CPP 5: Organic Semiconductors I: Solar Cells A (jointly with HL, DS)

Time: Monday 14:00–17:30 Location: ZEU 222

Topical Talk CPP 5.1 Mon 14:00 ZEU 222

Light harvesting in single polymer chains and inorganic nanostructures — •John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg — Department of Physics and Astronomy, University of Utah, Salt Lake City

Optimization of materials for energy conversion applications requires an understanding of intermolecular heterogeneity to ultimately formulate synthetic approaches to maximizing the fraction of a particular subensemble. Single molecule spectroscopy can offer such insight as an exquisitely sensitive tool to unravel the underlying complexity of organic semiconductors. In the context of solar cells, for example, the technique can help to identify purely intramolecular exciton migration and charge separation processes.

Recently, we have explored the migration of excitons in single molecules as a function of the initial excitation energy, thus offering information on thermalization processes within the polymer chain. The approach allows a direct spectroscopic identification of the absorption of individual chromophores on the chain, whereas mere emission tends to provide information only on the lowest-energy unit in the intramolecular excitonic cascade [1].

The heterogeneity in light-harvesting characteristics is particularly pronounced in semiconductor nanostructures, where particle morphology directly influences the heterojunction band structure and the excitonic spectrum [2].

[1]Walter et al., Phys. Rev. Lett. 103, 167401 (2009).

[2]Borys et al., Science (in press).

CPP 5.2 Mon 14:30 ZEU 222

Highly efficient vacuum processed BHJ solar cell based on merocyanines — •Vera Steinmann[1], Hannah Bürckstümmer[2], Nils M. Kronenberg[1], Martin R. Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität Köln, Germany — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems Universität Würzburg, Germany

Bulk heterojunction (BHJ) organic solar cells have attracted considerable interest due to their potential for large-scale, cost-effective and environmentally friendly power generation. Small molecules have been successfully introduced in solution- (SOL) as well as vacuum- (VAC) processed devices, reporting efficiencies (PCE) up to 4.4% and 5.7% respectively. For simple layer stack devices (2-3 layers) based on CuPc as electron donor and C60 as electron acceptor PCEs up to 5.0% have been achieved.

Recently, we presented a direct comparison of highly efficient SOL and VAC BHJ cells based on merocyanine dyes (MC) with a similarly simple layer stack as reported in the literature. Our most efficient devices exhibited PCEs up to 4.9%. Further optimizations on the VAC processed cells led to high PCEs exceeding 6% while keeping the same simple layer stack. In addition, these cells have demonstrated exceptional performance even at lower light intensities.

Due to the simple chemical variability of MC dyes, they are ideally suited for tandem solar cells. We will present first attempts in this direction.

CPP 5.3 Mon 14:45 ZEU 222

Efficiency-Limiting Processes in Bulk Heterojunction Organic Solar Cells — Ian Howard, Ralf Mauer, Fabian Etzold, Valentin Kamm, Michael Meister, Hannah Mangold, and •Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, MPI for Polymer Research, Mainz, Germany

Despite significant study, the efficiency-limiting processes that govern the efficiency of bulk heterojunction photovoltaic devices still remain ambiguous. In particular the role of interfacial charge-transfer (CT) states as potential intermediates of free charge carriers is diversely debated. In this contribution we directly observe charge generation and recombination processes in state-of-the-art polymer:methanofullerene photovoltaic blends by transient absorption spectroscopy and compare polythiophene (P3HT) of varying regioregularity and low-bandgap polymers as electron donor materials. We observe a common feature of these blends is ultrafast (< 100 fs) exciton dissociation at the donor-acceptor interface. However, a certain fraction of excitons create CT states that predominantly recombine geminately within a few nanoseconds. On the other hand the fraction of free charge carriers recombines bimolecularly on a time scale competing with charge extraction and can thus be swept out of the device as photocurrent. The results demonstrate the importance of ultrafast free carrier generation and suppression of interfacial CT state formation to achieve high power conversion efficiencies in various material systems. [1] I.A. Howard, R. Mauer, M. Meister, F. Laquai, J. Am. Chem. Soc. 2010, 132, 14866. [2] I.A. Howard, F. Laquai, Macromol. Chem. Phys. 2010, 211, 2063.

CPP 5.4 Mon 15:00 ZEU 222

Bias-Dependent Transient Absorption on Organic Solar Cells; Connection to Device Performance? — •Ian Howard, Ralf Mauer, Valentin Kam, Michael Meister, and Frédéric Laquai — Max Planck Forschungsgruppe für Organische Optoelektronik, Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

We directly observe the bias dependence of charge-transfer state separation in organic bulk heterojunctions using in-situ transient absorption on operating organic solar cells. The effect of bias on charge-transfer state lifetime (< 2ns) is found to be minimal, however suppression of nongeminate recombination with bias on later timescales (>10 ns) is observed and explains the bias dependence of the photocurrent. The bias independence of charge-transfer state separation is directly applicable to interpreting organic solar cell performance under standard AM1.5 illumination. However, due to the differences in charge densities and dynamic versus steady-state behavior between pulsed measurements and standard operating conditions, the effects of bias on the suppression of nongeminate recombination are not simplistically transferable. We consider to what extent pulsed transient absorbtion techniques on devices can be used to reveal nongeminate recombination mechanisms in devices operating under standard illumination conditions.

CPP 5.5 Mon 15:15 ZEU 222

Degradation effects related to the hole transport layer in organic solar cells — •Bernhard Ecker[1], Jairo Nolasco[2], Josep Pallarés[2], Lluis Marsal[2], Jörg Posdorfer[3], Jürgen Parisi[1], and Elizabeth von Hauff[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg (Germany) — [2]Departament d'Enginyeria Electrònica Elèctrica i Automàtica, Universitat Rovira i Virgili, Avda. Països Catalans 26, 43007 Tarragona (Spain) — [3]Enthone Nano Science Centre, Ormecon GmbH, Ferdinand-Harten-Str. 7, 22949, Ammersbek (Germany)

We discuss the influence of the hole transport layer on the device stability in organic bulk-heterojunction solar cells. Two water based hole transport layers, poly(3,4-ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT:PSS) and polyaniline : poly(styrene sulfonate) (PANI:PSS), and one isopropyl alcohol based PANI:PSS transport layer were investigated. Solar cells were prepared with the three different hole transport layers and degraded under illumination. Current-voltage, capacitance-voltage, and capacitance-frequency data were collected at varying light intensities over a period of 7 hours. Solar cell performance and stability were compared between non encapsulated and encapsulated samples to obtain understanding about degradation effects related to oxygen and water as well as degradation mechanisms related to the intrinsic instability of the solar cell materials and interfaces. We show that the properties of the hole transport layer can have a significant impact on the stability of organic solar cells.

15 min. break

CPP 5.6 Mon 15:45 ZEU 222

Characterization of trap states in small-molecule organic solar cells by using Impedance Spectrocopy. — •Lorenzo Burtone, Debdutta Ray, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden Germany

In this work, we focus on the characterization of trap levels in the electronic gap of organic semiconductors used in solar cells. These states can modify the electric field inside the device, considerably affecting charge generation and transport and consequently the solar cell efficiency. A method to characterize traps by using impedance spectroscopy is presented. We propose a new equivalent circuit based on previously reported theoretical models and we apply it in the fitting procedure of the measured data. In particular, we measure the impedance spectra of two flat heterojunction small molecule solar cells, where one of them has doped electron and hole transport layers. We observe the contribution of trap states at low frequencies in the capacitance spectra for the devices with doped transport layers. The experimental results can be understood with the equivalent circuit proposed and the trap state contribution can be evaluated. From a fitting procedure, we estimate the density of trap states to be around $1\mathrm{x}10^{17}\mathrm{cm}^{-3}\mathrm{eV}^{-1}$. Moreover we observe from the impedance analysis the presence of dopants in the intrisic layer with an estimated effective concentration of about $8.4\mathrm{x}10^{17}\mathrm{cm}^{-3}$. This value is in agreement with very low doping concentration and suggests the formation of a non-abrupt junction between intrinsic and doped layers.

CPP 5.7 Mon 16:00 ZEU 222

The effect of energetic disorder on open-circuit voltage in organic photovoltaics — •James C Blakesley, Ilja Lange, and Dieter Neher — University of Potsdam, Germany

Open-circuit voltage (VOC) is one of the most important figures of merit describing the quality of organic photovoltaics (OPVs). Usually it is assumed that VOC depends on the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, but large deviations from this trend are often found. In reality, there is a distribution of energy levels within the components, and this should also be taken into account.

We simulate bulk heterojunction OPVs using a simulation that includes the effects of energetic disorder [1].We find that VOC depends on: 1) the nominal donor-HOMO to acceptor-LUMO energy gap; 2) the charge-carrier generation and recombination rates; 3) the electrodes; and 4) the amount of energetic disorder. While the first three of these points have been much discussed previously, the effect of the fourth has not been conclusively demonstrated. An increase in the amount of energetic disorder leads to a reduction in the VOC due to relaxation of the carriers into the lowest lying energy levels. We find an analytical expression that predicts well the modelled VOC, and suggest the use of an effective donor-acceptor energy gap that takes energetic disorder into account. Measurements of Fermi-level pinning might be useful for determining this effective energy gap. [1] J. C. Blakesley and N. C. Greenham, J. Appl. Phys. 106, 034507 (2009)

CPP 5.8 Mon 16:15 ZEU 222

Modelling Temperature-Dependent Current-Voltage Curves of Organic Photovoltaic Devices — •Simon Züfle, Martin T. Neukom, Benjamin Perucco, Nils A. Reinke, and Beat Ruhstaller — ICP, ZHAW, Winterthur, Schweiz

Current-voltage curves allow to determine both fill-factor and efficiency of organic photovoltaic devices and are therefore a commonly used characterisation technique. Since analytical models for current-voltage curves fail in describing the fundamental processes of photogenerated current, more complex numerical calculations are mandatory for obtaining insight into the device physics. The analysis of multiple current-voltage curves at different temperatures calls for CPU-efficient algorithms combining state-of-the-art physical models and high calculation speed.

In order to model current-voltage curves simple drift-diffusion calculations with constant mobilities and thermionic emission as injection model are frequently used. In this study we investigate current-voltage curves measured at different temperatures with the help of a nonlinear least-square fitting algorithm in combination with a comprehensive physical model for charge carrier transport and injection. We evaluate the performance of different models for charge carrier transport, including the Gaussian Disorder Model, by simultaneously fitting multiple curves and discussing the mathematical quality of the fit. We employ an efficient algorithm for extracting material-specific parameters that allows modelling of measured current-voltage curves on a minute time-frame with a desktop PC.

CPP 5.9 Mon 16:30 ZEU 222

Role of drift and diffusion in organic solar cells measured by transient photocurrents — •Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

The role of the electric field and the contribution of diffusion to photocurrents are controversially discussed in the case of organic solar cells. We investigate flat heterojunction organic solar cells with systematically varied barriers at the contacts that are created by a HOMO offset between donor and hole transport layer. These barriers lead to S-kinks in the IV curve and to strong imbalanced and even reversed forces on charge carriers resulting from the field on the one hand and the concentration gradient on the other hand. By applying a rectangular illumination signal with varied light intensities, we observe in the photocurrent transients a pile-up of charge carriers at an extraction barrier. If an injection barrier is present, there exists a region in the IV curve where charges are extracted against the electric field by a strong diffusion gradient. These findings are based on the analysis of transient current data in the μs regime using electrical simulations based on a drift-diffusion model. The simulations show that observed overshoots in the photocurrent transients result from these imbalance effects and give new insights into the working principle of organic solar cells.

CPP 5.10 Mon 16:45 ZEU 222

Charge extraction with linearly increasing voltage: A numerical model for parameter extraction — •Martin Neukom, Simon Züfle, Nils Reinke, and Beat Ruhstaller — Institute of Computational Physics, Technikumstr 9, 8401 Winterthur, Switzerland

Device characterisation is an essential part in the process of improving the performance and lifetime of organic solar cells. Most of the device and material parameters are not accessible by measurements therefore sophisticated measurement techniques in combination with numerical simulations are needed to extract these parameters. A frequently used method to determine material parameters like charge carrier mobilities and the recombination coefficient is the CELIV technique (charge extraction by linearly increasing voltage). In this technique a voltage ramp is applied to the device in order to extract free charge carriers inside the bulk. With a simple analytical formula the mobility is commonly estimated on the basis of the temporal position of the current peak. We simulate the CELIV experiment, transient and steady-state measurement techniques with a fully-coupled opto-electronic model. On the one hand we investigate the limitations of the analytical formulas for mobility determination. On the other hand we use our model to fit several experimental datasets simultaneously to obtain elementary material parameters like the electron and hole mobility, recombination coefficient, photon to charge conversion efficiency and injection barriers in both printed and spin-coated bulk heterojunction solar cells. We deduce the influence of these material parameters on the overall device performance.

CPP 5.11 Mon 17:00 ZEU 222

Simulating electron transfer reactions in organic solar cell components — •Harald Oberhofer[1] and Jochen Blumberger[2] — [1]Department of Chemistry, University of Cambridge, UK — [2]Department of Physics and Astronomy, University College London, UK

Organic solar cells are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. To help overcome this deficiency we use advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified Fullerene crystals which are commonly used as electron-conducting component in organic solar cells.

In our contribution we will briefly discuss the techniques used to estimate electron transfer rates from computer simulations. Then we present our calculations on modified Fullerene crystals. We studied $C_{61}H_2$—a commonly used test system—and [6,6]-phenyl-C61-butyricacid-methyl-ester (PCBM) for 3 different crystal lattices which are commonly found in experiments. In the crystal we estimated electron transfer rates between next- and next-nearest neighbours with and without the application of an external electric field. These results where then used to estimate the electron mobility for the different lattice types. These results can represent a starting point for the optimisation of electron conduction in next-generation organic solar cells.

CPP 5.12 Mon 17:15 ZEU 222

Time resolved microwave conductivity reveals charge carrier dynamics in organic semiconductors — •Johannes Erben[1], Andreas Sperlich[1], Hannes Kraus[1], Tom J. Savenije[1,3], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Department of Chemical En-

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Understanding of the light induced charge carrier dynamics in organic semiconductors is essential to improve material properties and processing parameters, and, at long sight, device performance. Time Resolved Microwave Conductivity (TRMC) gives direct access to the microscopic transport properties, as the high frequency alternating electric field limits the drift of the charge carriers. After laser pulse excitation TRMC signal decays in P3HT:PCBM blends with varying PCBM content have been observed exhibiting a power law time dependence. The influence of morphology and temperature on the charge carrier recombination and mobility on a microscopic scale can thus be investigated.