

CPP 11: Focus: Organic Solar Cells Based on Non-fullerene Acceptors: Loss Mechanism and Options for Above 20 % Efficiencies II

Organized by Dieter Neher and Christoph J. Brabec

Time: Monday 15:00–17:15

Location: GÖR 226

Invited Talk CPP 11.1 Mon 15:00 GÖR 226
Quantifying the potential of organic solar cells using luminescence measurements and modelling — ●JENNY NELSON — Department of Physics, Imperial College London, SW7 2AZ, UK

In a molecular photovoltaic device, charge separation and energy conversion result from the evolution of a photogenerated exciton into a charge separated state, in competition with recombination to ground. Recently, new molecular materials have increased power conversion efficiency to approach 20%. To make further advances, we need to understand and isolate the effects of chemical structure, molecular packing, energetics and disorder on the competition between charge separation and recombination and hence on device efficiency. Electro- and photoluminescence have proved to be valuable tools to probe the energy and dynamics of excited states involved in photoinduced charge separation, and indirectly of the structure of molecular interfaces. Combined with other spectroscopic techniques, electrical measurements and modelling, luminescence can help us to understand how chemical and physical structure control the basic mechanisms in photovoltaic conversion. We show how such an approach can be used to study the properties and role of charge transfer states, the impact of structural and energetic disorder and to infer structure-property relationships. We apply a computational model that integrates the molecular charge transfer process with a one-dimensional drift-diffusion simulation to interpret experimental measurements and explore the effects of parameters on device performance. We consider the ultimate limits placed on solar to electric conversion by the molecular nature of the materials.

CPP 11.2 Mon 15:30 GÖR 226
Increasing the ionization offset to increase the quantum efficiency in non-fullerene acceptor based organic solar cells: How far can we go? — ●JULIEN GORENFLOT, WEJDAN ALSUFYANI, MARYAM ALQURASHI, SRI HARISH KUMAR PALETI, ANIRUDH SHARMA, DERYA BARAN, and FRÉDÉRIC LAQUAI — KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia

Molecular engineering offers a virtually unlimited number of unique semiconductors for organic photovoltaics applications, that can be tailored to adapt specific needs, but only a handful of combinations enables to reach state-of-the-art efficiencies. Rules are thus strongly needed to guide the design of promising systems. A recently unraveled rule is that the electron acceptor molecule requires an ionization energy 0.5 eV deeper than that of the electron donor to overcome the bending of the energy levels at the donor acceptor heterojunction interface, maximizing the charge transfer, hence the cell's quantum efficiency. Here we study the energy losses associated to this ΔIE increase. Based on 30+ blends, we show that those losses remain minimal up to an offset of 0.7 eV. We then use electroluminescence spectroscopy to evaluate the charge transfer state energy (E_{CT}) and find that this low energy losses range is associated to E_{CT} remaining at most similar to the NFA's optical bandgap ($E_{g,NFA}$), while further ΔIE increase pulls E_{CT} below $E_{g,NFA}$, accordingly decreasing V_{OC} . We finally study the evolution of the fill factor (FF) within this maximum quantum efficiency – minimal energy losses ΔIE range.

CPP 11.3 Mon 15:45 GÖR 226
The excess energy optimum to minimize recombination losses in organic solar cells — ●CLEMENS GÖHLER, ALEXANDER FLAMM, and MARTIJN KEMERINK — Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg, Im Neunheimer Feld 225, 69120 Heidelberg

Semiconductor blends that incorporate non-fullerene acceptors (NFA) have pushed organic solar cells to efficiency records based on an established principle: enhancing the generation yield of free charge carriers from tightly bound molecular excitations via interfacial charge transfer between donor and acceptor phases. Their success can in huge parts be attributed to an increase of the photocurrent; however, in comparison to less-effective systems, NFA blends possess a similar overall absorbance and lack the distinct low-energy absorption typically associated with charge transfer (CT) excitons.

The increased charge carrier densities are thus based on reduced recombination yields. As further improvements of the photocurrent are necessary to reach higher efficiencies, a thorough understanding of the mechanisms behind the cut in recombination losses compared to fullerene solar cells is invaluable. To contribute, we have investigated recombination signatures of both systems with respect to the available excess energy by combining field and excitation dependent electro-optical absorption spectroscopy in the steady state and close to solar cell working conditions with kinetic Monte-Carlo simulations. Our findings indicate towards an optimal excess energy which minimizes non-geminate recombination in CT processes.

CPP 11.4 Mon 16:00 GÖR 226
On the impact of the energy level offset on carrier recombination in organic non-fullerene acceptor-based solar cells — ●NURLAN TOKMOLDIN¹, BOWEN SUN¹, FLORIANA MORUZZI², OBAID ALQAHTANI³, BRIAN COLLINS³, IAIN MCCULLOCH², DIETER NEHER¹, and SAFA SHOAEI¹ — ¹University of Potsdam, Potsdam-Golm, Germany — ²University of Oxford, Oxford, UK — ³Washington State University, Pullman, USA

The energetic offset between the highest occupied molecular orbital (HOMO) levels of the donor and acceptor components of the organic photovoltaic (OPV) blends is well-known to affect the efficiency of the singlet exciton (S1) dissociation into separated charges (CS) via the charge-transfer (CT) state, however the impact of this offset on bimolecular recombination of free charge carriers has not been explored. In this study, using three different non-fullerene acceptors Y6, ITIC and o-IDBTR, blended with the same donor polymer PM6, we demonstrate that, apart from reducing the driving force for charge generation, diminishing HOMO-HOMO energy offset also activates exciton reformation as a channel for bimolecular recombination of free charges. This is accompanied by the rise in the respective bimolecular recombination coefficient, which in turn influences the device fill-factor. Using the comparison between PM6:ITIC and PM6:o-IDBTR, we show that neither morphology, nor carrier mobilities can on their own explain the observed difference in performance, signaling the importance of the energy landscape in controlling the OPV device efficiency, both through generation and recombination of charge carriers.

15 min. break

CPP 11.5 Mon 16:30 GÖR 226
Relating free charge carrier generation and field induced photoluminescence quenching in a non-fullerene-based organic blend with a low energy offset — ●MANASI PRANAV¹, THOMAS HULTZSCH¹, BOWEN SUN¹, RONG WANG², SAFA SHOAEI¹, LARRY LÜER², CHRISTOPH BRABEC², and DIETER NEHER¹ — ¹Institute of Physics and Astronomy, University of Potsdam, 14476 Germany — ²Institute of Materials for Electronics and Energy Technology (i-MEET), Friedrich-Alexander-Universität Erlangen-Nürnberg Martensstrasse 7, 91058 Erlangen, Germany

Many studies currently target the process of free charge carrier generation and recombination in relation to the energy level offset in organic blends based on non-fullerene acceptors (NFA). Here, we add to this discussion with a focus on the NFA Y5, characterized by a smaller highest occupied molecular orbital offset in PM6:Y5 compared to PM6:Y6, despite molecular similarity between Y5 and Y6. We find that the PM6:Y5 blend exhibits a pronounced field-dependence of free charge generation, as measured with the time-delayed collection field (TDCF) technique. We verify this with a new arbitrary-waveform TDCF technique that provides finer control over the time-delay parameters. In addition to this, we also observe a surprisingly pronounced effect of the electric field on both the steady state photoluminescence (PL) intensity and the transient PL lifetime. These results indicate that the field dependence of photo-current, free charge carrier generation and PL quenching in this low-offset system are governed by the same mechanism: likely field-induced exciton dissociation.

CPP 11.6 Mon 16:45 GÖR 226

Field Dependent Exciton Dissociation in Single-Component Organic Non-fullerene Acceptor Solar Cells — ●FLURIN EISNER, MOHAMMED AZZOUZI, and JENNY NELSON — Blackett Laboratory, Imperial College London, South Kensington, SW7 2AZ, UK

Improvements in the molecular design of non-fullerene acceptors (NFAs) has almost doubled the power-conversion efficiency (PCE) of organic photovoltaics in the last 5 years, from 11 to 19%. However, the exact molecular reasons behind why some acceptors (e.g. Y-series) perform better than others (e.g. ITIC-series) remain unclear. Interestingly, recent studies have shown that some the most efficient non-fullerene acceptors can achieve relatively high charge-generation efficiency in the absence of a donor-acceptor interface, challenging the current understanding of how photogenerated excitons dissociate into free charges in organic solar cells.

Here, we study the charge-generation processes in a series of NFA molecules in single-component devices, including A-DA*D-A-type acceptors (e.g. Y6) and A-D-A type acceptors (e.g. ITIC) using optoelectronic and spectroscopy characterisation methods under strong applied fields and at different temperatures. By combining experimental results with molecular and device-level calculations, we link exciton and charge dissociation efficiency in NFA films to molecular parameters such as reorganisation energy and electronic coupling. We use this to suggest how to design materials with both higher single-component device performance and how to improve heterojunction device performance beyond 20% PCE.

CPP 11.7 Mon 17:00 GÖR 226

Triplet Excitons and associated Efficiency-Limiting Pathways in NFA-based Organic Solar Cell Blends — JEANNINE GRÜNE^{1,2}, GIACOMO LONDI³, ALEXANDER J. GILLETT², YOANN OLIVIER³, VLADIMIR DYAKONOV¹, and ●ANDREAS SPERLICH¹ — ¹Experimental Physics 6, Julius Maximilian University of Würzburg, Germany — ²Cavendish Laboratory, University of Cambridge, UK — ³Laboratory for Computational Modeling of Functional Materials, Université de Namur, Belgium

Organic solar cells (OSC) have made great progress in recent years, but are now reaching a performance plateau. Triplet states are known to adversely affect efficiency by opening a channel for non-radiative recombination pathways. Here, we use the complementary spin-sensitive methods of photoluminescence detected magnetic resonance (PLDMR) and transient electron paramagnetic resonance (trEPR) corroborated by transient absorption and quantum-chemical calculations to unravel exciton pathways in OSC blends employing the (non-) halogenated polymer donors PBDB-T, PM6 and PM7 together with NFAs Y6 and Y7. We reveal that all blends form triplet excitons on the NFA populated via non-geminate hole back transfer and, in blends with halogenated donors, also by spin-orbit coupling driven intersystem crossing. Identifying these triplet formation pathways in all tested solar cell absorber films highlights the untapped potential for improved charge generation to further increase efficiencies.