

CPP 50: Organic Electronics and Photovoltaics III - Organic Photovoltaics

Time: Thursday 9:30–13:00

Location: H18

CPP 50.1 Thu 9:30 H18

Achieving suppressed recombination; kinetics of singlet and triplet charge transfer states defining charge generation and recombination in organic solar cells — ●SAFA SHOAI — University of Potsdam

In-depth understanding of charge carrier photogeneration and recombination mechanism in organic solar cells is still an ongoing effort in the community. In donor:acceptor (bulk) heterojunction organic solar cells charge photogeneration and recombination are inter-related via the kinetics of charge transfer states. While efficient charge photogeneration quantum yield can be achieved in many donor:acceptor systems, only very few systems have so far shown significantly reduced bimolecular recombination coefficient. Herein, we present a meta-analysis of the device performance for numerous BHJ OSC for which field dependent photogeneration, charge carrier mobility and fill factor are determined. From this analysis we find a spin-related factor which is dependent on the ratio of back electron transfer of the triplet CT states to the decay rate of the singlet CT states. This factor along with the dissociation efficiency of the CT states primarily define the charge generation efficiency and bimolecular recombination reduction factor. In systems with extremely efficient charge generation due to the very fast dissociation rate of the CT states, the recombination can be strongly suppressed regardless of the spin-related factor.

CPP 50.2 Thu 9:45 H18

The charge transfer state in organic solar cells: contribution of static disorder and molecular reorganisation — ●CLEMENS GÖHLER and CARSTEN DEIBEL — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Solar cells from organic semiconductors use an active layer consisting of a heterogeneous blend of electron acceptor and donor materials, such as fullerenes and conjugated polymers. The donor HOMO and acceptor LUMO level in these heterojunctions form an additional charge transfer (CT) state, which can be detected with electro-optical spectroscopy methods.

Molecular properties of donor copolymers, such as molecular weight, defects, or stoichiometry, are crucial to the solar cells performance - predominantly by affecting short circuit current and fill factor. Their impact upon the open circuit voltage, which is connected to the CT states energy, might not be as distinct. They are, however, affecting the CT states energetic distribution, which can be described as a convolution of its molecular reorganisation energy and the amount of energetic disorder. We are able to unravel both contributions using temperature dependent sub-gap photocurrent spectroscopy to contribute to a deeper understanding of the CT states role in solar cell performance.

CPP 50.3 Thu 10:00 H18

Evaluation of molecular donor-acceptor pairs forming charge-transfer or exciplex states — ●THOMAS ZEHEL, THOMAS SCHRÖTHER, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86159 Augsburg

Intermolecular excited states play a major role in various organic semiconductor applications. Charge-transfer (CT) states were shown to be a major contributor to large voltage losses in organic photovoltaic cells (OPVCs) and exciplex systems are becoming a viable alternative to heavy metal complexes in organic light emitting diodes (OLEDs). Both states are formed by at least two molecules of different kind (acceptor and donor). In both cases for the excited state the hole of the bound exciton resides on the donor and the electron resides on the acceptor molecule. The difference between the two being that the exciplex only exists in the excited state (no direct ground state absorption) while the CT state exhibits a small but measurable direct absorption from the ground state. This main difference is accompanied by considerably larger external electroluminescent quantum yields (EQE_{EL}) for exciplex systems compared to CT systems.

In this work a number of different donor-acceptor pairs which usually form exciplexes or CT states are investigated using electrical (current-voltage-luminescence, incident photon to current efficiency), optical (EL, PL) and computational (density functional theory simulations) methods to gain further insights into the differences and similarities of CT and exciplex systems on a basic material level.

CPP 50.4 Thu 10:15 H18

Exciton Dynamics in Pentacene-Perfluoropentacene Heterostructures — ●VIPILAN SIVANESAN¹, FRANK SCHREIBER², KATHARINA BROCH², and PETRA TEGEDER¹ — ¹Universität Heidelberg, Physikalisch-Chemisches Institut — ²Universität Tübingen, Institut für Angewandte Physik

Understanding the ultrafast electronically excited state dynamics in organic semiconductors after optical excitation is crucial for the optimization of organic optoelectronic devices. Moreover, the knowledge of the morphology and energetics at donor-acceptor interfaces is important for efficient charge separation in organic solar cells. Thereby, charge transfer (CT) states play a decisive role. To analyse the ultrafast processes at the interface more precisely, both well-defined structures of the samples and a very high time resolution in the experiment are required. In this work we investigated thin films of pentacene (PEN), perfluoropentacene (PFP), and various heterostructures of PEN and PFP by means of femtosecond time-resolved second harmonic generation. For the donor/acceptor configurations, depending on the molecular orientations at the interface and the excitation energies, the dynamics of CT-states were analyzed.

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Impact of Structural Defects on the Energy Level Alignment in planar Pentacene-Perfluoropentacene Heterojunctions — ●JAN HAGENLOCHER¹, ALEXANDER HINDERHOFER¹, SATOSHI KERA², and FRANK SCHREIBER¹ — ¹Universität Tübingen, Tübingen, Germany — ²Institute for Molecular Science, Okazaki, Japan

The majority of today's organic (opto-)electronic devices comprise a number of different organic-semiconductor layers. The functionality of such complex heterostructures depends on the relative alignment of the frontier molecular-orbital energies in the individual layers with respect to those in all others. In this study we investigated the dependence of this energy level alignment on structural defects in an organic-organic heterojunction of perfluoropentacene (PFP)-on-pentacene (PEN) using x-ray scattering, atomic force microscopy and ultraviolet photoelectron spectroscopy. The density of structural defects was varied by changing the growth temperature of the bottom PEN film. A direct relationship between the defect density and the energy level alignment was found, where the binding energies together with a change in the electrostatic potential at the interface vary systematically with the defect density. This indicates that a key factor affecting the energy level alignment is the number of transferred electrons from the substrate to unoccupied gap states in the PFP film. The described gap states originate from the structural defects and can be effectively controlled by adjusting the growth conditions of the organic films.

CPP 50.6 Thu 10:45 H18

Microscopic effects of the broadening of the density of states in donor-acceptor blends and their role in organic photovoltaics — ●MICHEL PANHANS¹, SEBASTIAN HUTSCH¹, JOHANNES BEDNUHN², KARL SEBASTIAN SCHELLHAMMER¹, KOEN VANDEWAL³, and FRANK ORTMANN¹ — ¹Center for Advancing Electronics Dresden, TU Dresden — ²Institut für Angewandte Physik, TU Dresden — ³Institute for Materials Research (IMO-IMOMECE), Hasselt University, Wetenschapspark 1, 3590 Diepenbeek, Belgium

Microscopic understanding and quantifying the density of states including linewidth broadening and dissipation mechanisms in organic semiconductors [1,2] plays a crucial role for designing efficient solar cells and transistors. We study models of fullerene based donor-acceptor systems regarding their response to optical excitations. We analyze the density of states (DOS) and excited-state DOS with electronic disorder and electron-phonon interaction based on ab initio simulations. The calculated temperature dependence of the absorption linewidth is compared to temperature dependent absorption measurements on the same blends where we find very good agreement. Finally, we discuss implications for the open-circuit voltage in organic solar cells.

[1] D. Venkateshvaran et al. Nature 515, 384 (2014).

[2] K. Vandewal et al. J. Am. Chem. Soc. 139, 1699 (2017).

CPP 50.7 Thu 11:00 H18

Energy Distribution of Charge-Transfer Excitons at Organic

Donor-Acceptor Interfaces: Simulations for Room Temperature — ●SEBASTIAN SCHELLHAMMER^{1,2}, GIANAURELIO CUNIBERTI^{1,2}, and FRANK ORTMANN² — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — ²Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

Charge transfer (CT) excitons at donor-acceptor interfaces determine the performance of organic solar cells. The subgap absorption by such excitons is also used to design sensitive near-infrared photodetectors based on the broad CT exciton bands. However, the prediction of the energetics of the CT exciton band has ever been a great challenge. We present an approach for an efficient computation of the CT energies at room temperature based on time-dependent density functional theory including the band tail broadening induced by thermal fluctuations in a semi-classical way. This method is demonstrated for different donor molecules with C60 as electron accepting material. A comparison to experimental CT band characteristics shows excellent agreement for both the linewidth broadening as well as the CT energies. The approach thus combines accuracy with modest computational cost.

15 min. break

CPP 50.8 Thu 11:30 H18

How to Interpret Absorption and Fluorescence Spectra of Charge Transfer States in an Organic Solar Cell — ●FRANK-JULIAN KAHLE¹, ALEXANDER RUDNICK¹, HEINZ BÄSSLER², and ANNA KÖHLER^{1,2} — ¹Soft Matter Optoelectronics, Department of Physics, University of Bayreuth, Germany — ²Bayreuth Institute of Macromolecular Science (BIMF), University of Bayreuth, Germany

The aim of the present work is to identify the appropriate framework for analyzing photoluminescence and photocurrent (EQE) spectra of charge transfer (CT) states in donor-acceptor blends used as active materials for organic solar cells. We applied gated photoluminescence (PL) spectroscopy within a temperature range from 5 to 295 K combined with EQE as well as electroluminescence (EL) experiments on 1:1 Me-LPPP:PCBM blends by weight. We find that the PL spectra are virtually temperature independent and the temporal decay of the emission features a power law with an exponent close to -3/2 as Hong and Noolandi predicted for distributed geminately bound electron-hole pairs. The results are inconsistent with both Marcus* electron transfer theory and the original Marcus-Levich-Jortner (MLJ) theory, and they prove that disorder effects are crucial. Both PL and EQE spectra can be rationalized in terms of the classic Franck-Condon picture of electronic transitions that couple to intra-molecular vibrations as well as low frequency modes of the donor-acceptor pair that forms the CT state.

CPP 50.9 Thu 11:45 H18

Absence of charge transfer state enables very low VOC losses in SWCNT:fullerene solar cells — ●ANDREJ CLASSEN¹, LUKAS EINSIEDLER¹, THOMAS HEUMÜLLER¹, ARKO GRAF², MAXIMILIAN BROHMANN², FELIX BERGER², SIMON KAHMANN¹, MOSES RICHTER¹, GEBHARD MATT¹, KAREN FORBERICH¹, JANA ZAUMSEIL², and CHRISTOPH BRABEC¹ — ¹Friedrich-Alexander-Universität Erlangen-Nürnberg — ²Ruprecht-Karls-Universität Heidelberg

Current state of the art organic solar cells (OSC) still suffer from high losses of open circuit voltage (VOC). Conventional polymer:fullerene solar cells usually exhibit band gap to VOC losses greater than 0.8 V. Here a detailed investigation of VOC is presented for solution processed OSCs based on (6,5) single-walled carbon nanotubes (SWCNT):[6,6]-phenyl-C71-butyric acid methyl ester (PC70BM) active layers [1]. Considering the very small optical band gap of only 1.22 eV of (6,5) SWCNTs, a high VOC of 0.59 V leading to a low $E_{gap}/q - VOC = 0.63$ V loss is observed. The low voltage losses are partly due to the lack of a measurable charge transfer state and partly due to the narrow absorption edge of SWCNTs. Consequently, VOC losses attributed to a broadening of the band edge are very small resulting in $VOC_{SQ} - VOC_{rad} = 0.12$ V. Interestingly, this loss is mainly caused by minor amounts of SWCNTs with smaller band gaps as well as (6,5) SWCNT trions. More intriguingly, we find a very low voltage loss due to nonradiative recombination, $\Delta VOC_{nonrad} = 0.26$ V, which is exceptional for fullerene based OSCs.

[1] Classen et al., Adv. Energy Mater., 2018, 1801913

CPP 50.10 Thu 12:00 H18

Investigating in-operando the effects of solvent additives

on the stability of organic solar cells based on PTB7-Th:PC71BM — ●DAN YANG¹, FRANZISKA LÖHRER¹, VOLKER KÖRSTGENS¹, ARMIN SCHREIBER¹, SIGRID BERNSTORFF², JILLIAN BURIK³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Elettra Sincrotrone Trieste, Basovizza, 34149 Trieste, Italy — ³University of Alberta, Department of Chemistry, Edmonton, Canada

Due to low cost, flexibility, solution processing and large-scale fabrication, enormous attention is focusing on the research and development for higher organic photovoltaics performance over the last decades. In recent years, the power conversion efficiency (PCE) of organic solar cells (OSCs) of single-junction OSCs has reached 14.6 %, which is still lower than the inorganic counterparts. To further optimize the performance, additive solvents are widely used in the solution of bulk heterojunction. While the influences of those additives on the device degradation behavior are essential to be disclosed. In this work, PTB7-Th:PC71BM solar cells with two different additive solvents are probed with in-operando GISAXS measurements to resolve the morphology changes during operation. Combining with the J-V performance, the degradation mechanisms behind the additive solvents is figured out.

CPP 50.11 Thu 12:15 H18

Toward a universal polymeric material for electrode buffer layers in organic and perovskite solar cells and organic light-emitting diodes — QIANG ZHANG¹, WEI-TING WANG², TOBIAS WÄCHTER³, ●MICHAEL ZHARNIKOV³, YIAN TAI², and DER-JANG LIAW¹ — ¹Polymer Science and Materials Lab., Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan — ²Nanohybrid Materials and Devices Lab., Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei 10607, Taiwan — ³Applied Physical Chemistry, Heidelberg University, 69120 Heidelberg, Germany

A novel concept of a "universal" electrode buffer layer material, exhibiting either hole transporting or reducing electrode work function properties, is demonstrated by the example of a polymeric compound PDTON. Depending on the composition ratio of acetic acid and ethyl acetate upon dispersing, PDTON forms two kinds of nanospheres, serving as building blocks and defining the properties of the respective materials, termed as A-PDTON and C-PDTON. These materials are suitable for hole transport (triphenylamine on the surface of A-PDTON nanospheres) and reducing the work function of electrode due to the formation of suitable interfacial dipole (C-PDTON), respectively. We demonstrate the versatility and high compatibility of these two types of the same polymer to organic solar cells, organic light-emitting diodes, and perovskite solar cells, exhibiting comparable or even superior performance compared to the standard device architectures.

CPP 50.12 Thu 12:30 H18

Growth kinetics of gold electrodes used in hybrid solar cells — ●VOLKER KÖRSTGENS¹, ADRIAN HAUSSMANN¹, FRANZISKA C. LÖHRER¹, MATTHIAS SCHWARTZKOPF², ALEXANDER HINZ³, OLEKSANDR POLONSKYI³, THOMAS STRUNSKUS³, HRISTO IGLEV⁴, STEPHAN V. ROTH², REINHARD KIENBERGER⁴, FRANZ FAUPEL³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²DESY, Notkestr. 85, 22607 Hamburg — ³CAU Kiel, Institut für Materialwissenschaft, Kaiserstr. 2, 24143 Kiel — ⁴TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Frank-Str. 1, 85748 Garching

The morphology of the gold electrode established at the metal-polymer interface between gold and the active layer of hybrid solar cells impacts the performance of devices. In this work the active layer consisting of a water-soluble polythiophene and laser-ablated titania nanoparticles including a blocking layer of PEDOT:PSS [1] is investigated. Gold sputter deposition is applied to the layered system and also the respective pure components. To obtain information of gold cluster growth kinetics during the sputter deposition process, in-situ time resolved grazing incidence small angle X-ray scattering (GISAXS) experiments and grazing incidence wide angle X-ray scattering (GIWAXS) are carried out. Different growth regimes of gold clusters are observed from the data analysis for the various films and the influence of surface roughness is discussed. [1] Körstgens et al., Nanoscale 7, 2900 (2015).

CPP 50.13 Thu 12:45 H18

Modelling of photoactive area spreading in unstructured photovoltaic cells — ●MATHIAS GRUBER^{1,2}, VLADISLAV JOVANOVIĆ¹, and VEIT WAGNER¹ — ¹Department of Physics and Earth Sciences, Ja-

cobs University Bremen, 28759 Bremen, Germany — ²PolyIC GmbH & Co. KG, 90763 Fürth, Germany

Photovoltaic cells incorporating unstructured conductive layers produce a significant amount of additional photocurrent outside the electrode overlap area by photoactive area spreading. This leads to a large error in the extraction of solar cell current density, fill factor and cell efficiency from I - V -measurements. To counteract this effect we present an analytical model which is able to describe the photoactive area spreading effect quantitatively, yielding more accurate results

than the conventional shadow masking approach. The presented model only requires layer sheet resistance data and the contact geometry to allow to calculate and remove the spreading current contribution from I - V -measurements of unmasked solar cells. This allows to extract accurate solar cell efficiency and j - V -data, which is demonstrated on the example of unstructured metal mesh based organic solar cells. The presented data demonstrates the problem of the conventional shadow masking approach and shows that our model yields more accurate results down to very low illumination light intensities.