CPP 20: Organic Electronics and Photovoltaics II

Time: Tuesday 13:45–16:15 Location: H37

CPP 20.1 Tue 13:45 H37

Spectroscopic signatures of C_{70}-Anions in Polymer-Fullerene composites — •Andreas Sperlich[1], Moritz Liedtke[2], Hannes Kraus[1], Oleg Poluektov[4], Carsten Deibel[1], Nazario Martin[3], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg — [3]Departamento de Quimica Organica, Facultad de Quimica, Universidad Complutense, E-28040 Madrid — [4]Chemical Sciences and Engineering Division, Argonne National Laboratory, 9700, USA

C_{70}-derivates are used in the most efficient organic bulk heterojunction solar cells. However, the detailed photophysical processes in composites containing C_{70} are still unresolved. In this contribution, our focus is on the light-induced charge transfer from the polymer to the fullerene, generating negatively charged C_{70} radicals. Photoinduced absorption (PIA), electron spin resonance (ESR 9.5GHz) and optically detected magnetic resonance (ODMR) were used to draw a picture of the photoinduced charge transfer from polymers to C_{70}. We provide the first experimental identification of the light induced C_{70} radical anion in blends with P3HT using high frequency ESR (130GHz). Comparing spectra from C_{70}-derivates with different sidechains, we could confirm that the electron is indeed localized on the C_{70}-cage. Further, we identify an additional absorption band at 0.9eV due to C_{70}^- by PIA.

CPP 20.2 Tue 14:00 H37

The Localized Nature of Charge Transfer in F_4TCNQ-Doped Thiophene-Based Donor Polymers — •Patrick Pingel[1], Lingyun Zhu[2], Kue Surk Park[1], Jörn-Oliver Vogel[1], Silvia Janietz[3], Eung-Gun Kim[2], Jürgen P. Rabe[1], Jean-Luc Brédas[2], and Norbert Koch[1] — [1]Department of Physics, Humboldt University Berlin, Germany — [2]School of Chemistry and Biochemistry, and Center for Organic Photonics and Electronics, Georgia Institute of Technology, USA — [3]Fraunhofer IAP, Potsdam, Germany

Recently, polymer layers exhibited exceptionally high conductivities upon p-type doping with the molecular acceptor tetrafluorotetracyanoquinodimethane (F_4TCNQ). Here, we present experimental and theoretical results on blend layers of F_4TCNQ and a series of poly(3-hexylthiophene-*co*-dithienyltetrafluorobenzene) (P3HT-TFT) copolymers with systematically varied TFT content. Regardless of the amount of TFT in the donor polymer, we find that only a single charge transfer (CT) species is formed, which we assign to the interaction of F_4TCNQ with an oligothiophene segment of the main chain. The degree of CT remains constant, even if the dopant concentration is increased up to a point, where closely neighbouring CT complexes exist at the same uninterrupted thiophene segment. Our findings show that the CT between F_4TCNQ and an oligothiophene segment has a localized, isolated nature, possibly comprising less than five connected thiophene units. Thus, CT is dictated by the local electronic structure on the nm scale, rather than depending, e.g., on the macroscopic ionization potential determined from photoemission methods.

CPP 20.3 Tue 14:15 H37

Charge Transfer Exciton Dynamics in Polymer/Fullerene Blend — •Josef M. Berger, Markus Hallermann, Enrico Da Como, and Jochen Feldmann — Lehrstuhl für Photonik und Optoelektronik, CeNS, LMU München

Polymer fullerene blends are one of the most promising material systems for organic photovoltaics. A major loss channel in these cells is the formation and recombination of charge transfer excitons. These excitons emit light as a consequence of radiative recombination of the hole on the polymer and the electron on the fullerene [1]. Here, we report on time resolved emission experiments with the aim of understanding the parameters controlling the recombination lifetime. For the blend of MDMO-PPV/PCBM we correlate the decay profile with the morphology obtained by transmission electron microscopy [2]. [1] Markus Hallermann, Stephan Haneder, and Enrico Da Como, Appl. Phys. Lett 93, 053307 (2008) [2] Markus Hallermann, Ilka Kriegel, Enrico Da Como, Josef M. Berger, Elizabeth von Hauff, Jochen Feldmann, Advanced Functional Materials 19, 3662 (2009)

CPP 20.4 Tue 14:30 H37

The Relationship between the Electric Field Induced Dissociation of Charge Transfer (CT) Excitons and the Photocurrent in Novel Hybrid Small Molecular/Polymeric Solar Cells — •Sahika Inal[1], Alan Sellinger[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam-Golm — [2]Institute of Materials Research & Engineering, Singapore 117602

Complete dissociation of coulombically bound interfacial states is an ultimate step accounting for photovoltaic performance. Recent work has proposed that the emission of CT-exciton, i.e. an exciplex, is a competing process to the generation of free charges [Appl. Phys. Lett. 2007, 90, 092117]. Here, we investigated the photophysical processes in a bulk heterojunction system using a soluble poly(p-phenylenevinylene) donor and a novel small molecular electron acceptor based on Vinazene (2-vinyl-4,5-dicyanoimidazole). Recent work has shown that this blend exhibits a featureless emission, prominent at long wavelengths of the spectrum, which was attributed to a CT-exciton [J. Chem. Phys. 2009, 130, 094703]. We monitored the field induced dissociation of these CT-excitons by means of steady state and time resolved PL spectroscopy. Shortened decay times and reduced PL emission in blend film evidence the dissociation of the emissive intermolecular pair by the external electric field. Analyzing the dependence of the photocurrent and external quantum efficiency on the external field, the fate of the separated exciplex pairs is tackled. It is suggested that the formation of free carriers involves channels other than CT-excitons in such blends.

CPP 20.5 Tue 14:45 H37

Study of Sub-Bandgap States in Polymer-Fullerene Solar Cells — •Martin Presselt[1], Felix Herrmann[1], Marco Seeland[1], Maik Bärenklau[1], Sebastian Engmann[1], Roland Rösch[1], Wichard J. D. Beenken[2], Sviatoslav Shokhovets[1], Harald Hoppe[1], and Gerhard Gobsch[1] — [1]Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

At present polymer-fullerene blends are widely used to build organic solar cells. The main contribution to their photocurrent originates from optical transitions between occupied states below the HOMO level and unoccupied states above the LUMO level of the polymer.

In this work, we investigated the origin of states contributing to the optical absorption in the sub-bandgap spectral range and the resulting photocurrent in P3HT-PCBM bulk heterojunction solar cells. Photothermal deflection spectroscopy, temperature dependent external quantum efficiency, photoluminescence and electroluminescence as well as spectroscopic ellipsometry measurements have been carried out. Effects due to different P3HT-PCBM blending ratios and annealing temperatures have been studied.

Two models are discussed to explain the experimental observations: optical transitions involving (a) disorder and/or defect related states, and (b) charge transfer complexes.

CPP 20.6 Tue 15:00 H37

Influence of system size on simulated charge mobility in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3) — •Alexander Lukyanov and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We present the results of a modeling study of the charge transport in amorphous films of tris(8-hydroxyquinolinato)aluminium (Alq3). In our multiscale approach we combine molecular dynamics to generate material morphologies, Marcus theory to evaluate charge hopping rates and kinetic Monte Carlo to simulate charge dynamics. Energetic disorder is taken into account by assigning partial charges to the hopping sites, obtained from DFT B3LYP, 6-311g(d) calculations. In contrast to the previous studies Poole-Frenkel behavior of the mobility is reproduced. Our results indicate strong finite-size effects, meaning that the absolute value of the calculated mobility decreases with the increase of the simulation box size. Simple analogy with a classical percolation problem suggests that very large systems are required to obtain a reliable estimate of the charge carrier mobility.

CPP 20.7 Tue 15:15 H37

Influence of injection and extraction barriers realized by choice of donor and HTL on organic solar cell performance — •Wolfgang Tress, Ellen Siebert, Karl Leo, and Moritz Riede — TU Dresden, Institut für Angewandte Photophysik

In the p-i-n solar cell architecture, the active materials of a donor/acceptor flat heterojunction are sandwiched between two doped transport layers, which provide a highly conductive contact to the cathode metal and the ITO, respectively. This concept allows for a systematic study of the influence of the HOMO of the donor and the adjacent hole transport layer (HTL) on the open circuit voltage (V_{oc}) and the shape of the IV curve. This approach avoids the main problems emerging by metal-organic interfaces like varying work functions, unpredictable interface dipoles, etc.. Additionally, extraction barriers, which cannot be realized by the choice of metal, can be adjusted in a controlled way by a HOMO of the HTL lying deeper than the HOMO of the donor. Using donor and HTL materials with a HOMO between 5.0 and 5.6 eV in combination with C_{60} as acceptor, we demonstrate a systematic dependence of V_{oc} on the HOMO of the donor, whereas the built in field is goverened by the HOMO of the strongly doped HTL. The fill factor (FF) is mainly influenced by the HOMO offset between donor and HTL. Both types of barriers (extraction and injection) decrease FF resulting in s-shaped curves with different characteristics. The experimental results are interpreted by comparison to simulation data of a drift-diffusion model, treating the HOMO barrier with a field dependent lowering effect.

CPP 20.8 Tue 15:30 H37

Hole transport characteristics of pentacene studied with Green functions and real-time propagation — •Sebastian Radke[1], Caroline Gollub[1,2], Stanislav Avdoshenko[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

For temperatures higher than 150 Kelvin the charge carrier mobility in organic semiconductors depends sensitively upon an interplay of band-like and hopping transport [1]. In this contribution, the hole transport characteristics of an organic semiconducting material are studied with two different theoretical methods and both approaches are compared. As a model system a pentacene structure is selected, which is well-characterized in the context of organic electronics. The first approach is based on a Green function formulation of the Holstein-Peierls model, accounting for local and non-local electron-phonon coupling and it addresses the transport problem in the energy space, so that fluctuations are taken into account only within a static picture. In the second approach, a real-time propagation of the charge carrier wave function is performed and this provides a deeper insight into the different time scales appearing in the problem. The Hamiltonian is formulated in the tight-binding representation, where the parametrization is evaluated for different levels of theory of the MD trajectories and of the electronic structure calculations.

[1] Y. C. Cheng, *et al.*, J. Chem. Phys. **118**, 3764 (2002).

CPP 20.9 Tue 15:45 H37

Ab initio based modeling of charge transport in organic semiconductors — •Caroline Gollub[1,2], Stanislav Avdoshenko[1], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology — [2]Max Planck Institute for the Physics of complex Systems, Dresden

In organic electronics, theory is expected to play an important role for the search of organic semiconducting materials with improved charge carrier mobilities. Current theoretical efforts are devoted to the understanding of the charge transport mechanism and the accurate prediction of the structure-mobility relationship. In this contribution, an approach for the charge migration in organic semicondutors is presented based on a self-consistent propagation of the charge carrier wave function effected by the molecular dynamics of the system, i.e. the electronic and nuclear dynamics are treated on an equal footing. The simulation comprises the evaluation of charge transfer parameters from ab initio calculations, the quantum dynamical calculation of the evolution of the charge carrier wave function and the molecular dynamics of the studied system. The method allows to follow the real-time and real-space transport and can be used to extract charge carrier mobilities in dependence of the chemical functionality, the temperature or the structure assembly. The technique will be demonstrated for hole transport in a 1D stack of coronene molecules.

CPP 20.10 Tue 16:00 H37

Energetics of Excited States in the Conjugated Polymer Poly(3-hexylthiophene) — Julien Gorenflot[1], •Daniel Mack[1], Daniel Rauh[4], Stefan Krause[2], Carsten Deibel[1], Achim Schöll[2], Friedrich Reinert[2,3], and Vladimir Dyakonov[1,4] — [1]Experimental Physics VI, University of Würzburg, D-97074 Würzburg — [2]Experimental Physics II, University of Würzburg, D-97074 Würzburg — [3]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — [4]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Although prototypes and first commercial polymer-based solar panels already exist, a comprehensive understanding of the fundamental processes and energetics involved in photocurrent generation is still missing and limits further device optimisations. We present a complementary set of experiments on poly(3-hexylthiophene(P3HT), which enables us to draw general conclusions on the energy levels and barriers involved in the processes from light absorption to polaron pair dissociation. From photoemission spectroscopy of occupied and unoccupied states we determine the transport gap to 2.6 eV, which we show to be in agreement with the onset of photoconductivity by spectrally resolved photocurrent measurements. We also find that photogenerated singlet excitons, generated with light at the absorption edge, require 0.7 eV of excess energy to overcome the binding energy. The intermediate charge transfer state, also called polaron pair, is situated only 0.3 eV above the singlet exciton. We discuss our results in view of their impact on charge generation.