

## HL 58: Focus Session: Structure and Transport in Organic Photovoltaics III (jointly with CPP)

Time: Wednesday 15:00–17:00

Location: ER 270

HL 58.1 Wed 15:00 ER 270

**Many-body perturbation theory calculations for organic photovoltaics** — ●CARINA FABER, CLAUDIO ATTACALITE, and XAVIER BLASE — Institut Néel, CNRS, Grenoble, France

We evaluate the performance of ab initio GW calculations for ionization energies (IEs) and for HOMO-LUMO gaps of thirteen gas phase molecules of interest for organic electronic and photovoltaics, including e.g. pentacene and free-base porphyrins. Our calculations are based on an efficient Gaussian-basis implementation of GW with explicit treatment of the dynamical screening through contour deformation techniques. We show that we significantly improve the IEs and gaps as compared to DFT Kohn-Sham results. Moreover, we study within the GW and Bethe-Salpeter approach the low lying singlet charge-transfer excitations in molecular donor/ acceptor complexes associating benzene, naphthalene and anthracene derivatives with the TCNE acceptor. Our calculations demonstrate that such techniques can reproduce the experimental data with a mean absolute error of 0.1-0.15 eV for the present set of dimers, which is in excellent agreement with the best time-dependent density functional studies with optimized range-separated functionals. The present results pave the way for the study of photoinduced charge-transfer processes in photovoltaic devices with a parameter-free ab initio approach showing equivalent accuracy for finite and extended systems. Finally, we show in the case of C60 that the magnitude of the electron-phonon coupling, an important quantity that governs the mobility of carriers in organic systems, is much better described within GW as compared to standard DFT calculations.

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**Transport and Electric Fields in Amorphous Silicon Organic Hybrid Solar Cells** — ●SEBASTIAN SCHAEFER<sup>1</sup>, TIM SCHULZE<sup>2</sup>, LARS KORTE<sup>2</sup>, AAD GORDIJN<sup>3</sup>, JAN WÖRDENWEBER<sup>3</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Universität Potsdam, Germany — <sup>2</sup>Helmholtz Zentrum Berlin, Germany — <sup>3</sup>Forschungszentrum Jülich GmbH, Germany

We investigated hybrid structures based on n-p a-Si:H cells where the p-type layer is replaced by the low band gap polymer PCPDTBT. In these devices the polymer acts as an extraction layer for holes generated in the intrinsic a-Si:H layer and additionally generates charge carriers in the red part of the spectrum, where a-Si:H does not absorb. IV- and quantum efficiency measurements of the hybrid cell show that both materials contribute to the photocurrent generation, indicating that exciton splitting at the hybrid interface as well as hole transfer from a-Si:H to the polymer are provided by the structure. However, low short circuit currents and fill factors lead to poor efficiencies. Simulations of the hybrid device band structure with AFORS-HET (Automat for Simulation of Heterostructures, Helmholtz Zentrum Berlin) indicate that low electric fields in the amorphous silicon layer may lead to the limited performance. This turns out to be a general problem of hybrid inorganic-organic devices since the dielectric constants differ remarkably between these materials. We investigated the electric fields in the hybrid cell with electroabsorption measurements which support our theoretical assumptions. Further studies show that by using doped organic layers the electric field is reconditioned in the amorphous silicon, leading to much better device performance.

HL 58.3 Wed 15:30 ER 270

**Field-dependent Charge Carrier Generation, Recombination and Extraction in Polymer Based Solar Cells** — ●JULIANE KNIEPERT, ILJA LANGE, JAMES BLAKESLEY, and DIETER NEHER — Universität Potsdam, Institut für Physik und Astronomie

Recently we used the time-delayed collection field (TDCF) method to show that charge generation in solvent annealed P3HT:PCBM solar cells is independent of the electric field[1]. In these blends solvent or thermal annealing leads to a phase-separated morphology and the corresponding solar cells exhibit high values for the external quantum efficiency and fill factor. By contrast, non-treated devices show significantly lower currents and fill factors.

A fundamental understanding of the processes leading to high fill factors and currents is of great importance for the development of a new generation of high efficiency polymer solar cells.

Here, we apply bias-dependent TDCF measurements to probe the generation and recombination of charge carriers in pristine and thermally annealed devices spincast from chloroform. In conjunction with

numerical modelling, we show that the differences in the I-V characteristics are not caused by field-dependent dissociation or by the enhanced recombination in non-treated blends, but rather by more efficient extraction of holes in the annealed blend.

[1] J. Kniepert et al., J. Phys. Chem. Lett. 2, 700 (2011)

HL 58.4 Wed 15:45 ER 270

**Phase separation in ternary charge-transfer-complexes** — ●DIANA NANOVA<sup>1,2</sup>, SEBASTIAN BECK<sup>2</sup>, MILAN ALT<sup>2</sup>, TOBIAS GLASER<sup>2</sup>, ANNEMARIE PUCCI<sup>2</sup>, KATRIN SCHULTHEISS<sup>1</sup>, RASMUS R. SCHRÖDER<sup>5</sup>, JENS PFLAUM<sup>4</sup>, WOLFGANG KOWALSKY<sup>1,3</sup>, and MICHAEL KRÖGER<sup>1,3</sup> — <sup>1</sup>Institute for High-Frequency Technology, TU Braunschweig, Germany — <sup>2</sup>Kirchhoff-Institute for Physics, U Heidelberg, Germany — <sup>3</sup>Innovation Lab GmbH, Heidelberg, Germany — <sup>4</sup>Institute for Experimental Physics VI, U Würzburg, Germany — <sup>5</sup>BioQuant, U Heidelberg, Germany

We studied, how mixing of two organic charge-transfer-complexes, which are deposited via thermal co-evaporation at different concentrations by substituting only the acceptor molecules, allows tuning of the optical and structural properties in analogy to inorganic III-V semiconductor compounds. The electron diffraction patterns we collected on samples of a so called ternary CT-system DB-TTF/F4-TCNQx/TCNQ1-x do not show any indication of a mixed crystalline phase or novel crystalline order. However, upon mixing of the complexes the crystallinity of the individual phases degrades. This effect is correlating with mixing ratio. We performed x-ray-diffraction measurements, which confirm the phase separation in the ternary system. Further, we do not observe a shift or the appearance of new peaks in the infrared spectra. Hence, there is no electronic interaction in the presented ternary system between the CT-complexes. In summary this means, that in the ternary system, a phase-separated growth mode dominates and mixing of the phases is not achieved.

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**Charge Carrier Dynamics in Blends of PCPDTBT/PC<sub>70</sub>BM: Influence of Solvent Additives** — ●STEVE ALBRECHT<sup>1</sup>, WOLFRAM SCHINDLER<sup>2</sup>, JONA KURPIERS<sup>1</sup>, SYBILLE ALLARD<sup>3</sup>, ULLRICH SCHERF<sup>3</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Universität Potsdam, Institute of Physics and Astronomy, Soft Matter Physics, D-14476 Potsdam, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany — <sup>3</sup>Bergische Universität Wuppertal, Macromolecular Chemistry and Institute for Polymer Technology, Gauss-Strasse 20, D-42097 Wuppertal, Germany

We have applied time delayed collection field (TDCF) and photo-CELIV to investigate the photogeneration, recombination dynamics and transport of charge carriers in blends composed of PCPDTBT:PC<sub>70</sub>BM processed with and without the solvent additive diiodooctane. We show that the solvent additive affects several elementary processes involved in the photon to electron conversion in these blends. First, there is a pronounced field dependence of the generation of free carriers for both blends, with the field dependence being more pronounced without the additive. Second and most important, addition of diiodooctane leads to a three-fold increase of the carrier mobility, enabling rapid extraction of the charge in competition with bimolecular recombination. On the other hand, both blends show rather high but similar bimolecular recombination coefficients. All together, the improvement in generation and extraction of the free carriers explains well the twofold increase in device efficiency upon addition of the processing agent.

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**Equivalent circuit analysis for understanding s-shaped IV-characteristics in organic solar cells** — ●BERNHARD ECKER<sup>1</sup>, HANS-JOACHIM EGELHAAF<sup>2</sup>, ROLAND STEIM<sup>2</sup>, JÜRGEN PARISI<sup>1</sup>, and ELIZABETH VON HAUFF<sup>3,4</sup> — <sup>1</sup>Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg, Germany — <sup>2</sup>Konarka Technology GmbH, Landgrabenstr. 94, Nürnberg, Germany — <sup>3</sup>Institute of Physics, Albert-Ludwigs University of Freiburg, 79104 Freiburg, Germany — <sup>4</sup>Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

In this contribution we investigate the origin of s-shaped current voltage (IV) characteristics in inverted solar cells with a TiO<sub>x</sub> interlayer

between the cathode and the P3HT:PCBM active layer. Initially, the solar cells demonstrate s-shaped IV characteristics, resulting in a low fill factor (FF). Upon light soaking with UV radiation the resistivity of the TiOx interlayer decreases, the s-shape disappears and the FF increases. Impedance spectroscopy (IS) is used to investigate the influence of the resistivity of the TiOx layer on the shape of the IV characteristics. A simple equivalent circuit is proposed to model the experimental data in both conditions, i.e. with s-shaped and regular shaped IV characteristics, respectively. The equivalent circuit elements can be attributed to the distinct layers in the solar cell, therefore giving insight into the origin of the s-shape. We show that IS in conjunction with equivalent circuit analysis can provide detailed information and we identify the resistivity of the TiOx interlayer ultimately influencing the shape of the IV characteristics.

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**Effect of AnE-PV copolymer blending on photophysical and photovoltaic properties** — ●CHRISTIAN KÄSTNER<sup>1</sup>, STEFAN TÜRK<sup>2</sup>, DANIEL AYUK MBI EGBE<sup>3</sup>, CHRISTOPH ULBRICHT<sup>3</sup>, ÖSLEM USLUER<sup>3,4</sup>, SILKE RATHGEBER<sup>5</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>Institute of Physics and Institute of Micro- and Nanotechnologies, Ilmenau University of Technology, Ilmenau, Germany — <sup>2</sup>Institute for Print and Media Technology, Chemnitz University of Technology, Chemnitz, Germany — <sup>3</sup>Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Austria — <sup>4</sup>Department of Chemistry, Mugla University, Mugla, Turkey — <sup>5</sup>Institute of Integrated Natural Science, University Koblenz-Landau, Koblenz, Germany

Abstract: Investigations on the effect of side-chain variation of anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymers (AnE-PVs) showed promising results for the design of bulk heterojunction solar cells.

Furthermore, statistical side-chain substitution of these AnE-PVs resulted in an increased solar cell performance. Thus, the question arose whether these results are similarly achievable by blending of different copolymers bearing different side-chain substitutions, instead of side-chain blending of only one polymer backbone. This concept has been applied to fabricate bulk heterojunction solar cells by blending mixtures of copolymers with PCBM within a common solution. It is shown that this concept is beneficial for the solar cell performance compared to single polymer based donor-acceptor blends.

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**Anisotropy of charge and exciton transport in organic semiconductors** — ●VERA STEHR<sup>1</sup>, REINHOLD FINK<sup>2</sup>, JOHANNES PFISTER<sup>2</sup>, BERND ENGELS<sup>3</sup>, and CARSTEN DEIBEL<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Würzburg, 97074 Würzburg — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Universität Tübingen, 72076 Tübingen — <sup>3</sup>Institut für Physikalische und Theoretische Chemie, Universität Würzburg, 97074 Würzburg

Organic solar cells become more and more interesting for applications due to their low production costs and easy processability. In order to increase their efficiency it is very important to understand the basic principles of charge and exciton transport in these materials. The charge carrier mobility and the exciton diffusion length are the crucial material parameters which decide on the applicability for solar cells. The transport properties and their orientational dependency have been studied theoretically by means of quantum chemical methods and a hopping approach using Marcus theory along with the master equation. This approach is straightforward and is shown to provide qualitatively good results concerning the directional and morphological dependency of the transport parameters.