

CPP 36: Organic Electronics and Photovoltaics III

Time: Thursday 9:30–13:00

Location: H 0110

CPP 36.1 Thu 9:30 H 0110

How 'Hot' are the Charges in OPV? — ●PRIYA VIJI, CONSTANTIN TORMANN, CLEMENS GÖHLER, DOROTHEA SCHEUNEMANN, and MARTIJN KEMERINK — IMSEAM, Universität Heidelberg, Germany

The question of whether charge transport in operational organic solar cells (OSC) occurs far-from-equilibrium or not is of practical and fundamental importance. While the equilibrium picture of the OSC assumes that the photogenerated charge carriers quickly lose their energy and attain lattice temperature, kinetic Monte Carlo (kMC) simulations of OSC have consistently shown that photogenerated charges are extracted before reaching thermal equilibrium energy: the population relaxes, albeit to an effective temperature that exceeds that of the lattice. In this work, we use Johnson thermometry to measure the temperature of the photogenerated carriers by noise spectroscopy. Two systems, P3HT:PCBM and PM6:Y6, are tested against their inorganic counterpart, silicon. The experiments prove, in contrast to silicon PV, charges in operational OSC are not thermalized and are almost twice as hot as the lattice. The experimental findings are confirmed by kMC simulations, which show that the energetic disorder in organic semiconductors is the reason for slow thermalization as well as high effective temperature. Our results imply that OSCs are far from equilibrium systems, which opens realistic prospects to mitigate the thermalization losses and eventually beat the near-equilibrium thermodynamic limit. In fact, the results show that a regular OSC is Hot-Carrier Solar Cell in the sense that excess energy contributes to output power.

CPP 36.2 Thu 9:45 H 0110

Energetic landscape of fluorinated and non-fluorinated donors and non-fullerene acceptors in bulk heterojunction organic photovoltaics — SHAHIDUL ALAM¹, JAFAR I. KHAN², VOJTECH NÁDAŽDY³, TOMÁŠ VÁRY³, AURELIEN D. SOKENG⁴, MD MOJIBUL ISLAM⁴, CHRISTIAN FRIEBE⁴, WEJDAN ALTHOBAITI¹, WENLAN LIU⁵, MARTIN HAGER⁴, ULRICH S. SCHUBERT⁴, CARSTEN DEIBEL⁶, DENIS ANDRIENKO⁵, FRÉDÉRIC LAQUAI¹, and ●HARALD HOPPE⁴ — ¹KAUST, Saudi Arabia — ²University of Hull, UK — ³Slovak Academy of Sciences, Slovak Republic — ⁴IOMC/CEEC, Jena, Germany — ⁵MPIP, Mainz, Germany — ⁶TU Chemnitz, Germany

Performance improvement of OSCs via fluorination of the D and/or NFA is an effective method. The end-group fluorination of the well-known NFA ITIC yields further extension of the absorption to the NIR, which increases the SC's J_{ph} compared to the non-fluorinated version. Herein, ITIC and two of its fluorinated variants were synthesized and systematically investigated concerning the influence of end-group fluorination on physicochemical, optical, and photovoltaic properties. DFT calculations show that fluorination increases the EA of the acceptor and, therefore, reduces the Voc of the built devices. On the other hand, the molecular quadrupole moment increases with the degree of fluorination leads to more efficient dissociation and reduced recombination of CT-states at the D-A interface. At the same time, IE increases, thus increasing the driving force for CT-state formation. The collected and presented results herein shed light on the importance of the energetic landscape at the D-A interface and how this deviates from general expectations when consulting the pristine materials.

CPP 36.3 Thu 10:00 H 0110

Optimizing Thermal Annealing Sequences for Enhanced Photovoltaic Performance in Organic Solar Cells — ●HAYA ALDOSARI^{1,2}, SHAHIDUL ALAM¹, JOSÉ JURADO¹, and FRÉDÉRIC LAQUAI¹ — ¹King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia — ²Department of Physics, College of Science, Imam Abdulrahman Bin Faisal University, P.O. Box 383, 31113, Dammam, Saudi Arabia

Thermal annealing is a widely used approach in organic solar cell research aimed at enhancing the performance of these devices. Therefore, the bulk heterojunction of PBDB-T:IT-2F was subjected to thermal annealing at various phases of the fabrication process to examine the impact of annealing on the photovoltaic characteristics. Several optoelectronic methods were employed to investigate the kinetics of charge recombination and the process of charge extraction. Based on

the results of our investigation, it has been observed that both post-annealing and 2-stage-annealing methods contribute to the enhancement of fill factor and power conversion efficiency. However, the latter method has even greater advantages. Further research explores the impact of annealing on the hole transport layer (MoOx). The work function of MoOx was enhanced during the annealing process, leading to an increase in the internal electric field and a higher rate of charge carrier extraction. Finally, field-dependent charge generation processes were investigated using time-delayed collection field measurements.

CPP 36.4 Thu 10:15 H 0110

Role of energetic offset in low-offset organic solar cells and its effect on loss pathways — ●BOWEN SUN and SAFA SHOAEI — Institute of Physics and Astronomy, University of Potsdam, Germany

While efficient charge generation despite ultra-low energy offsets (down to 0 eV offsets) between donor and acceptor in non-fullerene acceptor (NFA) based organic solar cells (OSCs) has been often reported, the physical meaning of this observation is discussable and unclear.

In this work, we have performed advanced optoelectronic and morphology characterization, as well as optical simulation for a series of donor:NFA systems. The energetic offsets between CT and excitons, as well as the effect of this energetic offset on the carrier loss pathways in different bias conditions have been studied in detail. From our work, we reached several important conclusions: 1) the short circuit current density and fill-factor of low-offset systems are largely determined by a field-dependent exciton dissociation yield. 2) The energetic offset also affects the recombination dynamics. Our analysis clearly shows that this enhanced recombination is contributed by a highly non-radiative channel, indicating the significance of triplet states in the recombination process. 3) It is strongly indicated that the charge generation and recombination (losses) proceed via different energetic states. The losses during charge generation process occur via highly radiative channels, while that during charge recombination process proceed via highly non-radiative channels. In general, our study clarifies the role and effect of energetic offset in low-offset OSCs, and provides a guideline for the further improvement of OSCs.

CPP 36.5 Thu 10:30 H 0110

Photophysics of Poly(3-hexylthiophene): Non-Fullerene Acceptor Based Organic Solar Cells — ●WEJDAN ALTHOBAITI, JULIEN GORENFLOT, CATHERINE DE CASTRO, JAFAR KHAN, SHAHIDUL ALAM, CHRISTOPHER PETOUKHOFF, 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, Saudi Arabia

The efficiency of P3HT:Non-fullerene acceptor (NFA) based solar cells lacks considerably behind many other polymer donor:NFA systems. For reasons which are yet incomprehensible. Here, we report on a series of P3HT:NFA solar cells, and elucidate the origin of performance losses in terms of the photophysical processes. It is a matter of fact that the interfacial ionization energy (IE) offset is a critical parameter in NFA-based blends in determining the efficiency of the exciton-to-charge transfer (CT) state conversion. We show that while large IE offsets in excess of >0.9 eV still facilitate complete exciton quenching, the device internal quantum efficiency (IQE) is limited by geminate and / or non-geminate recombination processes in P3HT-based photoactive blends. Our finding shows a drop in IQE when the diagonal bandgap of the photoactive blend i.e the difference between the IE of the donor and the electron affinity (EA) of the acceptor is small irrespective of the IE offset. Understanding the relation between the IE offsets, EA offsets at the interface of donor and acceptor materials, and the performance of organic solar cells could improve the charge generation efficiency.

CPP 36.6 Thu 10:45 H 0110

Correlating the morphology of PTQ-2F:BTP-4F organic solar cells through scattering and real space methods — ●LUKAS V. SPANIER¹, JULIAN E. HEGER¹, RENJUN GUO¹, MATTHIAS SCHWARTZKOPF², HARISHANKAR BALAKRISHNAN³, RACHID HOUSSAINI³, STEPHAN V. ROTH², ACHIM HARTSCHUH³, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — ²DESY, 22607 Hamburg, Germany — ³LMU, Department Chemie und CeNS, 81377

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Lately, organic solar cells (OSCs) have gained increasing attention due to their rapidly increasing efficiencies as well as the relatively easy scalability in their manufacture. To make the manufacturing process of the bulk-heterojunction (BHJ) more environmentally friendly, increased efforts have recently been made to use halogen-free solvents, which, however, can lead to reduced efficiencies.

We investigate the changes in morphology and performance stability of PTQ-2F:BTP-4F organic solar cells processed from various halogenated and non-halogenated solvents, utilizing operando grazing-incidence wide and small angle X-ray scattering (GIWAXS/GISAXS) during illumination and solar cell operation. We further show the impact of solvents on the mesoscopic distribution of small molecules within the bulk heterojunction through scattering-type scanning near-field optical microscopy.

CPP 36.7 Thu 11:00 H 0110

Polymer Donors vs. Small Molecule Donors for Solar Cells — ●ELIFNAZ SAĞLAMKAYA and SAFA SHOAE — Disordered Semiconductor Optoelectronics, Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam-Golm, Germany

All small molecule (ASMs) solar cells have great potential to actualize the commercialization of organic photovoltaics owing to their higher solubility, lesser batch-to batch variety and simpler synthesis routes compared to the blend systems that utilize conjugated polymers. However, the efficiency of the ASMs are slightly lacking behind the polymer: small molecule single heterojunctions. To address this discrepancy, we compare a small molecule donor ZR1 and polymer PM7 blended with Y6 acceptor. Our temperature dependent electroluminescence quantum efficiency analysis reveals the same energetic offset between the charge transfer state and the singlet energy (ΔE_{S1-CT}) in PM7:Y6 and ZR1:Y6. Surprisingly, the ZR1:Y6 has noticeably stronger field-dependency of charge generation. Furthermore, the energy barrier for charge generation is quite high (100 meV) for the ZR1:Y6 system unlike the PM7:Y6 (10 meV). Low charge carrier mobilities of ZR1:Y6 measured from the space charge limited currents entail a viable explanation for energy barrier for the charge generation. On the other hand, the maximum power point tracking measurements show a higher stability of ZR1:Y6, exhibiting a tradeoff between efficiency and stability.

15 min. break

Invited Talk CPP 36.8 Thu 11:30 H 0110
Digital luminescence: Novel platform for minimalistic photonic applications based on programmable luminescent tags

— ●SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Information is everywhere and with the ever-growing thirst for data in the digital age, solutions for information storage and exchange need to advance. Barcodes and QR-codes are the current systems for passive information distribution in all sectors (B2B, B2C, and private). In this talk, I will present an advanced system for information storage and exchange based on luminescence of organic molecules. In contrast to passive printed codes, these programmable luminescent tags (PLTs) allow for non-contact writing, erasing, and re-writing, thus allowing much more use scenarios where the interaction with the data is essential. The system's core functionality is based on the phosphorescence of organic emitters, which can be turned on or off depending on the presence or absence of nearby molecular oxygen, respectively. These emitters are embedded in special transparent polymer foils, rendering the PLTs invisible when not used. Following the discussion of the general concept of PLTs, I will give an update on our recent efforts towards such systems made from biodegradable materials to demonstrate their potential as environmentally-harmless functional systems.

CPP 36.9 Thu 12:00 H 0110

The Photocurrent in Organic Solar Cells does not Vanish at Open-Circuit — ●CLEMENS GÖHLER, MÓNICA DYREBY, ALEXANDER FLAMM, and MARTIJN KEMERINK — Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg, Im Neunheimer Feld 225, 69120 Heidelberg

Organic solar cells (OSCs) have reached close to 20% of power conversion efficiency and 100% conversion yield between incident photons to extracted charge carriers, but still suffer from unexpected losses to the open-circuit voltage and fill factor. Non-thermalized charge car-

rier distributions—due to incomplete relaxation in a disordered density of states—can explain their current-voltage-characteristics, yet with at times uncommon ramifications: here, we will show that a non-negligible photogenerated current under open-circuit conditions is a general feature of OSCs. In more detail, we have investigated the internal quantum efficiency in non-fullerene acceptor OSCs in the steady state. Utilizing a small signal light source, modulated at low frequencies, and varying the working conditions from reverse (collection) to forward (injection regime) fields, we are able to determine the extraction efficiency of photogenerated charges at any point on the current-voltage-curve. We find that while the yield decreases towards open-circuit, it does not vanish completely; therefore, the resulting photocurrent has to be compensated by charge injection in order to reach zero net current. We were further able to reproduce these experimental findings with kinetic Monte-Carlo device simulations involving non-equilibrium dynamics.

CPP 36.10 Thu 12:15 H 0110

Structure-function properties in a water soluble polymer via single-molecule spectroscopy — ●ERIK F. WOERING¹, MARIA DUMA¹, JANE KARDULA^{1,2}, RYAN C. CHIECI^{1,2}, and RICHARD HILDNER¹ — ¹University of Groningen, ZIAM, The Netherlands — ²University of Groningen, Stratingh Institute for Chemistry, The Netherlands

Conjugated polymers represent a promising class of versatile and easy to produce high-performance materials. Due to their (chemically) adjustable nature, they find use in bioelectronics or organic solar cells. However, the interplay of the polymers' chemical structure of the backbone and of the side groups on optical and electronic properties remain largely unexplored due to their large conformational flexibility. Here, we perform temperature-dependent single-molecule photoluminescence (PL) spectroscopy on p(ProDOT-TetEster), a water-soluble polythiophene-derivative bearing two dimethyloctane-dioate side chains. In particular, we explore the influence of polarity of the surrounding environment through statistical analysis of spectral features upon embedding single chains into a PS, PMMA or PVA matrix. The granular analysis on the single-chain scale will be valuable for deriving structure-function relationships and ultimately for the design of optimized and specialized conjugated polymers.

CPP 36.11 Thu 12:30 H 0110

On the competition between exciton emission and free charge generation in organic solar cells with low energetic offsets —

●MANASI PRANAV¹, ATUL SHUKLA¹, BOWEN SUN¹, RONG WANG², DAVID MOSER³, JULIA RUMENY³, SANDER SMEETS⁴, WOUTER MAES⁴, SABINE LUDWIG³, LARRY LÜER², CHRISTOPH BRABEC², SAFA SHOAE¹, and DIETER NEHER¹ — ¹University of Potsdam, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — ³University of Stuttgart, Germany — ⁴Hasselt University, Belgium

Organic blends with low energy-offset are the fruit-flies of today's organic photovoltaics research. Low photocurrent efficiencies for low offset blends draw attention to the link between energetic offset and free charge generation. Here, we take a quantitative, methodical approach to probing the origin of field-dependent free charge generation. Blending Y6 and Y5 with different molecular weights of the PM6, we progressively tune the photovoltaic parameters from a very efficient to inefficient device with severe field dependence of generation. We find the same pronounced field-dependence in transient absorption spectroscopy, and steady state and transient photoluminescence (PL) for inefficient low offset blends. The free charge generation and PL show a strict anticorrelation as a function of bias across all model systems. Thereby, we theoretically evaluate the quantum yields of PL to demonstrate inefficient charge transfer state formation from the local exciton, without any indication of hybridization, and that the decay of the singlet exciton is the only competing process to free charge generation.

CPP 36.12 Thu 12:45 H 0110

Directed exciton transport highways in organic semiconductors — KAI MÜLLER^{1,2}, SEBASTIAN SCHELLHAMMER^{1,3}, NICO GRÄSSLER^{3,4}, BIPASHA DEBNATH⁴, FUPIN LIU⁴, YULIA KRUPSKAYA⁴, KARL LEO³, MARTIN KNUPFER⁴, and ●FRANK ORTMANN^{1,5} — ¹cfaed, TU Dresden — ²Institut für Theoretische Physik, TU Dresden — ³IAPP and IAP, TU Dresden — ⁴Leibniz Institute for Solid State and Materials Research Dresden — ⁵TUM School of Natural Sciences, Technische Universität München

Exciton bandwidths and exciton transport are difficult to control by

material design. We showcase the intriguing excitonic properties in an organic semiconductor material with specifically tailored functional groups, in which extremely broad exciton bands in the near-infrared-visible part of the electromagnetic spectrum are observed by electron energy loss spectroscopy and theoretically explained by a close contact between tightly packing molecules and by their strong interactions. This is induced by the donor-acceptor type molecular structure and

its resulting crystal packing, which induces a remarkable anisotropy that should lead to a strongly directed transport of excitons. The observations and detailed understanding of the results yield blueprints for the design of molecular structures in which similar molecular features might be used to further explore the tunability of excitonic bands and pave a way for organic materials with strongly enhanced transport and built-in control of the propagation direction.