments are presented which - when analyzed in the same way as reported in literature - result in a field dependence of the charge carrier generation and the recombination coefficient even though field-independent values are used. For the carrier generation this discrepancy is consistently shown to be caused by (unavoidable) bi-molecular recombination in the short time scale prior to and during extraction. The apparent field dependency becomes more pronounced with increasing recombination coefficient and decreasing charge carrier mobilities, well in accordance with TDCF data from literature. The apparent field dependence of the bimolecular recombination coefficient is due to the fact that its derivation from experimental TDCF data is based on spatially averaged values of carrier densities. In contrast, electrons and holes in real devices are distributed inhomogeneously as a consequence of the boundary conditions. Our study shows clearly that in order to explain results from TDCF experiments it is not required to include any field-dependence nor of the photocurrent generation nor of the recombination coefficient.

CPP 23.11 Tue 12:30 C 243

Effect of the RC time on photocurrent transients and determination of charge carrier mobilities — ●JULIANE KNIEPERT and DIETER NEHER — University of Potsdam, Germany

We present a closed analytic model to describe time dependent photocurrents upon pulsed illumination in the presence of an external RC circuit. In combination with numerical drift diffusion simulations, it is shown that the RC time has a severe influence on the shape of the transients. In particular, the maximum of the photocurrent is delayed due to a delayed recharging of the electrodes. This delay increases with increasing RC constant. As a consequence, charge carrier mobilities determined from simple extrapolation of the initial photocurrent decay will be in general too small and feature a false dependence on the electric field. Here, we present a recipe to correct charge carrier mobilities determined from measured photocurrent transients by taking into account the RC time of the experimental set-up. We also demonstrate how the model can be used to more reliably determine the charge carrier mobility from experimental data of a typical polymer/fullerene organic solar cell. It is shown that further aspects like a finite rising time of the pulse generator and the current contribution of the slower charge carriers influence the shape of the transients and may lead to an additional underestimation of the transit time.[1]

[1] Kniepert et al., J. Appl. Phys. 122, 195501 (2017)

CPP 23.12 Tue 12:45 C 243

Parameter extraction from measured solar cell IV curves using CELIC model — ●VLADISLAV JOVANOVIĆ, ARNE MÜLLER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Current voltage (IV) characteristic of solar cells with low mobility of charge carriers cannot be described using classical Shockley model. To properly describe behavior of low-mobility solar cells, we have developed analytical CELIC model based on simplified drift-diffusion calculations [1]. This model assumes a constant electric field (CE) and linearly increasing current (LIC) contributions of holes and electrons inside the semiconductor layer. Furthermore, the developed model takes into account recombination processes within the semiconductor bulk and at the contact interfaces. We have already shown that CELIC model is not limited only to solar cells with low mobility of charge carrier, and it can be also used for modeling of perovskite and silicon solar cells. In this study, we show how to extract material parameters from measured solar cell IV curves using CELIC model. For this purpose, we have fabricated organic bulk heterojunction solar cells for different composition ratio of polymer and fullerene using solution processing. By applying CELIC model, we can analyze the crossing point between dark and light curves and access mobility and contact properties in dependence of composition of the semiconductor layer.

[1] A.Müller, V.Jovanović, V.Wagner, Appl.Phys.Lett. 111 (2017) 023506