

## CPP 70: Organic Electronics and Photovoltaics V: OPV (joint session CPP/DS/HL, organized by CPP)

Time: Friday 10:15–13:15

Location: ZEU 255

CPP 70.1 Fri 10:15 ZEU 255

**Non-Radiative Voltage Losses Reduce the Upper Limit of the Power Conversion Efficiency in Fullerene-Based Organic Solar Cells** — ●JOHANNES BENDUHN<sup>1</sup>, KRISTOFER TVINGSTEDT<sup>2</sup>, FORTUNATO PIERSIMONI<sup>3</sup>, SASCHA ULLBRICH<sup>1</sup>, DIETER NEHER<sup>3</sup>, DONATO SPOLTORE<sup>1</sup>, and KOEN VANDEWAL<sup>1</sup> — <sup>1</sup>IAP, TU Dresden — <sup>2</sup>EP VI, University of Würzburg — <sup>3</sup>University of Potsdam

The open-circuit voltage of organic solar cells (OSCs) is low as compared to the optical gap of the absorber molecules, indicating high energy losses per absorbed photon. These voltage losses arise only partly due to necessity of an electron transfer event to dissociate the excitons. A large part of these voltage losses is due to recombination of photo-generated charge carriers, including inevitable radiative recombination. In this work, we study the non-radiative recombination losses and we find that they increase when the energy difference between charge transfer (CT) state and ground state decreases. This behavior is in agreement with the energy-gap law for non-radiative transitions, which implies that internal conversion from CT state to ground state is facilitated by skeletal molecular vibrations. This intrinsic loss mechanism, which until now has not been thoroughly considered for OSCs, is different in its nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination. As a consequence, the theoretical upper limit for the power conversion efficiency of a single junction OSC reduces by 25% as compared to the Shockley-Queisser limit for an optimal optical gap of the main absorber between (1.45-1.65) eV.

CPP 70.2 Fri 10:30 ZEU 255

**Quantifying Coupling Rate Constants of Bound Charges to the Ground State and Free Charges in Organic Semiconductors** — ●SAFA SHOAAE<sup>1</sup>, MARTIN STOLTERFOHT<sup>1</sup>, and ARDALAN ARMIN<sup>2</sup> — <sup>1</sup>Institute for Physics and Astronomy, University of Potsdam, Potsdam, Germany — <sup>2</sup>School of Mathematics and Physics, University of Queensland, Australia

Bimolecular recombination of the free charges in the donor/acceptor organic solar cells has been considered as the main loss mechanism. For very few donor/acceptor systems the bimolecular recombination rate constant is shown to be lower than what predicted by the classic Langevin model. We and others have recently shown that this suppression may originate from weaker coupling rate of the so called interfacial charge transfer states to the ground state [Burk et al. AEM 2015, Armin et al. AEM 2016]. In Particular we have shown that recombination can be 150 times less than that predicted by Langevin model, resulting in efficiencies as high as 9%, at junction > 300 nm. These studies show the importance of the kinetic constants of the charge transfer states. Recently we have developed methodology to quantify these kinetic rates as well as charge generation efficiency in organic photovoltaic systems [Stolterfoht, Shoaee et al. Nature Comm 2016, Shoaee et al. Unpublished results], as well as determining the kinetic rate constants of the charge transfer states. These are pathway towards better understanding donor acceptor solar cells and optimise their photovoltaic performance for better efficiencies.

CPP 70.3 Fri 10:45 ZEU 255

**Energy losses in organic small molecule photovoltaics** — ●THERESA LINDERL, ALEXANDER HOFMANN, THOMAS ZECHEL, and WOLFGANG BRÜTTING — Universität Augsburg, 86135 Augsburg, Germany

One of the most important factors that limits the efficiency of organic photovoltaics is the relatively large energy loss between the optical gaps of the neat materials and the open-circuit voltage  $V_{OC}$ . Partly, this can be explained by the energetic offset between the energy levels of the donor and acceptor material, which is often called the driving force to form the charge transfer complex. The energy of this charge transfer complex is regarded as the upper limit for  $V_{OC}$  at 0 K. In contrast, at room temperature  $V_{OC}$  is further reduced by radiative and non-radiative recombination losses.

By combining different donors with fullerene and non-fullerene acceptor materials, we have investigated the influence of interface energetics, molecular orientation and morphology on the total energy loss in organic small molecule solar cells. We find, that for proper non-fullerene

acceptor materials the overall loss can be significantly reduced to about 0.6 eV, which is comparable to the best polymer solar cells.

CPP 70.4 Fri 11:00 ZEU 255

**Sensitive charge transfer state spectroscopy in organic solar cells** — ●MARTIN STREITER, ALEXANDER WAGENPFAHL, and CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The understanding of recombination mechanisms at donor-acceptor interfaces is of high importance for improving organic solar cells as the former determine both photocurrent and open circuit voltage. In order to investigate the influence of interface structure on charge transfer state recombination, we use confocal emission and excitation spectroscopy which we developed and applied to study the reorganisation energy of single molecules [1]. Sensitive measurements of both emission and excitation spectra on the timescale of seconds enable the characterisation of environmental and molecular conformational influences on dynamic spectral properties. Using this technique, we investigate the donor-acceptor charge transfer state in diluted bulk heterojunction systems. We discuss the impact of reorganisation energy and energetic disorder on the charge transfer state distribution in systems directly relevant for organic solar cells.

[1] M. Streiter, S. Krause, C. von Borczyskowski, C. Deibel, J. Phys. Chem. Lett., 7, 4281 (2016).

Invited Talk

CPP 70.5 Fri 11:15 ZEU 255

**Charge transfer states for organic opto-electronics** — ●KOEN VANDEWAL — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, George-Bähr-Strasse 1, 01062, Dresden, Germany

Intermolecular charge transfer (CT) states at the interface between electron-donating and electron-accepting (A) materials in organic thin films are characterized by absorption and emission bands within the optical gap of the interfacing materials. Depending on the used donor and acceptor materials, CT states can be very emissive, or generate free carriers at high yield. The former can result in rather efficient organic light emitting diodes, via thermally activated delayed fluorescence, while the latter property is exploited in organic photovoltaic devices and photodetectors. In this contribution, we will discuss the fundamental properties of CT states and link them to organic opto-electronic device performance. Furthermore, we introduce a new device concept, using an optical cavity resonance effect to boost CT absorption at photon energies below the optical gap of both donor and acceptor, enabling narrow-band, near infrared (NIR) photo-detection.

15 min break

CPP 70.6 Fri 12:00 ZEU 255

**Interfacial Energetics in Organic Multi-Heterojunctions by Charge-Transfer Emission** — ●CHRISTIAN KÄSTNER<sup>1</sup>, KOEN VANDEWAL<sup>2</sup>, DANIEL A. M. EGBE<sup>3</sup>, and HARALD HOPPE<sup>4</sup> — <sup>1</sup>Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Am Helmholtzring 1, 98693 Ilmenau, Germany — <sup>2</sup>Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), George-Bähr-Str. 1, 01069 Dresden, Germany — <sup>3</sup>Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Altenbergerstr. 69, 4040 Linz, Austria — <sup>4</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

Charge generation via exciton dissociation in organic solar cells requires donor-acceptor interfaces. Semi-crystalline phases of polymer and fullerene domains result in smaller energy gaps between the highest occupied molecular orbital and the lowest unoccupied molecular orbital as compared to the situation for amorphous phases. These molecular energy level shifts result in different interfacial charge transfer (CT) transitions depending on the disordered or ordered character of interfacing domains. In this work, a systematic variation of the order at the donor-acceptor interface was obtained via ternary blending of semi-crystalline and amorphous model polymers with a fullerene acceptor (PCBM). Using photo- and electroluminescence spectroscopy, various transition energies due to recombination across different donor-

acceptor interfaces could be detected.

CPP 70.7 Fri 12:15 ZEU 255

**Charge transfer recombination at planar hybrid inorganic/organic interfaces** — ●ULRICH HÖRMANN<sup>1</sup>, FORTUNATO PIERSIMONI<sup>1</sup>, STEFAN ZEISKE<sup>1</sup>, LUKAS HOFFMANN<sup>2</sup>, THOMAS RIEDL<sup>2</sup>, and DIETER NEHER<sup>1</sup> — <sup>1</sup>Universität Potsdam, Potsdam, Germany — <sup>2</sup>Bergische Universität Wuppertal, Wuppertal, Germany

The role of the intermolecular energy gap in all-organic donor/acceptor heterojunction (HJ) solar cells is well established. In the case of hybrid inorganic/organic HJs the situation is less clear. Recently, Piersimoni et al. have shown that the energy of the hybrid charge transfer (HCT) emission in electroluminescence experiments correlates with the interface energetics determined by UPS and with the open circuit voltage ( $V_{oc}$ ) of hybrid solar cells [1]. Here we focus on photovoltaic characterization of planar HJs between ZnO or SnO<sub>x</sub> acceptor layers and different organic donor materials. Tools well established for all-organic solar cells are carefully transferred to these hybrid systems and their validity is confirmed. Reconstruction of the dark jV-curve from light intensity dependent measurement of  $V_{oc}$  and the short circuit current gets rid of the otherwise drastic influence of the series resistance in these devices and allows access to the ideality factor associated with the hybrid interface. Temperature dependent characterization in a carefully chosen operation regime allows the extraction of an effective energy gap, whose origin is – opposed to all-organic HJs – not completely clear, yet. With our combined analysis, we shed light on the nature of HCT states and their role for recombination at metal oxide/organic interfaces.

[1] Piersimoni et al. / Phys. Chem. Lett. 6, 500 (2015)

CPP 70.8 Fri 12:30 ZEU 255

**Overcoming interfacial losses in solution-processed organic multi-junction solar cells** — ●XIAOYAN DU<sup>1</sup>, OLE LYTKEN<sup>1</sup>, HANSPETER STEINRÜCK<sup>1</sup>, RAINER H. FINK<sup>1</sup>, NING LI<sup>2</sup>, and CHRISTOPH BRABEC<sup>2</sup> — <sup>1</sup>Physical Chemistry 2 and ICMF Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Institute of Materials for Electronics and Energy Technology (i-MEET) Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) Martensstraße 7, 91058 Erlangen, Germany

We report on a systematic study of interface losses in both single- and multi-junction solar cells based on representative polymer donors and hole transporting layers (HTLs). It is found that a facile mixed HTL containing PEDOT:PSS and MoO<sub>x</sub> nanoparticles successfully overcomes the interfacial losses in both single- and multi-junction solar cells based on various active layers by reducing interface protonation, promoting better energy-level alignment, and forming a dense and smooth layer. Multi-junction solar cells with different polymers containing nitrogen atoms as the first layer and the mixed PEDOT:PSS and MoO<sub>x</sub> nanoparticles as HTL reach fill factor (FF) of over 60%, and power conversion efficiency (PCE) of over 8% [1], while the identical stack with pristine PEDOT:PSS or MoO<sub>x</sub> nanoparticles show significantly lower performance. This work is funded by the DFG within GRK 1896. [1] X. Du, et al, Adv. Energy Mater. 2016, DOI:10.1002/aenm.201601959

CPP 70.9 Fri 12:45 ZEU 255

**Following the Formation of Metal Electrodes for Organic Photovoltaics** — ●FRANZISKA LÖHRER<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, ALEXANDER HINZ<sup>3</sup>, OLEKSANDR POLONSKYI<sup>3</sup>, THOMAS STRUNSKUS<sup>3</sup>, FRANZ FAUPEL<sup>3</sup>, STEPHAN ROTH<sup>2,4</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, D-85748 Garching — <sup>2</sup>Deutsches Elektronensynchrotron DESY, D-22607 Hamburg — <sup>3</sup>CAU zu Kiel, Institut für Materialwissenschaft, D-24143 Kiel — <sup>4</sup>KTH, Teknikringen 56-58, SE-100 44 Stockholm

With their easy processability, high flexibility and tunable optical properties, organic photovoltaics offer a wide range of potential applications. Although based on organic materials, photovoltaic devices typically contain metal contacts due to their unrivaled electronic conductivity. These contacts have a major influence on the solar cell performance. Our work focuses on the nanostructure evolution of metal-polymer interfaces inherent in organic solar cells. We follow the morphological changes during the sputter deposition of metal electrodes onto photoactive layers using in-situ GISAXS and GIWAXS. This technique allows us to investigate the deposition process with a high spatial as well as temporal resolution. Comparing the deposition behavior of typical electrode materials (such as Au or Al) on thin films of photoactive organic materials (e.g. PTB7) helps to understand their influence on the respective photovoltaic performance.

CPP 70.10 Fri 13:00 ZEU 255

**Procedures and Practices for Evaluating Thin-Film Solar Cell Stability** — ●ROLAND RÖSCH<sup>1</sup>, TOBIAS FABER<sup>1</sup>, MONICA LIRACANTU<sup>2</sup>, ELIZABETH VON HAUFF<sup>3</sup>, THOMAS BROWN<sup>4</sup>, and HARALD HOPPE<sup>1</sup> — <sup>1</sup>CEEC Jena, FSU Jena — <sup>2</sup>ICN2, Barcelona — <sup>3</sup>Vrije Universiteit Amsterdam — <sup>4</sup>University of Rome "Tor Vergata"

Novel thin film PV technologies require an attestation of their stability in order to get ready for their qualification. In order to improve the understanding of degradation effects and how they can be prevented, stress testing under different conditions is commonly applied. By careful combination of stress factors and thorough analysis of photovoltaic parameter decaying curves, an understanding of the underlying degradation pathways can be gained. With the help of standardized and accelerated stress tests, as described in the ISOS-protocols [1], statements concerning application lifetimes can finally be made and compared among different labs. Once a photovoltaic technology has proven long lasting durability, the ultimate barrier for entering the commercial market are the IEC tests, taking a deeper look on overall safety and reliability, not only on durability. Here, the most prominent stress tests are reviewed, discussed and extended with respect to learning the most about photovoltaic device stability [2]. The most prominent outcome of this discussion an analytical determination of the \*burn-in\* time (tS) and furthermore the operational lifetime (tS80) and the lifetime energy yield (LEY), a newly introduced figure of merit as a measure for the energy a solar cell can produce during its lifetime. [1] Reese, SOLMAT, 95 (2011) 1253-1267 [2] Roesch, AEM, 5 (2015) 1501407