

CPP 10: Poster: Charge transfer effects in molecular materials (related to symposium SYCT)

Time: Monday 17:30–19:30

Location: Poster C

CPP 10.1 Mon 17:30 Poster C

Foam-like structures of titania films for application in flexible photovoltaic — ●BO SU, MARTIN A. NIEDERMEIER, MONIKA RAWOLLE, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics, for example in hybrid solar cells and dye-sensitized solar cells (DSSC). The nanoporous titania layers are responsible for the electron transporting and directing dye layers' structure. In our studies, the morphology of titania films is investigated with respect to a possible incorporation into hybrid solar cells. The titania films are prepared by a sol-gel process in combination with block copolymer templating. Via this route we have a very high level of control over the final morphology. The films are typically prepared via spin-coating, followed by a calcination step to remove the polymer template and obtain crystalline titania. Additionally, our method is even suitable for low-temperature synthesis by changing the titania precursor. The structure of these films is probed with the imaging techniques such as scanning electron microscopy and atomic force microscopy. To determine the optical and opto-electronical properties UV/Vis spectroscopy and photoluminescence are used.

CPP 10.2 Mon 17:30 Poster C

Field dependent charge carrier generation via charge transfer states: A blending ratio dependent study — ●JULIA KERN¹, CLEMENS GRÜNEWALD¹, HANNES KRAUS¹, FRANZISKA FUCHS¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilians University of Würzburg, 97074 Würzburg, Germany — ²Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), 97074 Würzburg, Germany

In organic bulk heterojunction solar cells, the mechanism of exciton dissociation at the polymer–fullerene interface is still controversially debated. This work studies the charge carrier generation via charge transfer states by investigating the electric field dependence of the process for a model system consisting of MDMO-PPV and PC₆₁BM. Focusing on the influence of different donor–acceptor blend ratios, the complementary techniques of field dependent photoluminescence quenching and transient absorption are employed to reveal a substantial change in the electric field behavior. Thus, the binding energy of the respective charge transfer excitons (CTE) is reduced from ~ 320 meV for a 4:1 blend ratio to ~ 200 meV for a 1:1 blend, decreasing even further for higher PC₆₁BM concentrations. The observed phenomenon may be ascribed to a change in the average dielectric constant or in the CTE delocalization length of the system. The relevance of these influencing factors is unveiled by combined morphological studies comprising atomic force microscopy and optically detected magnetic resonance. This study demonstrates the importance of a high dielectric constant for charge carrier generation in organic photovoltaics.

CPP 10.3 Mon 17:30 Poster C

Effect of Polymorphism, Regioregularity and Paracrystallinity on Charge Transport in Poly(3-Hexyl-Thiophene) [P3HT] Nanofibers — ●CARL POELKING, KURT KREMER, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

We establish the link between molecular order and charge-transport parameters in poly(3-hexyl-thiophene) (P3HT) accounting for different polymorphic structures and regioregularities. Using atomistic molecular dynamics, we study structural transitions related to side-chain melting and a conversion from a non-interdigitated metastable (form Γ') to the stable (form I) P3HT polymorph, as also observed experimentally, thus providing structural models for side-chain arrangement and backbone-backbone stacking. We investigate how packing modes and regioregularity effect paracrystalline and side-chain order and analyse effects thereof on the dynamics and distribution of electronic couplings and site energies. In particular, we demonstrate how a small concentration of defects in side-chain attachment can lead to a dramatic decrease in charge-carrier mobility due to a strong intermolecular contribution to the energetic disorder, which we attribute to fluctuations in backbone-backbone distances. Our simulated mobil-

ities indicate excellent agreement with experimental values obtained for P3HT nanofibers.

CPP 10.4 Mon 17:30 Poster C

Microscopic simulations of charge and energy transfer in crystalline PCPDTBT and PSBTBT — ●ANTON MELNYK, BJÖRN BAUMEIER, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Charge and exciton transfer processes in two semi-crystalline polymers, PCPDTBT and PSBTBT, are compared using a combination of classical molecular dynamics to simulate semi-crystalline morphologies, quantum chemistry to evaluate the electronic structure of conjugated segments, and charge/energy transfer theories to study charge and energy transfer/transport. By linking local molecular arrangements of two polymers to the changes in distributions of site energies and electronic coupling elements we rationalize the improved charge mobility, reduced bimolecular recombination, and formation of charge transfer states in PSBTBT.

CPP 10.5 Mon 17:30 Poster C

Multifrequency electron spin resonance analysis of organic polymer:fullerene blends — ●MAX GESSNER¹, ANDREAS SPERLICH¹, HANNES KRAUS¹, STEFAN VÁTH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University Würzburg, 97074 Würzburg, Germany — ²ZAE Bayern, 97074 Würzburg, Germany

Understanding of the light-induced charge transfer in organic solar cells is essential to improve material properties and processing parameters, and, at long sight, device performance. Since the charge carriers are spin- $\frac{1}{2}$ particles they can be studied by electron paramagnetic resonance (EPR). Several solar cell blends of fullerene-derivatives PC₆₀BM and PC₇₀BM with conjugated polymers P3HT, C-PCPDTBT and Si-PCPDTBT were investigated with light induced X-band EPR. The resulting spectra consist of overlapping signals from electrons and holes. By performing the same measurements with the high frequency Q-band EPR we were able to study the individual signals of charges localized on either fullerene or polymer domains in more details with higher resolution. By comparing the experimental spectra with simulations performed with EasySpin we have the tool for learning more about the local order and geometry as well as the electric properties of these promising materials for organic photovoltaics.

CPP 10.6 Mon 17:30 Poster C

Influence of charge density on microscopic transport in amorphous organic semiconductors — ●PASCAL KORDT and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The effect of finite charge carrier density on microscopic transport parameters, such as occupation probabilities, local currents, and charge mobility is analyzed by means of the off-lattice kinetic Monte Carlo method as well as the Fokker-Planck equation in a mean-field approximation. Implications for the macroscopic description of organic field effect transistors and light emitting diodes are discussed.

CPP 10.7 Mon 17:30 Poster C

Energy Level Alignment for Many-Body Resonant Tunneling — ●JESSICA WALKENHORST¹, HEIKO APPEL², NICOLE HELBIG^{3,1}, and ANGEL RUBIO¹ — ¹NanoBio Group and ETSF, UPV/EHU, Spain — ²NanoBio Group and ETSF, Fritz-Haber-Institut der MPG, Germany — ³PGI and IAS, Forschungszentrum Jülich, Germany

Electron tunneling plays a fundamental role in many chemical and physical processes and provides evidence of quantum mechanics at the macroscopic level. In addition to the fundamental physics, electron tunneling at surfaces also attracts much attention due to its importance for charge transfer and carrier injection mechanisms e.g. in organic devices. Resonant tunneling is governed by the alignment of energy levels of donor and acceptor. While the separate systems are described well by standard approaches, the alignment of their chemical potentials is problematic since bringing donor and acceptor in contact changes the respective energy levels due to the electronic interaction. We investigate resonant many-body tunneling in a one dimensional donor-acceptor system, where the electrons interact via a softened Coulomb

potential. For a system of few electrons, we solve the Schrödinger equation exactly. As a first step we analyze the case of adiabatic tunneling. Starting from the description of tunneling between non-interacting systems, we derive the necessary energy correction terms for the case of the complete fully interacting donor-acceptor many-body system. We then extend our adiabatic model to a time-dependent description to study the deviation of the dynamic tunneling behavior from the adiabatic case.

CPP 10.8 Mon 17:30 Poster C

Microscopic simulations of electronic excitations at donor-acceptor interfaces — •BJÖRN BAUMEIER, CARL POELKING, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Fundamental processes involving electronic excitations govern the

functionality of molecular materials, in which the motion of excitons and charges is determined by an interplay of molecular electronic structure and morphological order. To understand, e.g., charge separation and recombination at donor-acceptor heterojunctions in organic solar cells, knowledge about the microscopic details influencing these dynamics in the bulk and across the interface is required.

Using a combination of molecular dynamics and quantum-chemistry (DFT/GW-BSE), we first obtain atomistically resolved morphologies of prototypical planar heterojunctions of dicyanovinyl-substituted quaterthiophene (donor) and C₆₀ (acceptor) and then analyze the charged and neutral electronic excitations therein. We pay special attention the spatially-resolved electron/hole transport levels (band bending and offsets), as well as the relative energies of Frenkel and charge-transfer excitations at the interface. Finally, we link our results to the molecular architecture of the donor material and its orientation on the fullerene substrate.