TT 60: Organic Electronics and Photovoltaics: OPV II (jointly with CPP, HL)

Time: Wednesday 9:30–13:00 Location: C 130

TT 60.1 Wed 9:30 C 130

Impact of Mesoscale Order on Energetics in Organic Semiconductors — •Carl Poelking[1], Max Tietze[2], Chris Elschner[2], Selina Olthof[3], Dirk Hertel[3], Björn Baumeier[1], Frank Würthner[4], Klaus Meerholz[3], Karl Leo[2], and Denis Andrienko[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institut für Angewandte Photophysik, Dresden, Germany — [3]Physikalische Chemie, Universität zu Köln, Germany — [4]Institut für Organische Chemie, Universität Würzburg, Germany

The interaction of charged excitations with the molecular surrounding in organic semiconductors is strictly long-ranged, due to their quadrupolar building blocks and preferential or absolute structural order. We show how atomistic simulations access the resulting energetics of charges and charge pairs and derived quantities, notably the charge-density-dependent open-circuit voltage across organic heterojunctions, with excellent accuracy. We compute level diagrams for a variety of donor-fullerene interfaces, with direct experimental validation. The underlying simulation approach takes into account long-range electrostatic effects that persist up to the mesoscale. The resulting mesoscale fields not only produce flat level profiles, but provide orientation-dependent push-out forces across a donor-acceptor interphase that can drive the charge-separation process. Correct polarity of these push-out forces is a requirement for functional solar cells, with operation closely above an isopolar point as the optimum tradeoff between magnitude of these push-out forces and the photovoltaic gap.

TT 60.2 Wed 9:45 C 130

Signature of the Dirac cone in the excitation gaps of linear oligoacenes — •Richard Korytár — Institut für Nanotechnologie, Karlsruher Institut für Technologie, Herrmann-von-Helmholtzplatz 1, 76344 Eggenstein-Leopoldshafen

Linear oligoacenes (linearly fused benzene rings) are one of the prototypical examples of quantum wires and the simplest realization of the so called nano-graphene. We show that contrary to a widely held belief, the excitation gaps of oligoacenes can display oscillations of period 11 (rings) as a function of the molecule's length. By inspection of the polyacene electronic band-structure, we show that the incommensurate oscillations are caused by the presence of an accidental degeneracy at the Fermi level, reminiscent to the Dirac cone of graphene. Our predictions are supported by calculations based on density functional theory. We clarify the role of interactions by studying a parameterized Hubbard model with density matrix renormalization group. Our findings may have implications for organic electronics and research of materials for energy conversion.

TT 60.3 Wed 10:00 C 130

Probing Interfacial Properties in Polymer:Fullerene Bulk Heterojunctions — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

We investigated the properties of donor-acceptor interfaces occurring in fine-tuned ternary bulk heterojunctions and were able to quantitatively correlate spectroscopic information with domain phase order. Relaxation energies for AnE-PV donor polymers as well as of PCBM were found to range within 100-200 meV.

TT 60.4 Wed 10:15 C 130

The Effect of Solvent Additive on Generation, Recombination and Extraction in PTB7:PCBM Solar Cells: A conclusive Experimental and Numerical Simulation Study — •Juliane Kniepert[1], Ilja Lange[1], Thomas Brenner[1], Jan Anton Koster[2], and Dieter Neher[1] — [1]Universität Potsdam, Germany — [2]University of Groningen, The Netherlands

Time delayed collection field (TDCF), bias amplified charge extraction (BACE) and space charge limited current (SCLC) measurements are combined with complete numerical device simulations to unveil the effect of the solvent additive 1,8-diiodooctane (DIO) on the performance of PTB7:PCBM bulk heterojunction solar cells. DIO is shown to increase the charge generation rate, reduce geminate and bimolecular recombination and increase the electron mobility. In total, the reduction of loss currents by processing with the additive raises the power conversion efficiency of the PTB7:PCBM blend by a factor of almost three. Our device simulations show unambiguously that the effect of the additive on the shape of the current-voltage curve cannot be ascribed to the variation of only the mobility, the recombination or the field-dependence of generation. It is only when the changes of all three parameters are taken into account that the simulation matches the experimental J-V-characteristics under all illumination conditions and for a wide range of voltages.

TT 60.5 Wed 10:30 C 130

Quantification of loss channels in bulk heterojunction organic solar cells based on DPP-type donor-acceptor copolymers blended with PC71BM — •Julian Robert Ochsmann[1], Deepak Chandran[2,3], Kwang-Sup Lee[3], and Frédéric Laquai[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Dublin City University, Dublin, Ireland — [3]Hannam University, Daejeon, South Korea

A promising approach to improve the performance of bulk-heterojunction (BHJ) organic solar cells (OSC) is to use low-bandgap polymers as electron donor materials as they enhance the photon absorption of the photoactive layer in the near infrared wavelength range and thereby increase the photocurrent. In addition, low-bandgap polymers are suitable for use in tandem solar cells, since their absorption spectrum is complementary to that of mid-bandgap polymers such as P3HT or PCDTBT, which allows for photocurrent matching of front and back cells. A promising class of low-bandgap polymers for single- and multijunction solar cells are donor-acceptor type copolymers based on diketopyrrolopyrrole (DPP) units. In this study we investigate the photovoltaic performance and the photophysics of two DPP-based copolymers, namely PTDPP-TT and PFDPP-TT, blended with PC71BM and applied in single junction BHJ solar cells. The photophysics of the OSC devices were investigated with broadband transient absorption pump-probe spectroscopy (TA) and analyzed with a previously reported model of charge recombination that allows to quantify the loss channels in devices.

TT 60.6 Wed 10:45 C 130

Efficiency-Limiting Processes in Low-Bandgap Polymer:Perylene Diimide Photovoltaic Blends — •Dominik Gehrig[1], Steffen Roland[2], Ian Howard[1], Dieter Neher[2], and Frédéric Laquai[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz — [2]Institut für Physik und Astronomie, Physik weicher Materie, Universität Potsdam

In this work, we present a photophysical study on blends of a low-bandgap polymer, namely PBDTTT-C, as donor in combination with a PDI-based electron acceptor.[1] Exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to microsecond pump-probe transient absorption (TA) and time-resolved photoluminescence (TRPL) spectroscopy in combination with multivariate curve resolution (MCR) data analysis. A largely diffusion-limited exciton dissociation at the donor acceptor interface and consequently a slow charge generation is observed. Time-delayed collection field (TDCF) experiments reveal a strongly field-dependent charge generation process in turn leading to low fill factors in devices. However, once free charges are generated they recombine non-geminately on a ns-us timescale indicating that they can be potentially extracted as photocurrent. By comparison of the PBDTTT-C:PDI charge generation efficiency with that of a PBDTTT-C:fullerene blend, we identify inefficient charge generation and fast non-geminate recombination competing with charge extraction to be the main bottlenecks of photocurrent generation in the investigated polymer:PDI blends.

[1] Gehrig et al., J. Phys. Chem. C 2014, 118, 20077

TT 60.7 Wed 11:00 C 130

Effect of solvent vapor annealing on perylene-based solar cells — •Stefan Grob[1], Mark Gruber[1], Andrew Bartynski[2], Theresa Linderl[1], Mark Thompson[2], and Wolfgang Brütting[1] — [1]University of Augsburg, Augsburg, Germany — [2]University of Southern California, Los Angeles, USA

Diindenoperylene (DIP) and Tetraphenyldibenzoperiflanthene (DBP) are two common materials used in organic solar cell devices. While DIP is growing crystalline, showing good charge and exciton transport but only weak absorption, DBP exhibits an amorphous character, leading to lower carrier mobility and a short exciton diffusion length, however, DBP reveals a distinctly higher absorption. For both materials we investigate the influence of solvent vapor annealing (SVA) on solar cell performance. In general, SVA leads to a reorganization of the treated materials due to a partial re-solubilization of the layers, allowing the molecules to rearrange into structures characterized by a higher degree of order [1]. Though, for DBP, extended annealing times lead to a strong aggregation of the molecules, resulting in inhomogeneous layers unfavorable for solar cells. For DIP cells however, SVA leads to an increase in fill factor (FF) and also a slight increase in short-circuit current density (Jsc) due to interface roughening. Nevertheless, the best results are obtained by combining annealed DIP layers with strongly absorbing DBP and C70 on top. Thereby, we obtain the same increase in FF but a higher gain in Jsc, elevating the power conversion efficiency by almost 20 % up to more than 4 %.

[1] G. De Luca et al., J. Mater. Chem., 2010, 20, 2493-2498

15 min. break

TT 60.8 Wed 11:30 C 130

Morphology Tuning by Side-chain Variation in Bulk-Hetero-Junction Solar Cells Based on Merocyanines — •Dirk Hertel, Julian Nowak, Stephanie Rüth, Ruth Bruker, Jürgen Schelter, and Klaus Meerholz — Universität zu Köln, Department Chemie, Luxemburgerstrasse 116, 50939 Köln

Organic photovoltaics (OPV) offers the potential of mass-produced renewable energy. Within the last decade the efficiency of organic solar cells has increased from 3 % to 10 %, mainly based on better understanding and control of morphology. We investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Despite these impressive numbers the understanding of the influence of morphology on charge generation, transport and recombination in MCs is in its infancy. To aim towards even higher PCEs we have systematically varied the side-chain of a prototypical donor-acceptor MC with a high ground state dipole moment. By applying atomic-force mircroscopy, transmission electron microscopy and x-ray diffraction we are able to elucidate the thin film structure and show how side-chain variation reduces domain size and improves device data. We are able to correlate crystal size to optical, morphological and device data. There is an optimum side chain length and contrary to previous observations the MC:PCBM blend layers processed from solution perform better in OPVs than layers processed by thermal deposition under vacuum.

TT 60.9 Wed 11:45 C 130

Exploring the performance enhancement potential of the tapering technology for block-copolymer solar cells using a novel particle-based multiscale solar-cell algorithm — Anton Pershin, Sergii Donets, and •Stephan Baeurle — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, 93040 Regensburg, Deutschland

Tapered block copolymers offer an exciting opportunity to tailor the interfacial region between different components by conserving their phase-separated mesoscale structure, which enable the generation of polymer systems with the desired spatio-dynamic properties. In this presentation, we explore their usefulness for optimizing the photovoltaic performance of polymer bulk heterojunctions. To this end, we apply a recently developed particle-based multiscale solar-cell algorithm [1,2] and investigate the effect of random tapering at the chemical junctions between the electron-donor- (D) and electron-acceptor- (A) blocks on the photovoltaic properties of various lamellar-like polyfluorene-based block-copolymer systems. Our simulation results [2] reveal that introducing a tapered middle block with optimal length leads to a significant increase of the exciton dissociation efficiency, but deteriorates the charge transport efficiency only moderately. This results in a gain of the internal quantum efficiency from 25 up to 39 % by increasing the thickness of the active layer of the solar cell from 10 up to 50 nm in direction to the DA interface. Literature: [1] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 3736 (2014); [2] A. Pershin, S. Donets, S.A. Baeurle, Polymer 55, 1507 (2014).

TT 60.10 Wed 12:00 C 130

Effect of alcohol treatment on the morphology and performance of PTB7:PC71BM bulk heterojunction solar cells — Shuai Guo[1], Biye Cao[1], Weijia Wang[1], Jean-Francois Moulin[2], and •Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]Helmholtz-Zentrum Geesthacht am MLZ, Lichtenbergstr. 1, 85747 Garching

The environmentally friendly alcohol treatment of bulk heterojunction (BHJ) polymer solar cells using the low bandgap copolymer based on thieno[3,4-b]thiophene-alt-benzodithiophene units (PTB7) and [6,6]-phenyl-C71-butyric acid methyl ester (PC71BM) is studied. Different alcohols are tested and besides the most commonly used methanol treatment, other alcohols such as ethanol, 2-propanol, and 1-butanol also improve the device performance as compared to untreated solar cells. Changes of the surface structure caused by the alcohol treatment are probed with AFM and the modification of inner film morphology is probed by time of flight-grazing incidence small angle neutron scattering (TOF-GISANS). UV/Vis measurements show that the thickness of all BHJ films remains unchanged by the different solvent treatments. Thus, the enhanced device performance induced by the alcohol treatments is correlated to the reconstruction of the inner film structures probed with TOF-GISANS and the modified energy levels at the interfaces between the BHJ layer and the aluminum electrodes, evident by the enhanced short-circuit current and open-circuit voltage of the I-V curves.

TT 60.11 Wed 12:15 C 130

Control of Structural Order and Phase Separation in Polymer-Fullerene Solar Cells — •Christian Kästner[1], Daniel A. M. Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Technische Universität Ilmenau, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University, Linz, Austria

It is common knowledge that polymer aggregation and phase separation in blends with fullerene derivatives is a delicate issue and crucially impacts the photovoltaic parameters of polymer based solar cells. On the one side, strongly intermixed polymer:fullerene phases provide large interfacial area and consequently large exciton dissociation rates and thus charge carrier generation. On the other side, pristine, and eligibly ordered, polymer or fullerene domains support exciton delocalization and efficient charge transport. Herein, we present versatile routes to control the morphology by applying side-chain modifications to the polymer and fullerene, tuning the polymer:fullerene blend ratio and controlling the order within the bulk heterojunction via ternary blends. On the basis of an anthracene-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene) (PPE-PPV) copolymer backbone we investigated a number of these structure-property-relations. As an imposing result it is demonstrated that via manipulation of molecular structure and processing parameters enables tuning bulk morphologies at will.

TT 60.12 Wed 12:30 C 130

Influence of post-production thermal stress on organic photovoltaic cells — •Arne Hendel, Marlis Ortel, and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

One of the mayor challenges of organic photovoltaic cells towards large scale industrial production is the lifetime of the organic solar cells. Accelerated lifetime tests can be performed by applying thermal stress to the devices. In this study, PTB7:PCBM bulk hetero-junction solar cells were exposed in a post-production thermal heat step to temperatures up to 140°C. The reaction to thermal stress was investigated by impedance analysis and light intensity dependent I-V characteristics. It was found that the overall conductivity improved by thermal stress. In addition, an asymmetric series resistance which depends strongly on the light intensity was found by the light intensity dependent measurements. Furthermore, an investigation of the diode characteristic in dark revealed a deterioration of the blocking behaviour for reverse voltages. The results of the impedance analysis and light intensity dependent measurements were compared to AM1.5G I-V characterization, which was used to monitor the degradation of the device performance. A physical device model including the contact properties of the solar cells is presented to explain the findings.

TT 60.13 Wed 12:45 C 130

How intrinsic photo-degradation impacts photovoltaic device performance in organic solar cells — •Thomas Heumueller[1], Timothy Burke[2], William Mateker[2], Michael McGehee[2], and Christoph Brabec[1,3] — [1]Universität Erlangen-Nürnberg — [2]Stanford University — [3]ZAE Bayern

As organic PV efficiencies exceed 10%, the science of stabilization and lifetime gains importance. Several degradation phenomena in organic solar cells are related to an increase in trap density, but the mechanisms of how different types of traps affect open-circuit voltage, short-circuit current and fill factor need considerably more investigation. To separate effects from several different degradation mechanisms that usually occur at the same time, we perform tests under controlled environmental conditions and distinguish between bulk and interface effects by de-laminating and replacing electrodes. Interfacial degradation is observed to predominantly affect the fill factor, most likely due to the formation of energetic barriers and can be reversed by reapplying new electrodes. Bulk degradation in amorphous systems, like PCDTBT, results in a loss of open circuit voltage. Using charge extraction and transient photovoltage we show that the Voc losses are not caused by increased recombination, but rather by a broadening in the density of states. Crystalline materials demonstrate an increased stability against Voc losses, most likely due to a high charge carrier density at Voc. Sometimes a characteristic loss of short circuit current is observed in crystalline materials. We show that those losses can be prevented by choosing a different acceptor material.