

CPP 1: Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies I

Organized by Dieter Neher and Christoph J. Brabec

Time: Monday 9:30–13:00

Location: GÖR 226

Invited Talk CPP 1.1 Mon 9:30 GÖR 226
Strategies for advancing the performance of organic photovoltaics — ●THOMAS ANTHOPOULOS — King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Kingdom of Saudi Arabia

The dramatic advances in the power conversion efficiency (PCE) of organic photovoltaics (OPVs) witnessed in recent years have been primarily driven by the development of new materials and the minimization of performance losses associated with conventional cell architectures. This talk will discuss our recent OPV work, focusing on practical strategies for boosting cell performance. I will first discuss using low-dimensional charge-extracting interlayers and the numerous advantages of these innovative materials for next-generation OPVs. I will then present recent progress in using molecular dopants to improve the PCE of OPVs and how their combination with innovative interlayers can improve the material utilisation and circularity of the ensuing OPV cells without compromising their performance.

CPP 1.2 Mon 10:00 GÖR 226
Can Organic Solar Cells Beat the Near-Equilibrium Thermodynamic Limit? — TANVI UPRETI¹, ●CONSTANTIN TORMANN², and MARTIJN KEMERINK^{1,2} — ¹Complex Materials and Devices, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — ²Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany

Switching to non-fullerene acceptors has led to an impressive increase in power conversion efficiencies (PCEs) of organic photovoltaic cells over the past decade. Despite this, the PCE of such devices is still below the near-equilibrium limit of the corresponding material, which is particularly evident from losses in the open-circuit voltage (V_{oc}). A prominent yet incompletely understood loss channel affecting V_{oc} is the thermalization of photogenerated charge carriers in the density of states, which is broadened by energetic disorder. In contrast to symmetric morphologies like classic bulk heterojunctions, morphologies with a gradient in the donor:acceptor ratio can mitigate this loss channel by rectifying the diffusive motion of the thermalizing photogenerated charge carriers. Here, we show by extensive numerical modelling how funnel-shaped donor and acceptor-rich domains in a phase-separated morphology promote directed transport of positive and negative charge carriers towards the anode and cathode, respectively. In such optimized funnel morphologies, this kinetic, nonequilibrium effect even allows one to surpass the near-equilibrium thermodynamic limit for the same active material in the absence of gradients.

CPP 1.3 Mon 10:15 GÖR 226
Transparent Conductive Electrodes: Figure of Merit Revisited for Photovoltaics — ●HARALD HOPPE — Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany — Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany

Figure of Merits (FOMs) are meant to provide a simple means for assessing the suitability of a certain material for or compartments within devices in general. In case of photovoltaic devices, the role of the transparent conductive electrode is to allow as much as possible light to enter into the device as well as to enable current flow out of the device. Over the last 5 decades a number of FOMs were introduced based on several approaches. Here we present a rather novel, yet implicit approach for an FOM, which is highly suitable for photovoltaics, allowing to assess the potential photovoltaic performance quantitatively.

CPP 1.4 Mon 10:30 GÖR 226
Reconnoitering the impact of fluorination on both donor and non-fullerene acceptor in bulk heterojunction organic photovoltaics — ●SHAHIDUL ALAM¹, JAFAR I. KHAN¹, VOJTĚCH NÁDAŽDÝ³, TOMÁŠ VÁRY³, AURELIEN D. SOKENG², MD MOJIB ISLAM², CHRISTIAN FRIEBE², WEJDAN ALTHOBAITI², MARTIN HAGER², ULRICH S. SCHUBERT², CARSTEN DEIBEL⁴, DENIS ANDRIENKO⁵, FRÉDÉRIC LAQUAI¹, and HARALD HOPPE² — ¹KAUST

Solar Center (KSC), Kingdom of Saudi Arabia — ²FSU Jena, Germany — ³Slovak Academy of Sciences, Bratislava — ⁴TU Chemnitz, Germany — ⁵MPIP, Mainz, Germany

Organic solar cells' performance can be often effectively improved through fluorination of the donor and/or non-fullerene acceptor (NFA). The end-group fluorination of the well-known NFA ITIC yields further extension of the absorption spectrum to the near infrared, which results in an increment of the device's photocurrent as compared to the non-fluorinated version. Herein, ITIC and two fluorinated variants of ITIC (ITIC-2F* and ITIC-4F) were synthesized and systematically investigated the influence of end-group fluorination physicochemical properties, optical properties, and photovoltaic performance. Photovoltaic parameters are discussed in terms of exciton quenching, charge generation, charge dissociation, and recombination losses. Specifically, it is found that fluorinated acceptors control the devices' open circuit voltage. All the results shed light on the importance of the energy landscape and the quadrupole moment of acceptor beyond the underlying donor-acceptor interface.

CPP 1.5 Mon 10:45 GÖR 226
Synthesis and Characterization of Organic Heterojunction Model Interfaces — ●HANBO YANG¹, JARVIST MOORE FROST¹, JENNY NELSON¹, and HUGO BRONSTEIN² — ¹Imperial College London, London, UK — ²Cambridge University, Cambridge, UK

Control of the molecular configuration at the interface of an organic heterojunction is key to the development of efficient optoelectronic devices. Due to the difficulty in characterizing these buried and (likely) disordered heterointerfaces the interfacial structure in most systems remains a mystery. Here, we demonstrate a novel synthetic strategy to design and control model interfaces, allowing for their detailed study in isolation from the bulk material. This is achieved by the synthesis of a donor polymer-non-fullerene acceptor 'through space' linked system, where the exact position and orientation of the moieties is completely controlled and we furthered showed that the kinetics of charge separation can be tuned using transient absorption spectroscopy and excited state calculations.

CPP 1.6 Mon 11:00 GÖR 226
Direct Determination of the Photogenerated Free Charge Carrier Luminescence in Organic Solar Cells via Transient Photoluminescence Measurements — ●JARED FAISST, MATHIAS LIST, and ULI WÜRFEL — Fraunhofer ISE, Freiburg, Deutschland

Photoluminescence (PL) measurements have shown to be a valuable tool characterizing the optoelectronic properties of semiconductors. In organic solar cells, the PL measurement of free charge carriers is hindered by the strong and spectrally broad luminescence of non-dissociated local exciton recombination. Therefore, the PL of free charge carriers under steady state condition is not directly detectable. To overcome this problem, we make use of the vastly different lifetimes of local excitons (ps-ns) and free charge carriers (μ s). In this work, we present experimental time resolved PL data of a fullerene based D18:PC₇₁BM and two non-fullerene based D18:Y6 and PV-X plus organic solar cells and demonstrate the possibility to separate the luminescence of local excitons from the one of free charge carriers. We further show that the luminescence of the free charge carriers indeed correlates with the quasi-Fermi level splitting as expected. Hence, this novel measurement technique eventually allows to investigate free charge carriers in organic absorber layers directly. This is of great importance to further understand recombination mechanisms and degradation effects and to identify optimization potentials.

15 min. break

Invited Talk CPP 1.7 Mon 11:30 GÖR 226
Lost in translation? Transport resistance in organic solar cells — ●CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

With the advent of non-fullerene acceptors, breaking the 20 % power

conversion efficiency limit is within close reach for organic solar cells. Understanding the efficiency-limiting processes remains important.

I will discuss how losses in the fill factor can be due to the transport resistance, a voltage loss because of a low conductivity in the active layer. Its relevance for organic solar cells was only shown a half dozen years ago [1]. I will present transport resistance limiting different organic solar cell types, and then focus on fresh and thermally degraded PM6:Y6 solar cells (heated to 85°C, in the dark, under nitrogen atmosphere), a state-of-the-art system based on the non-fullerene Y6. The increasing fill factor losses on this degradation path are because of the transport resistance [2]. The reason seems to be trap formation in the tail states, which decrease the active layer conductivity.

- [1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat. Commun. 6, 6951 (2015).
- [2] C. Wöpke, C. Göhler, M. Saladina, X. Du, L. Nian, C. Greve, C. Zhu, K. M. Yallum, Y. J. Hofstetter, D. Becker-Koch, N. Li, T. Heumüller, I. Milekhin, D. R. T. Zahn, C. J. Brabec, N. Banerji, Y. Vaynzof, E. M. Herzog, R. C. I. MacKenzie, C. Deibel. Nat. Commun. 13, 3786 (2022).

CPP 1.8 Mon 12:00 GÖR 226

Thermal Degradation Mechanism in PM6: Y-series Acceptors Organic Solar Cells — •SI CHEN, JULIEN GORENFLOT, and LAQUAI FREDERIC — Abdullah University of Science and Technology Thuwal 23955-6900, Saudi Arabia

The stability issue is the core restriction for the application of organic solar cells (OSCs), and the study of the degradation mechanism of high-efficient PM6: Y-series systems is an urgent problem to be solved. We concluded one specific pathway of FF degradation for typical PM6:Y-series acceptors organic solar cells since FF changed most obviously after thermal aging. After developing several characterization measurements, including time-delayed collection field (TDCF), light intensity dependent measurements, etc. to study the photo-physics of PM6:Y-series solar cells before and after thermal degradation, we can quantify FF degradation with field-dependent charge generation, non-geminate recombination, and transport resistance factors. The effect of transport resistance is quantified by the Suns-Voc method. The results show that the increase of charge transport resistance is the primary factor leading to FF degradation, which can be further explained by excessive phase separation with the information from GIWAXS and AFM. Our work can not only provide material design ideas for highly efficient and stable organic solar cells by figuring out the thermal degradation mechanism of PM6:Y-series organic solar cells but also come up with a new methodology to quantify the FF degradation of organic solar cells.

CPP 1.9 Mon 12:15 GÖR 226

Photophysics of Poly(3-hexylthiophene):Non-Fullerene Acceptor Based Organic Solar Cells — •WEJDAN ALTHOBAITI, JAFAR KHAN, JULIEN GORENFLOT, SHAHIDUL ALAM, GEORGE HARRISON, STEFAAN DE WOLF, and FRÉDÉRIC LAQUAI — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Saudi Arabia

Charge generation can proceed through two different paths in Bulk Heterojunction based organic solar cells which are electron transfer from donor to acceptor and hole transfer from acceptor to donor. These processes can be controlled by Electron Affinity (EA) offsets and Ionization Energy (IE) offsets, respectively. Understanding the relationship between the IE offsets, EA offsets between donor and acceptor materials, and the performance of OSCs could improve the charge generation efficiency. We characterized the impact of large IE and EA

offsets on device performances and more precisely on the internal quantum efficiency (IQE) using a wide bandgap polymer donor which has shallow IE such as P3HT and Non Fullerene Acceptor (NFA). This provides a wide range of diagonal bandgap (IE of the donor and EA of the acceptor). Thus, enables us to find the relation between small diagonal bandgap and the decrease of the IQE in energy gap law framework. Low IQE while high exciton quenching observed can be explained due to charge recombination as our results demonstrated by geminate and non-geminate recombination.

CPP 1.10 Mon 12:30 GÖR 226

Efficient Nanoscale Exciton Transport in Non-fullerene Organic Solar Cells Enables Reduced Bimolecular Recombination of Free Charges — •DREW B. RILEY¹, OSKAR J. SANDBERG¹, NASIM ZARRABI¹, RYUN KIM², PAUL MEREDITH¹, and ARDALAN ARMIN¹ — ¹Swansea University, Swansea, Wales. — ²Cambridge University, Cambridge, UK

The origins of reduced bimolecular recombination in high efficiency OPV-based solar cells are debated, and mechanisms related to the charge-transfer (CT) state and free-carrier encounter dynamics have been proposed as underlying factors.[1] Further, it is expected that the CT-state dynamics is strongly influenced by exciton dynamics in low off-set blends.[2]

In this presentation I will explore the role exciton dynamics play in the charge generation and recombination processes. Specifically, I will introduce a photoluminescence-based probe to quantify the acceptor domain size in OPV blends. It will be shown that NFA-based blends form larger domains than fullerene-based systems but that this increase is unable to account for the observed non-Langevin recombination. Further, I will show that the reduction of bimolecular recombination is correlated with enhanced exciton dynamics within the NFA domains. This indicates that the processes responsible for efficient exciton transport also enable strongly non-Langevin recombination in high efficiency NFA-based solar cells with low energy offsets.

- [1] A. Armin, et.al. AEM, 11, 2003570, 2021.
- [2] A. Classen, et.al. Nat. Energy, 5, 2020.

CPP 1.11 Mon 12:45 GÖR 226

Power-law density of states in organic solar cells revealed by the open-circuit voltage dependence of the ideality factor — •MARIA SALADINA¹, CHRISTOPHER WÖPKE¹, CLEMENS GÖHLER¹, IVAN RAMIREZ², OLGA GERDES², CHAO LIU^{3,4}, NING LI^{3,4,5}, THOMAS HEUMÜLLER^{3,4}, CHRISTOPH J. BRABEC^{3,4}, KARSTEN WALZER², MARTIN PFEIFFER², and CARSTEN DEIBEL¹ — ¹Technische Universität Chemnitz, Germany — ²Heliatic GmbH, Germany — ³FAU Erlangen-Nürnberg, Germany — ⁴Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Germany — ⁵South China University of Technology, China

We determine the density of states (DOS) in disordered semiconductors via the diode ideality factor (n_{id}). We employ illumination intensity and temperature-dependent open-circuit voltage measurements. In amorphous silicon, we found that n_{id} only depends on the temperature, and can be explained by an exponential DOS distribution.

For the organic donor-acceptor solar cells, we find that n_{id} is not only temperature but also light intensity-dependent. The seemingly unsystematic dependence of n_{id} on the light intensity becomes systematic once the former is displayed in dependence of the open-circuit voltage, which is a means to sample the DOS distribution at a certain energetic depth. This evaluation approach leads to our central result: the DOS follows a power-law distribution over a broad range of energies. In particular, for the investigated organic solar cells under working conditions the DOS is best represented by the power-law, not a gaussian or exponential one.