CPP 22: Fokus: Conjugated Polymers

Time: Wednesday 9:30–12:30 Location: ZEU 160

Topical Talk CPP 22.1 Wed 9:30 ZEU 160

Charge transport in doped poly(p-phenylene vinylene) — Y. Zhang, B. de Boer, and •P. W. M. Blom — Zernike Institute for Advanced Materials and Dutch Polymer Institute, University of Groningen, The Netherlands

The hole transport in poly(dialkoxy-p-phenylene vinylene) (PPV) based diodes is known to be space-charge limited (SCL) for Ohmic contacts. At room temperature the SCL current in PPV-derivatives is governed by the dependence of the hole mobility on charge carrier density, whereas at low temperatures the field-dependence prevails [1]. We present controlled p-type doping of MEH-PPV deposited from solution using tetrafluoro-tetracyanoquinodimethane (F4-TCNQ) as a dopant. By using a co-solvent aggregation in solution can be prevented and doped films can be deposited. Upon doping the current-voltage characteristics of MEH-PPV based hole-only devices are increased by several orders of magnitude and a clear Ohmic behavior is observed at low bias. Taking the density dependence of the hole mobility into account the free hole concentration due to doping can be derived. We find that a doping concentration of 1.0 wt.% leads to a free carrier density of $2 \times 10^{22}\,\mathrm{m}^{-3}$. Neglectance of the density-dependent mobility would lead to an overestimation of the free hole density by an order of magnitude. The free hole densities are further confirmed by impedance measurements on Schottky diodes based on F4-TCNQ doped MEH-PPV and a silver electrode.

1. C. Tanase, P.W.M. Blom, and D.M. de Leeuw, Phys. Rev. B.70, 193202 (2004)

Topical Talk CPP 22.2 Wed 10:00 ZEU 160

A realistic description of the charge carrier wavefunction in microcrystalline polymer semiconductors — •Alessandro Troisi, David L. Cheung, and David P. McMahon — Department of Chemistry, University of Warwick, Coventry, UK

The electronic structure of the charge carrier in one of the most commonly used semiconducting polymer (P3HT) is investigated using a combination of classical and quantum chemical methods. It is shown that the carriers are localized in correspondence of long lived traps which are present also in the crystalline phase of the polymer and these traps are characterized with chemical detail. The existence of activated transport also for very ordered polymer phases (regardless of the strength of the polaron formation energy) is explained and the provided chemical description of the trapped states can be used to design materials with improved mobility. It is shown that is possible to use computational chemistry methods to fill the gap between phenomenological descriptions of charge transport in polymers and microscopic description of the individual quantum dynamic process.

Topical Talk CPP 22.3 Wed 10:30 ZEU 160

Influence of microstructure on transport and recombination in conjugated polymer:fullerene blend films — •Jenny Nelson[1], Amy Ballantyne[1], Mariano Campoy-Quiles[1], Toby Ferenczi[1], Jarvist Frost[1], Panos Keivanides[1], Ji-Seon Kim[1], James Kirkpatrick[1], Christian Mueller[2], Donald Bradley[1], James Durrant[1], Paul Smith[2], and Natalie Stingelin[3] — [1]Imperial College London, UK — [2]ETH Zuerich, Switzerland — [3]Queen Mary University of London, UK

The dynamics of charge carriers in conjugated polymer:small molecule blend solar cells are strongly influenced by the microstructure of the blend films. Efficient photocurrent generation appears to require, at the same time, a high degree of order in local molecular packing (benefitting charge transport and charge separation), a large interface (for charge separation) and significant phase segregation (to minimise charge recombination). In this work, we will show how a combination of spectroscopic techniques, electrical measurements and studies of phase behaviour can be used to build up a picture of the microstructure in a polymer: fullerene blend film, and to relate the microstructure to the dynamics of charge separation, transport and recombination. To interpret the results we use coarse grained models of the evolution of phase morphology and kinetic Monte Carlo models of charge transport and recombination. Finally, we demonstrate that the optimum blend composition for photocurrent generation can be related in a rational way to the phase behaviour of the binary system and in particular to the self-organising tendency of the component materials.

Topical Talk CPP 22.4 Wed 11:00 ZEU 160

Charge transport along isolated conjugated molecular wires — •Ferdinand C. Grozema and Laurens D.A. Siebbeles — DelftChemTech, Delft University of Technology, The Netherlands

In the majority of measurements of charge transport in single molecular wires the molecule is connected to two electrodes. The results obtained from these measurements are often to a large extent determined by the molecule-electrode interface and the transport occurs by direct tunneling with the charge never being fully located on the wire. Therefore is difficult to obtain information on the mobility of charges when they are actually on the molecule. We use a unique combination of techniques that enables us to measure the mobility of charges along conjugated polymers chains that are isolated from each other by bringing them in a dilute solution. Charges are generated by irradiation with pulses of high-energy electrons and the mobility of these charges is determined by contact-less time-resolved microwave conductivity measurements. These experiments have been performed for a wide variety of different types of conjugated polymers and it was found that charge carrier mobility strongly depends on the molecular structure [1-3].

1. P. Prins, F.C. Grozema, J.M. Schins, S. Patil, U. Scherf and L.D.A. Siebbeles, Phys. Rev. Lett., 2006, 96, 146601

2. P. Prins, F.C. Grozema and L.D.A. Siebbeles, J. Phys. Chem. B, 2006, 110, 14659

3. F.C. Grozema, C. Houarner-Rassin, P. Prins, L.D.A. Siebbeles and H.L. Anderson, J. Am. Chem. Soc., 2007, 129, 13370

Topical Talk CPP 22.5 Wed 11:30 ZEU 160

Charge transport: a multiscale model in polymers — •James Kirkpatrick — Department of Physics, Imperial College London, UK

This contribution addresses the relationship between charge transport and polymer chain morphology. It attempts to determine whether our instinctive model of charges rapidly moving along chains and slowly between them is consistent with charge transport parameters computed using state of the art computational methods.

The morphology of polymer films is simulated using molecular dynamics, charge transport parameters are computed using semi classical methods and charge transport is simulated by solution of rate equations. The model system considered is polypyrrole. Global arrangement is manipulated by preparing morphologies with chains aligned along one axis ("fiber"), lying in the plane ("slice") or disordered in all directions ("isotropic"). Local molecular arrangement can also be manipulated by making the chains stiffer, simulating their morphology when oxidized.

Non-adiabatic semi-classical theory will be used to describe hops between different chains. The motion of charges along polymer chains will be approximated as adiabatic hops. The influence of parametrization of charge transport rates on mobility will be studied.

Topical Talk CPP 22.6 Wed 12:00 ZEU 160

From amorphous polymers to discotic liquid crystals - Measuring charge carrier mobility with the time-of-flight technique — •Frederic Laquai[1], Dirk Hertel[2], Marcel Kastler[1], Klaus Muellen[1], and Gerhard Wegner[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]University of Cologne, Germany

The charge carrier mobility is one of the key parameters of conjugated materials that greatly determines the performance of electronic devices. It can be measured by various techniques, for instance, the time-of-flight (TOF) technique, space-charge limited current measurements or pulsed radiolysis time resolved microwave conductivity measurements. Here, the charge-generation-layer TOF technique has been used to study hole mobility of a series of amorphous poly-spirobifluorene copolymers. The copolymers contain different concentrations of triarylamine units in the polymer backbone and have mobilities in the range of $10^{-6} - 10^{-4}\,\mathrm{cm}^2/\mathrm{Vs}$. The results of the field and temperature dependent measurements can be well interpreted in the framework of the 3D-Gaussian disorder formalism. The experiments show that high hole mobility does not necessarily lead to high performance in OLEDs. Secondly, the TOF technique has been employed to study hole transport in hexa-peri-hexabenzocoronene molecules that can be organised into face-on or edge-on arrangements between substrates depending on

the nature of the alkyl-chains attached to the molecule. Mobilities of $10^{-3}\,\mathrm{cm}^2/\mathrm{Vs}$ have been determined and results could be well analysed in the framework of a 1D-transport model.