

CPP 49: Organic Electronics and Photovoltaics II (joint session CPP/DS/HL/O, organized by CPP)

Time: Thursday 9:30–12:45

Location: H40

Invited Talk CPP 49.1 Thu 9:30 H40

Patterned organic ferroelectric memory diodes by solution micromolding — ●PAUL BLOM, THOMAS LENZ, SIMON BENNECK-ENDORF, KAMAL ASADI, and DAGO DE LEEUW — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, D-55128

Ferroelectric polymers are promising candidates for memory technology, since they provide two bistable non-volatile polarization states corresponding to a Boolean 1 and 0, which can repeatedly be switched by an external field. The most widely investigated organic ferroelectric is the copolymer of poly(vinylidene fluoride) and trifluoroethylene (P(VDF-TrFE)). However, implementation of ferroelectric capacitors into integrated circuits is hampered by the read-out of the information being destructive. This problem can be overcome by using phase separated blends of P(VDF-TrFE) with a semiconducting polymer. The bistable polarization state of the P(VDF-TrFE) yields the binary information that can be read-out non-destructively by the current through the semiconducting columns. Phase separation however is a random process that yields a spatially undefined microstructure. Here we use solution micromolding to obtain a linear grating of P(VDF-TrFE). The space in between the lines is backfilled with a semiconducting polymer, resulting in a binary array between two electrodes. The resulting ferroelectric diode can be programmed reversibly in a low resistive on-state and high resistive off-state. When the bias is turned off, the information is retained. The performance can be optimized by down scaling the lateral dimensions of the binary array.

CPP 49.2 Thu 10:00 H40

A new Figure of Merit for Organic Solar Cells with Transport-limited Photocurrents — ●DIETER NEHER¹, JULIANE KNIEPERT¹, ARIK ELIMELECH¹, and L. JAN ANTON KOSTER² — ¹University of Potsdam, Potsdam, Germany — ²Zernike Institute for Advanced Materials, Groningen, The Netherlands

Organic semiconductors exhibit superior absorption properties but suffer from low mobilities. Organic solar cells, therefore, display non-ideal JV-curves. Here, we present a closed-form analytical expression for the JV-curves of organic solar cells, based on the model in reference [1]. The expression is able to reproduce simulated JV-curves for a wide range of mobilities, generation rates and recombination parameters. Most importantly, the model delivers a novel figure of merit α to express the balance between free charge recombination and extraction in low mobility photoactive materials. This figure of merit is shown to determine critical device parameters such as the apparent series resistance and the fill factor. We also find α to be related to the parameter θ as defined in reference [2], showing that the approaches published in [1] and [2] are closely related. With that, we can accurately reproduce the gradual decrease of the fill factor with increasing recombination coefficient, decreasing mobility and increasing thickness.

[1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat Commun 2015, 6, 6951 [2] D. Bartsch et al., Nat Commun 2015, 6, 7083

CPP 49.3 Thu 10:15 H40

Design Rules for Organic Donor-Acceptor Heterojunctions: Pathway for Charge Splitting and Detrapping — ●CARL POELKING and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic solar cells rely on the conversion of a Frenkel exciton into free charges via a charge-transfer state formed on a molecular donor-acceptor pair. These charge-transfer states are strongly bound by Coulomb interactions and yet efficiently converted into charge-separated states. A microscopic understanding of this process, though crucial to the functionality of any solar cell, has not yet been achieved. Here we show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase. Comparing a variety of small-molecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices.

[1] J. Am. Chem. Soc., 2015, **137**, 6320-6326

[2] Nature Materials, 2015, **14**, 434-439

CPP 49.4 Thu 10:30 H40

Investigation of the hybrid charge transfer state at ZnO/organic interfaces — ●FORTUNATO PIERSIMONI¹, STEFAN ZEISKE¹, JOHANNES BENDUHN², RAPHAEL SCHLESINGER³, NORBERT KOCH³, KOEN VANDEWAL², and DIETER NEHER¹ — ¹Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — ²Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — ³Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Berlin, Germany

This contribution aims to study the Charge Transfer States (CTS) in hybrid systems based upon organic small molecules and ZnO. Those systems were investigated by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE). The presence of Hybrid CTSs is proven by the appearance of a distinct peak in the EL and EQE spectra located below the energy gap of the molecules or ZnO. The energy gap (E_{gap}) between the ZnO conduction band and the donor HOMO was tuned either by varying the ZnO work function through self-assembled monolayers of polar molecules, or by employing organic donors with different HOMO energy. The correspondence between the EL peak position and the E_{gap} attributes this emission to radiative recombination between an electron on the ZnO and a hole on the organic material. Notably all samples displayed a linear relation between the maximum of the EL spectrum and the $2/3$ power of the electric field F , in accordance to the confinement of the HCTS in a rectangular electrostatic potential well, implying a certain degree of delocalization perpendicularly to the donor/acceptor interface.

CPP 49.5 Thu 10:45 H40

PBDT[2F]T: Insight into the Secrets of a Wide Band-Gap Polymer with 7% Power Conversion Efficiency — ●JULIEN GORENFLOT^{1,2}, ANDREAS PAULKE³, FORTUNATO PIERSIMONI³, FEDERICO CRUCIANI², DIETER NEHER³, PIERRE M BEAUJUGE², and FRÉDÉRIC LAQUAI² — ¹Max Planck Institut für Polymerforschung, Mainz, Germany — ²Universität Potsdam, Potsdam, Germany — ³King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

PBDT[2F]BT:fullerene blends exhibit performance up to 75% higher than the reference P3HT:PCBM solar cells [1]. Using femto- to microsecond transient absorption, we investigate the origin of those outstanding properties. We find that geminate recombination losses of photogenerated charge carriers are nearly absent in PBDT[2F]BT:fullerene blends. Field-dependent measurement as well as morphological and energy levels characterization reveal efficient and field-independent charge generation, enabling excellent short-circuit current and fill factor. Strikingly, this outstanding generation is achieved in spite of a rather low offset between the polymer's excitons and the blend's charge transfer state energy levels, which allows for an open circuit voltage as high as 0.9 V. Replacing the fluorine substituents by hydrogen in those polymers results in only moderate performances, thus highlighting the importance of molecular design. This is discussed in terms of energy levels and blends morphology.

[1] J. Wolf et al., Chem. Mater. 27, 2015

15 min. break

CPP 49.6 Thu 11:15 H40

The Meaning of Charge Carrier Density in Charge Extraction Experiments — ●JULIANE KNIEPERT, EDGAR NANDAYAPA, and DIETER NEHER — University of Potsdam, Potsdam, Germany

Charge extraction experiments are a powerful tool to extract important information on the charge carrier dynamics, such as the effective charge carrier mobility and the order and coefficient of nongeminate recombination, from charge carrier densities under steady state conditions. However, it is often neglected that the extracted carrier density in these experiments is highly sensitive to the actual carrier distribution in the device, which can be very inhomogeneous due to high carrier injection at the contacts, imbalanced mobilities or fast recombination. This is particularly true for organic solar cells, which usually have thin active layers and low intrinsic carrier densities. These condi-

tions may lead to an erroneous interpretation of the results. We show with numerical simulations and experiments how the extracted carrier density is influenced by intrinsic (mobility, recombination coefficient, injection barriers) and extrinsic (layer thickness, illumination, bias) parameters. From these results we deduce experimental conditions for which reliable values for the carrier density, mobility and recombination coefficient can be obtained.

CPP 49.7 Thu 11:30 H40

Rapid non-geminate recombination in organic solar cells — ●JONA KURPIERS¹, JOHN LOVE¹, CHRISTOPHER PROCTOR², THUC-QUYEN NGUYEN², and DIETER NEHER¹ — ¹Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany — ²Department of Chemistry & Biochemistry, University of California, Santa Barbara, USA

In the last years a dramatic increases in the efficiency of solution processed bulk heterojunction (BHJ) solar cells have been reported. However, the fundamental processes involved in the conversion of absorbed photons to free charges are still not fully understood. In this work, we use time delayed collection field (TDCF) experiments with exceptionally high time resolution to investigate the charge carrier dynamics in polymer-fullerene and small molecule-fullerene systems. TDCF experiments reveal rapid non-geminate recombination on the 20 ns time-scale, even for charge carrier densities comparable to one sun illumination. This loss becomes significantly accelerated at higher pulse fluences for the polymer-fullerene device. To identify the reason for this rapid loss, the recombination dynamics were further investigated on devices with different thicknesses. It is concluded that the primary reason for the nongeminate loss observed at the short time scale in the polymer blend is recombination of charges close to the contacts. In the small-molecule system however, the loss mechanism differs completely. Specifically, we find a rapid filling of traps on short time scales. Our work shows evidence that these rapid loss channels are essential to understand and can dramatically affect device operation.

CPP 49.8 Thu 11:45 H40

Temperature dependent competition between different recombination channels in organic heterojunction solar cells — ●THERESA LINDERL, ULRICH HÖRMANN, SERGEJ BERATZ, MARK GRUBER, STEFAN GROB, ALEXANDER HOFMANN, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg

A modification of the Shockley-Queisser theory is presented with a special focus on constellations, where a linear extrapolation of the temperature dependence of the open circuit voltage V_{OC} results in the optical gap of the absorber rather than in the intermolecular charge transfer (CT) gap. Depending on the electronic coupling strength between donor and acceptor molecules, either singlet or CT recombination is dominant in different temperature regimes. These regimes are separated by a transition temperature T_{tr} that is, in the case of small energy level offset and weak electronic coupling, around 300 K or even below. For α -sexithiophene (6T)/diindenoperylene (DIP) solar cells with elevated substrate temperature during 6T deposition the linear extrapolation of the temperature dependent V_{OC} yields a value of 2.07 eV, whereas the extrapolation for the device evaporated at room temperature results in a value of 1.90 eV. Heating the substrate during 6T deposition leads to a molecular configuration at the interface where the coupling between donor and acceptor molecules is strongly reduced compared to the device evaporated at room temperature. This results in a transition temperature well below room temperature which is confirmed by temperature dependent electroluminescence measurements.

CPP 49.9 Thu 12:00 H40

Ambipolar Charge Transfer In Single-Wall Carbon Nanotube Based Bulk-Heterojunctions — ●MICHAEL AUTH¹, ANDREAS SPERLICH¹, FLORIAN SPÄTH², TOBIAS HERTEL², and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg — ²Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, — ³Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The exceptional electrical conductivity of Single-Wall Carbon Nano-

tubes (SWNT) makes them potentially interesting to improve charge transport in organic photovoltaics (OPV). Additionally, their near infrared absorption bands can improve the spectral response of conventional polymer-fullerene bulk-heterojunctions. Until now, only few OPV devices containing purified semiconducting SWNTs were reported regarding the charge transfer properties of solar cell absorbers. For this study we prepared highly purified semiconducting (6,5)-SWNT samples, which we investigated in combination with known OPV donors and acceptors, namely the fullerene acceptor PC₆₀BM and the conjugated polymer P3HT. Using Electron Paramagnetic Resonance, we found specific signatures for charge carriers localized on either SWNTs, P3HT or PC₆₀BM and revealed the potential ambipolarity of SWNTs, leading to either hole transfer from PC₆₀BM or electron transfer from P3HT. Furthermore our measurements confirmed exceptional SWNT purity, with respect to doping, dangling bonds or catalyst residue. In conclusion, we see a high application potential of (6,5)-SWNTs in OPV and, generally, in optoelectronic devices.

CPP 49.10 Thu 12:15 H40

Influence of the Heterojunction's Interface on the Dynamics of Separated Charges Recombination in Organic Photoactive Materials — ●JULIEN GORENFLOT^{1,2}, NIVA ALINA RAN³, MIKE HEIBER³, GUILLERMO BAZAN^{3,4}, THUC-QUYEN NGUYEN^{3,4}, and FRÉDÉRIC LAQUAI^{1,2} — ¹Max Planck Institut für Polymerforschung, Mainz, Germany — ²King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — ³University of California Santa Barbara, Santa Barbara, California, United States — ⁴Faculty of Science King Abdulaziz University, Jeddah, Saudi Arabia

A recent study has indicated that the energetic density of shallow trap states, specifically at the interface between the electron donor and the electron acceptor, could be responsible for the apparent high recombination order observed in organic photoactive blends [1]. In order to elucidate this issue, we carried out investigations on a material system that allows for well-controlled donor/acceptor interactions. Films of the small-molecule donor, H1, can be processed such that H1 molecules are either stacking with their pi-face perpendicular or parallel to the substrate. By evaporating a layer of the acceptor molecule C60 on the films, we study the effect of molecular orientation at the donor/acceptor interface on charge recombination using transient absorption spectroscopy. We compare the two bilayer systems to a bulk heterojunction also using H1, which is expected to have a mixture of face-on and edge-on donor/acceptor interactions as well as a much larger interface area. [1] J. Gorenflot et al., J. Appl. Phys.115, 144502 (2014)

CPP 49.11 Thu 12:30 H40

Resonant GISAXS on ternary thin film systems — ●MIHAEL CORIC¹, NITIN SAXENA², JAN WERNECKE³, STEFANIE LANGNER³, PETER MÜLLER-BUSCHBAUM², MICHAEL KRUMREY³, and EVA M. HERZIG¹ — ¹Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — ²TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ³Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

Using additives to influence the properties of a material is an extensively used method in material science. It is also an approach to achieve morphological control in binary thin film systems like in organic photovoltaic systems. If the third component is also a polymer the morphological characterization poses a challenge since the sophisticated thin film characterization methods like grazing incidence small angle x-ray scattering (GISAXS) carried out a high x-ray energies can only distinguish between different electron densities. Using x-ray energies near the absorption edges of certain elements contained in the polymers enables a much higher contrast between the different materials, increasing the distinguishability of the different components within the active film of the organic solar cell. However, it is also challenging to interpret the scattering data correctly since some approximations routinely carried out in the theory used for interpretation of hard x-rays are no longer valid. We show our systematic measurements at the sulphur and chlorine edge and explain the advantages we can take out of the measurements to analyze the morphology of this ternary thin film.