# HL 68: Photovoltaics: Organic Semiconductors

Time: Wednesday 17:45–19:30 Location: ER 270

HL 68.1 Wed 17:45 ER 270

**Quantum coherence controls the charge separation in a prototypical artificial light harvesting system** — •Sarah Maria Falke[1], Carlo Andrea Rozzi[2], Nicola Spallanzani[2], Angel Rubio[3], Elisa Molinari[2], Daniele Brida[4], Margherita Maiuri[4], Giulio Cerullo[4], Heiko Schramm[1], Jens Christoffers[1], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]CNR, Centro S3, Modena, Italy — [3]Fritz-Haber-Institut, Berlin, Germany — [4]IFN-CNR, Politecnico di Milano, Italy

In artificial light harvesting systems the conversion of light into electrical or chemical energy happens on the femtosecond time scale and is thought to involve the incoherent jump of an electron from the optical absorber to an electron acceptor. Here we investigate the primary process of electronic charge transfer dynamics in a supramolecular triad, a prototypical elementary component for an artificial photosynthetic/photovoltaic system. Combining coherent femtosecond spectroscopy and first-principles quantum dynamics simulations, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a quantum correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. Our work highlights the fundamental role played by the chemical interface between the light-absorbing chromophore and the charge acceptor in triggering the coherent wavelike electron-hole splitting.

HL 68.2 Wed 18:00 ER 270

**Doping induced performance enhancement in low bandgap polymer:fullerene solar cells** — •Antonietta De Sio[1], Ali Veysel Tunc[1], Daniel Riedel[2], Enrico Da Como[2], Jürgen Parisi[1], and Elizabeth von Hauff[3] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany — [2]Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität München, 80799 Munich, Germany — [3]Institute of Physics, Albert-Ludwigs University of Freiburg, 79104 Freiburg, Germany

We investigate the effect of molecular doping in poly[2,6(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b0]-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) and its blend with [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). Tetrafluorotetracyanoquinodimethane (F4-TCNQ) is used to dope PCPDTBT via co-solution at different concentrations. The effect of doping on the transport properties of the neat polymer as well as of the blends is investigated with field effect measurements while photoinduced absorption spectroscopy is employed to get information on the charge separation efficiency. Bulk heterojunction solar cells with molecularly doped active layers were also prepared and characterized. We demonstrate that molecular doping is a simple and effective method to improve the performance in polymer:fullerene solar cells by reducing the recombination and increasing the hole mobility.

HL 68.3 Wed 18:15 ER 270

**Field dependence of charge carrier generation in MDMO-PPV based organic solar cells** — •Julia Kern[1], Clemens Grünewald[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

One of the key issues of organic photovoltaics is the fundamental understanding of charge photogeneration and recombination. The dissociation of the singlet excitons created in the polymer is likely to occur via one of two distinct routes, the first one being direct dissociation to free charge carriers and the second one involving an intermediate step comprising the formation of an interfacial charge transfer exciton (CTE). In order to shed light onto the relevance of the respective dissociation patterns, we investigated the field dependence of CTE photoluminescence as a means of probing geminate recombination as well as of the photocurrent, being a direct indicator for free charge carriers. Starting with MDMO-PPV blended with PCBM as a reference system, we employed various fullerene derivatives, systematically changing the lowest unoccupied molecular orbital (LUMO) and thus the open circuit voltage, correspondingly. This approach allows us to study the influence of the different parameters on the CTE binding energy, which can be derived from the dissociation probability predicted by the Onsager Braun model. In view of our results, we discuss the correlation between this binding energy and the field dependent charge generation.

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**Field- and Temperature Dependence of charge Photogeneration in organic bulk heterojunction solar cells** — •Stefan Walter[1], Markus Mingebach[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

A topic of high interest is to understand the principles of charge carrier generation and recombination in organic bulk heterojunction solar cells. Generation of free charge carriers with high yield is a crucial step to ensure high power conversion efficiencies. The dissociation of singlet excitons into free charge carriers may occur either directly or via the intermediate step involving Coulomb bound charge transfer states. The field dependence of charge carrier generation can help to distinguish between these two channels. In the case of the poly(3-hexylthiophene-2,5-diyl):[6,6]-phenyl-C61 butyric acid methyl ester (P3HT:PC60BM) blends almost no field dependence of extracted charge carrier density under positive bias between 0V and open circuit voltage was observed at room temperature [1], thus indicating a direct generation. In contrast we show a strong field dependence for poly[2-methoxy-5-(3′,7′-dimethyloctyloxy)-1,4-phenylenevinylene] :[6,6]-phenyl-C61 butyric acid methyl ester (MDMO-PPV:PC60BM) blends by applying field- and temperature dependent time delayed collection field measurements.

[1] J. Kniepert, M. Schubert, J.C. Blakesley and D. Neher, J. Phys. Chem. Lett., 2, 700-705 (2011).

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**Recombination Processes in Disordered Organic Bulk-Heterojunction Solar Cells** — •Alexander Wagenpfahl[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, 97074 Würzburg, Germany — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany

In recent years the charge carrier recombination mechanisms in organic bulk-heterojunction solar cells have been controversially discussed. For blended organic semiconductors recombination orders between one, two or even higher have been reported. The origin of these observations, the recombination pathways as well as their impact on the device performance, still need further investigations to be understood in detail. In an organic bulk-heterojunction solar cell two blended but spatially separated semiconductor phases are used to gain current from the incident light. Due to their spatial disorder organic semiconductors generally show a Gaussian distribution of the molecular orbitals. Introducing this disorder into our macroscopic numerical device simulation, we show the possible interaction pathways of conducting and trapped electrical charges within the multiple trapping and release model. Based on these results we illustrate the impact of various recombination pathways for charge carriers on the observed current-voltage characteristics under consideration of phase separation aspects. Our results clearly show that it is crucial for the performance which recombination pathway is dominant in organic bulk-heterojunction solar cells and which role the energetic disorder plays in these processes.

HL 68.6 Wed 19:00 ER 270

**Time and Spatially Resolved 1D-MonteCarlo Simulations on Charge Transport** — •Manuel Ruf[1], Jens Lorrmann[1], Vladimir Dyakonov[1,2], and Carsten Deibel[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg

Charge transport in organic materials is one of the limiting steps for highly efficient solar cells. Further insight into the microscopic processes promise a better unterstanding of the underlying charge transport.

In this study we describe charge transport by a one dimensional Monte Carlo (1D-MC) simulation, which is based on multiple trapping and release events of charge carriers into a density of trap states while moving through the sample due to thermal and electric field energy. As

long as a charge carrier is trapped, its contribution to current is zero. The actual form of the density of trap states determines the charge carrier release time therefore affecting the shape of the transient. The time dependence of the model allows simulation of transient measurement techniques, such as Time-Of-Flight (TOF) or charge extraction by linear increasing voltage (CELIV).
Hence we can probe the individual behaviour of single charge carriers, which allows studies of propagation of the spatial charge carrier distribution and energetic relaxation for different model parameters. The simplicity of this model provides low computing times, yet allows to reproduce physical behaviour as observed in measurements on regio regular poly(3-hexyl thiophene-2,5-diyl) (P3HT 4002E).

HL 68.7 Wed 19:15 ER 270

**Thermodynamic efficiency limit of molecular donor-acceptor solar cells and its application to diindenoperylene (DIP)-based devices** — •Mark Gruber[1], Julia Wagner[1], Ulrich Hörmann[1], Andreas Opitz[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, Germany — [2]Institute of Physics, Humboldt University, Berlin, Germany

Based on the principle of detailed balance we have developed a modified Shockley-Queisser theory including the effects of interfacial charge transfer (CT) states that allows for a quantitative assessment of the thermodynamic efficiency limits of molecular donor(D)/acceptor(A) solar cells. Key parameters entering the model, apart from the optical gap of the absorber material, are the energy ($E_{CT}$) and relative absorption strength ($\alpha_{CT}$) of the CT state. We demonstrate how the open-circuit voltage and thus the power conversion efficiency are affected by different parameter values. Furthermore, we show that temperature dependent device characteristics can serve to determine the CT energy, and thus the upper limit of $V_{OC}$ for a given D/A combination, as well as to quantify non-radiative recombination losses. The model is applied to DIP based photovoltaic devices, where open-circuit voltages between 0.9 and 1.4 V, depending on the partner, have recently been reported [1,2].
[1] J. Wagner et al., *Adv. Func. Mater.* 2010, 20, 4295.
[2] U. Hörmann et al., *Phys. Stat. Sol. RRL* 2011, 5, 241.