

## CPP 6: Poster: Structural Ordering and Electronic Transport (joint focus with HL)

Time: Monday 17:30–19:30

Location: Poster A

CPP 6.1 Mon 17:30 Poster A

**Multiscale molecular simulations of P3HT:PCBM blends** — ●OLGA GUSKOVA<sup>1</sup>, ANDREAS JOHN<sup>1</sup>, PETER FRIEDEL<sup>1</sup>, and JENS-UWE SOMMER<sup>1,2</sup> — <sup>1</sup>Leibniz Institute of Polymer Research, Dresden, Germany — <sup>2</sup>TU Dresden, Dresden, Germany

We apply a multi-level approach including micro- and mesoscale simulation to investigate the nanoscale morphologies of bulk heterojunction blend films comprising poly(3-hexylthiophene) (P3HT) and the methanofullerene derivative phenyl-C61-butyric acid methyl ester (PCBM). DFT provides the information about local system morphology and the electronic properties that are important for device performance. Full-atomistic MD simulations expand the accessible length and time scale to ranges of heterojunction regions. Combination of these methods provides a deeper insight into the relations between structural and electronic properties of polymer-based donor/acceptor materials. Since existing force-fields do not properly reproduce the torsion angle between neighboring thiophene rings, we optimized dihedral angle potential between neighboring thiophene rings and validated the empirical force field PCFF for PCBM and P3HT. Simulations of blended P3HT and PCBM molecules were carried out to study the conformations at the P3HT/PCBM interface which crucial to our understanding of both the morphology evolution of the active layer in photovoltaic devices and charge separation/recombination rules. Since morphology has a direct impact on the electronic properties of the device, DFT studies of the realistic morphologies, based on MD simulations, enables a more accurate prediction of the device performance.

CPP 6.2 Mon 17:30 Poster A

**Distribution of States and Energetic Disorder in P3HT:PCBM Blends** — ●ILJA LANGE, JULIANE KNIEPERT, PETER BRÜCKNER, JAMES C. BLAKESLEY, and DIETER NEHER — University of Potsdam

P3HT:PCBM has been widely used as a promising candidate for research on organic photovoltaic because of its relatively high efficiency of 3-5%. However, this system is still not fully understood and some basic fundamental processes are still lacking. One reason for this incomplete picture is the lack of information about the energetic landscape of these devices. Established techniques like photoemission spectroscopy or cyclic voltammetry only deliver a rough approximation of the position of relevant transport bands and states. Instead, exact information about the distribution of states and their broadening is preferable for a comprehensive insight into e.g. open-circuit voltage, charge carrier generation, recombination and extraction.

Recently, we showed that charge injection into the low densities of tail states of organic semiconductors can be detected sensitively by Kelvin Probe [1]. By careful numerical analysis of the measurements, the distribution of tail states can be quantified. Here we apply this technique to explore the energetic structure of P3HT:PCBM blends. Surprisingly, we find that the energetic structure of both the donor and acceptor components change dramatically upon thermal treatment. These results open up interesting new insights into fundamental processes of this popular material system that have wider implications for all organic solar cells.

[1]Phys. Rev. Lett. 106, 216402 (2011)

CPP 6.3 Mon 17:30 Poster A

**Recombination process in organic photovoltaic solar cells based on BTD/DPP copolymers studied by IV-characteristics** — ●OLESA SYNOOKA — Physics institute, TU Ilmenau, 98693 Ilmenau, Germany

The short-circuit current density ( $J_{sc}$ ) of polymer/fullerene bulk heterojunction solar cells based on benzothiadiazole (BTD) and/or diketopyrrolopyrrole (DPP) is investigated as a function of light intensity. The influence of light intensity and recombination strength on  $J_{sc}$  is consistently explained by a model based on the notion that the quasi-Fermi levels are constant throughout the device, including both drift and diffusion of charge carriers. A typical feature of polymer/fullerene based solar cells is that  $J_{sc}$  does not scale exactly linearly with light intensity ( $I$ ). Instead, a power law relationship is found given by  $J_{sc}(I)$ , where  $a$  ranges from 0.7 to 0.8. In a number of reports this deviation from unity is attributed to the occurrence of bimolecular recombination. Here is demonstrated the model calculations which shows that

bimolecular recombination leads not a 100% of a typical loss of all free charge carriers at  $J_{sc}$  for these devices but it also governed by the build-up of space charge in the device.

CPP 6.4 Mon 17:30 Poster A

**Influence of different organic ligands on the charge transport and charge transfer characteristics of CuInS<sub>2</sub>/polymer hybrid mixtures** — ●CHRISTOPHER KRAUSE, NIKOLAY RADYCHEV, FLORIAN WITT, MARTA KRUSZYNKA, DOROTHEA SCHEUNEMANN, JOANNA KOLNY-OLESIK, HOLGER BORCHERT, and JÜRGEN PARISI — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, 26111 Oldenburg

CuInS<sub>2</sub> (CIS) nanoparticles embedded into a conductive polymer are a promising candidate for hybrid photovoltaic application due to unique features of the CIS nanomaterials. One of the key problems of the hybrid solar cells functionality is the creation of an efficient bulk heterojunction itself. In most cases, nanoparticles in the polymer matrix have to be stabilized by organic ligands, which can impede efficient charge transport through the hybrid blends as well as charge separation at the polymer/nanoparticle interface. Therefore an exchange of the initial ligand is required and might significantly improve the performance of semiconductor nanoparticle based hybrid solar cells. In the present work, the influence of different organic ligands on the charge transport in CIS and CIS/polymer blends is investigated by current-voltage measurements in a device geometry similar to solar cells and compared to mobility measurements in organic field-effect transistors (OFETs). Additionally, the charge transfer process at the donor/acceptor interface is studied by electron spin resonance.

CPP 6.5 Mon 17:30 Poster A

**Subsurface imaging of P3HT:PCBM blends** — ●MARTIN DEHNERT<sup>1</sup>, MARIO ZERSON<sup>1</sup>, SVEN HÜTTNER<sup>2</sup>, ZHUXIA RONG<sup>2</sup>, ULLRICH STEINER<sup>2</sup>, and ROBERT MAGERLE<sup>1</sup> — <sup>1</sup>Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — <sup>2</sup>Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K.

We investigate the surface morphology of thin films of poly(3-hexylthiophene) (P3HT) and [6,6]-phenyl C61-butyric acid methyl ester (PCBM) blends using AFM based amplitude-phase-distance-curves (APD). We use the indentation of the tip into the soft surface layer to measure the mechanical properties as a function of the tip indentation which allows reconstructing three dimensional depth profiles of the top 10 nm of the film. We show surface depth profiles of blends with varying ratio of P3HT:PCBM and study structural changes after different thermal annealing steps. The soft amorphous layer on the surface are formed to be between five and ten nanometers thick. We discuss the impact of the surface morphology and the amorphous top layer on the efficiency of organic solar cells.

CPP 6.6 Mon 17:30 Poster A

**Ordered TiO<sub>2</sub> single crystal nanowire arrays for hybrid solar cells** — ●JULIAN REINDL<sup>1</sup>, JONAS WEICKERT<sup>1</sup>, ANDREAS WISNET<sup>1</sup>, CHRISTINA SCHEU<sup>1</sup>, and LUKAS SCHMIDT-MENDE<sup>2</sup> — <sup>1</sup>Ludwig-Maximilians-University, Munich — <sup>2</sup>University of Konstanz

Organic Solar cells are an interesting technology where remarkable efficiencies beyond 8 % have been realized with the bulk heterojunction concept. Here a donor-acceptor blend is fabricated as absorbing and charge transporting layer. Even though this concept is striking for thin films, the unordered inner morphology of the active layer has detrimental effects in thicker layers due to higher charge trapping and charge carrier recombination. A promising approach to realize thicker active layers with accordingly higher absorptivity is the hybrid solar cell concept, where the organic donor is substituted by a wide band gap metal oxide like titania (TiO<sub>2</sub>). The TiO<sub>2</sub> can be nanostructured, resulting in a controlled phase separation of donor and acceptor.

Here we present a possibility of synthesizing a layer of ordered monocrystalline rutile titania wires with controllable properties such as wire length, diameter and spacing. This layer acts as electron transporting matrix and should provide enhanced electron mobility compared to polycrystalline titania layers. In order to fabricate hybrid solar cells we fill these structures with the commonly used polymer P3HT. For better structure filling novel attempts using different methods are studied, including interface engineering and an approach

using diethylfluorene monomers, which can be polymerized inside the structure.

CPP 6.7 Mon 17:30 Poster A

**Nanostructured Hybrid Solar Cells** — ●JONAS WEICKERT<sup>1,2</sup>, ANDREAS WISNET<sup>1</sup>, CHRISTINA SCHEU<sup>1</sup>, and LUKAS SCHMIDT-MENDE<sup>2</sup> — <sup>1</sup>Ludwig-Maximilians-University Munich, Munich, Germany — <sup>2</sup>University of Konstanz, Konstanz, Germany

Organic solar cells have gained remarkable interest during the past two decades and have reached high power conversion efficiencies of 8%. However, efficiencies are still limited by relatively low absorptivity. Only thicker active layers could allow more complete photon harvesting. However, the active layer thickness of conventional organic solar cells is conceptually limited due to the relatively uncontrolled morphology of their active layers, which promotes charge carrier recombination for films thicker than 100-200 nm.

One way to overcome these limitations is the substitution of the organic acceptor material with wide band-gap semiconductors like TiO<sub>2</sub> in so-called hybrid solar cells. TiO<sub>2</sub> also acts as electron acceptor but can be nanostructured in order to meet the competing demands of high interfacial area and consistent pathways for charge transport.

TiO<sub>2</sub> nanotubular arrays with dimensions comparable to exciton diffusion lengths in typical organic materials are synthesized on conductive glass substrates via electrochemical anodization of thin Ti films and can be readily infiltrated with donor material to realize ordered hybrid heterojunctions.

The properties of the metal oxide-organic junction can be further tuned by introduction of interfacial modifiers like dye molecules and are investigated in detail.

CPP 6.8 Mon 17:30 Poster A

**Solvent additives for tuning the photovoltaic properties of polymer-fullerene solar cells** — ●ANNA GÖRITZ<sup>1</sup>, ANTONIETTA DE SIO<sup>2</sup>, THOMAS MADENA<sup>2</sup>, RALPH HUBER<sup>2</sup>, JÜRGEN PARISI<sup>2</sup>, SHANY NEYSHADT<sup>3</sup>, FELIX DESCHLER<sup>3</sup>, ENRICO DA COMO<sup>3</sup>, SALVATORE ESPOSITO<sup>4</sup>, and ELIZABETH VON HAUFF<sup>1,2</sup> — <sup>1</sup>Physics Institute, University of Freiburg — <sup>2</sup>Physics Institute, University of Oldenburg — <sup>3</sup>Dep. of Physics and CeNS, LMU, Munich — <sup>4</sup>ENEA Research Center, Localita Granatello, Portici, Italy

We demonstrate that using solvent additives to prepare P3HT:PCBM blends increases the performance of bulk heterojunction solar cells by inducing favorable phase segregation and increased polymer ordering in the active layer<sup>[a]</sup>. The solvent additives 1,2,3,4-tetrahydronaphthalene (THN) and chlorobenzene were added to the host solvent 1,2-dichlorobenzene (oDCB) to influence the film formation properties. Solar cells prepared using solvent additives resulted in higher photocurrents than solar cells prepared using pure oDCB, and blends prepared from THN resulted in best efficiencies. Structural investigations with TEM, AFM, and Kelvin probe force microscopy indicated that the solvent additives lead to preferential in-plane phase segregation between the polymer and fullerene and increased P3HT ordering in the blends. The solvent additives led to a decrease in the PCBM content at the top of the blend, resulting in lower fill factor in the solar cells and reduced bulk electron transport. We discuss these results considering the effects of morphology on charge separation.

<sup>[a]</sup>A.De Sion et al., Solar Energy Materials and Solar Cells 95/12(2011)

CPP 6.9 Mon 17:30 Poster A

**Charge transport investigation in electrochemical environment** — ●ZHIWEI YI<sup>2</sup>, BASTIAN KOPP<sup>2</sup>, DIRK MAYER<sup>1</sup>, ANDREAS OFFENHÄUSSER<sup>1</sup>, and ELKE SCHEER<sup>2</sup> — <sup>1</sup>Research Center Jülich, 52425 Jülich, Germany. — <sup>2</sup>Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Here, an electrochemical mechanical break junction setup is introduced, which combines electrodeposition techniques and mechanical breaking techniques. Using such setup, the charge transport through electrostatically assembled molecular junctions of Au/cysteamine/1,1-ferrocene dicarboxylic acid (FDA)/cysteamine/Au was measured in liquid. The conductance across those single-molecule junctions ( $0.34 \times 10^{-4} \text{ G}_0$ ) is one order of magnitude smaller than the conductance of covalently linked ferrocene molecular junctions ( $3.4 \times 10^{-4} \text{ G}_0$ ), which indicates that the electrostatic coupling is strong enough to form an electron transport pathway, but the electron transfer rate across electrostatic interfaces is lower than across the covalent bonds. Molecular monolayers assembled on Au surface and Au/molecule/Au junctions are often used to investigate the influence of light on the electron trans-

port across molecules. However, the influence of light on the charge transport at the liquid/metal interface has not been investigated yet. Here, using an indium tin oxide (ITO) electrode with gold nanoparticles on top as the working electrode, light induced signals were observed when performing cyclic voltammetry. We discuss voltage and wave-length dependence of the light-induced signals and first results obtained for photochromic molecules assembled with this technique.

CPP 6.10 Mon 17:30 Poster A

**Time resolved microwave conductivity (TRMC) and transient absorption (TAS) measurements reveal charge carrier dynamics in organic semiconductors** — ●ANDREAS FRITZE<sup>1</sup>, ANDREAS SPERLICH<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, TOM J. SAVENIJE<sup>3</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — <sup>2</sup>ZAE Bayern, D-97074 Würzburg — <sup>3</sup>Department of Chemical Engineering, Delft University of Technology, NL-2628 BL Delft, The Netherlands

Understanding of the light induced charge carrier dynamics in self arranged organic semiconductors is essential to improve material properties and processing parameters and, at long sight, device performance. We performed combined TRMC and TAS measurements on organic semiconductors to gain direct access to the microscopic transport properties and charge carrier densities, respectively comparing both data yields us a complete picture about the generation, transport and recombination of charges on a microscopic length-scale. After laser pulse excitation TRMC and TAS signal decay in the blend of PCPDTBT:PCBM with varying PCBM content have been observed at different temperatures. This polymer:fullerene blend is a promising candidate for new high efficiency organic photovoltaic devices. We discuss the influence of morphology on light induced charge carrier density, recombination and mobility on a microscopic scale.

CPP 6.11 Mon 17:30 Poster A

**Influence of PEDOT:PSS on the Morphology of P3HT:PCBM:PSS Solar Cells** — ●BEN STAFFORD, KLAUS WAGENBAUER, EVA M. HERZIG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany

In organic photovoltaics the binary system poly(3-hexylthiophene) (P3HT) and phenyl C61-butyric acid methylester (PCBM) is well known for the active layer. By adding a third component, in our case polystyrenesulfonate (PSS), the performance of a solar cell can be improved. [1] PSS has no conductive or absorbing properties, consequently it must influence the morphology of the ternary system as compared with the two component system. Indeed, we have observed an ordering effect on P3HT when adding PSS to the binary blend. Of great interest is the interface between PEDOT:PSS and the active layer and its influence on the P3HT morphology. To optimise device performance different layer thicknesses of the PEDOT:PSS blocking layer are examined via electrical characterization.

[1] Kim et al., Solar Energy Materials and Solar Cells, 92:1188 (2008)

CPP 6.12 Mon 17:30 Poster A

**Simulations of charge transport in lamellar PBTTT** — ●ALEXANDER MALAFEEV<sup>1,3</sup>, EUNKYUNG CHO<sup>2</sup>, CHAD M. RISK<sup>2</sup>, JEAN-LUC BREDAS<sup>2</sup>, VICTOR IVANOV<sup>3</sup>, and DENIS ANDRIENKO<sup>1</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, USA — <sup>3</sup>Physics Department, Moscow State University, Moscow, Russia

The force-field of poly(2,5-bis(3-alkylthiophen-2-yl)thieno[3,2-b]thiophenes) (PBTTT), a compound with a charge carrier mobility of up to  $1 \text{ cm}^2/\text{Vs}$ , is parametrized using first-principles calculations. Subsequently, molecular dynamics simulations of a lamellar molecular arrangement are performed and the charge carrier mobility is determined by solving rate equations<sup>1</sup> in large-scale morphologies of PBTTT. We find that the unit cell parameters, as well as charge carrier mobilities, are in a good agreement with experimental data.

<sup>1</sup> V. Rühle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, D. Andrienko, J. Chem. Theory Comput., 7, 3335 (2011)

CPP 6.13 Mon 17:30 Poster A

**Subsurface Mapping of Amorphous Surface Layers on different types of P3HT** — ●M. ZERSON<sup>1</sup>, E.-C. SPITZNER<sup>1</sup>, C. RIESCH<sup>1</sup>, R. LOHWASSER<sup>2</sup>, M. THELAKKAT<sup>2</sup>, A. SPERLICH<sup>3</sup>, H. KRAUS<sup>3</sup>, V. DYAKONOV<sup>3</sup>, and R. MAGERLE<sup>1</sup> — <sup>1</sup>Technische Uni-

versität Chemnitz, Chemnitz, Germany — <sup>2</sup>Universität Bayreuth, Bayreuth, Germany — <sup>3</sup>Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of different types of poly(3-hexylthiophene) (P3HT) using depth-resolved amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance (APD) curves, the tip indentation into the soft (compliant) amorphous surface layer is measured. This spatial information serves as depth coordinate for reconstructing high resolution cross sections and 3D depth profiles of the top 10 nm of the specimen. Furthermore, the shape of the unperturbed (true) surface and the thickness of the amorphous top layer can be determined. With this depth profiling technique we discovered that the entire surface of different types of (P3HT) is covered by an amorphous layer of P3HT. We determine the amorphous layer thickness of commercial P3HT with a wide range of molecular weight (PDI 1.97), purified commercial P3HT (PDI 1.59) and of a well-defined type of P3HT with a low polydispersity index (1.19). Its thickness is between 4 and 10 nm, depending on the type of material, sample preparation conditions and annealing. We discuss the possible impact of these amorphous surface layers on the electronic properties of the surfaces and the performance of thin-film electronic devices using these polymers.

CPP 6.14 Mon 17:30 Poster A

#### Tuning of Crystal Orientation in Conducting Polymer Blends

— •EVA M. HERZIG<sup>1</sup>, KLAUS WAGENBAUER<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, WEIJIA WANG<sup>1</sup>, YUAN YAO<sup>1</sup>, ADELINE BUFFET<sup>2</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>2</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>HASYLAB at DESY, 22603 Hamburg, Germany

Surface sensitive x-ray diffraction is a powerful method to investigate molecular orientation in thin conducting polymer films [1]. In organic electronics successful charge transport depends strongly on the structural arrangement of the organic components because charge transport is anisotropic in such materials. Therefore control over crystallization and crystal orientation is highly desirable to improve device performance.

Using grazing incidence wide angle x-ray scattering we are able to show that the addition of an amorphous, electrolytic polymer results in an increased molecular ordering in standard organic photovoltaic films. This ordering is examined with respect to different parameters like temperature and substrate surface thereby showing ways of deliberately influencing the polymer crystal orientation.

[1] J. Perlich, J. Rubeck, S. Botta, R. Gehrke, S. V. Roth, M. A. Ruderer, S. M. Prams, M. Rawolle, Q. Zhong, V. Körstgens, and P. Müller-Buschbaum, *Rev. Sci. Instrum.* 81, 105105 (2010)

CPP 6.15 Mon 17:30 Poster A

#### Increase in performance of polymer based field effect transistors with dielectric nanoparticles

— •ALI VEYSEL TUNC<sup>1</sup>, JÜRGEN PARISI<sup>1</sup>, and ELIZABETH VON HAUFF<sup>2</sup> — <sup>1</sup>University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — <sup>2</sup>Institute of Physics, University of Freiburg, Germany

We have investigated the effect of nanomorphologic manipulation by SiO<sub>2</sub> nanoparticles and PCBM [6,6]-phenyl-C<sub>61</sub>-butyric acid methyl ester (PCBM) in poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) based field effect transistors. PCBM has already been observed to improve hole mobility when added to the polymer. The explanation of this improvement with PCBM is still controversial in the literature. We investigate the effect of conducting and insulating nanomaterials (SiO<sub>2</sub> and PCBM) on the transport properties of PPV based field effect transistors. Scanning electron microscopy (SEM) is used to image the morphologies of the blends. We observe that both PCBM and SiO<sub>2</sub> nanoparticles lead to an increase in the hole current and effect mobility, and additionally reduce the contact resistance and the threshold voltage. We discuss these improvements in terms of improved chain ordering and conformation. To confirm this, we additionally investigate the influence of SiO<sub>2</sub> nanoparticles in blends prepared with PPVs of varying molecular weight. We demonstrate that using SiO<sub>2</sub> nanoparticles then can be a simple and cost effective method to improve the performance in polymer based OFETs.

CPP 6.16 Mon 17:30 Poster A

#### Host-Guest Complexes of $\beta$ -Cyclodextrin-Substituted Silicon (IV) Phthalocyanines and a Tetrasulfonated Porphyrin: MD Simulations and Estimates on Electron Transfer

— •JULIE KRAINAU<sup>1</sup>, JÖRG MEGOW<sup>1</sup>, ALEXANDER KULESA<sup>2</sup>, and VOLKHARD MAY<sup>1</sup> — <sup>1</sup>Institut für Physik, Humboldt Universität zu Berlin, Germany — <sup>2</sup>Institut für Physik, Freie Universität zu Berlin, Germany

The development of artificial photosynthesis requires an assembly of molecules that can mimic light harvesting and charge separation. Two host-guest complexes are formed between a tetrasulfonated porphyrin and several silicon (IV) phthalocyanines. The latter are substituted axially with two permethylated  $\beta$ -cyclodextrin units via different spacers. For these compounds it had been shown that they satisfy the needed requirements by exhibiting photoinduced fluorescence resonance energy transfer and charge transfer. The experimental measurements led to the hypothesis that the host-guest complex with the longest spacer has two conformations: One folded conformation in which the spacer is bended in such a way that the donor-acceptor distance is decreased and one conformation in which the donor and the acceptor are not close to each other [1]. In order to analyse this hypothesis, room-temperature MD simulations, using water as solvent, have been conducted that proved the made assumption. Furthermore, the trajectory gained by MD simulations was used to estimate the charge transfer rate in its dependence on the conformation.

[1] Ermilov et al., *Phys. Chem. Chem. Phys.*, DOI: 10.1039/c1cp21930h

CPP 6.17 Mon 17:30 Poster A

#### Role of Structural Order on Ultrafast Free Charge Generation in Polythiophene/Si Photovoltaics

— •CHRISTINA SCHARSICH<sup>1</sup>, DANIEL HERRMANN<sup>2</sup>, SABRINA NIESAR<sup>3</sup>, MARTIN STUTZMANN<sup>3</sup>, EBERHARD RIEDLE<sup>2</sup>, and ANNA KÖHLER<sup>1</sup> — <sup>1</sup>Universität Bayreuth — <sup>2</sup>Ludwig-Maximilians-Universität München — <sup>3</sup>Technische Universität München

In hybrid and organic solar cells, the precise process for the generation of free charge carriers is still not fully understood. This is partially due to the ultrafast time scale of a few-10 fs on which charge transfer between e-donor and acceptor takes place. Here, we use a novel broadband ultrafast transient absorption spectroscopy with a time resolution of 40 fs to probe charge generation and recombination in thin films of poly(3-hexylthiophene)/silicon (P3HT/Si). The fundamental photo-physical processes accompanying charge generation depend strongly on morphology of the heterojunction. For this reason, we study the role of structural order on the ultrafast charge generation by applying regioregular (rr) and regiorandom (rra) P3HT as electron donor material. [1,2] We show that singlet excitons dissociate to subsequently form polarons within 140 fs. Aggregated rrP3HT/Si films show recombination of non-geminate pairs. In comparison, geminate recombination appears to be the dominant loss mechanism for rraP3HT/Si films. Therefore, we find that polymer structural order is the key criterion for free charge generation in hybrid P3HT/Si solar cells.

[1] D. Herrmann et al. *J. Am. Chem. Soc.* 2011, 133, 18220-18233  
[2] C. Scharisch et al. *J. Polym. Sci., Part B: Polym. Phys.* - in press

CPP 6.18 Mon 17:30 Poster A

#### Electronic trap states in organic polymer-fullerene solar cells

— •JULIA RAUH<sup>1</sup>, STEFAN NEUGEBAUER<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius-Maximilian University of Würzburg, D-97074 Würzburg — <sup>2</sup>ZAE Bayern, D-97074 Würzburg

Trap states can have a significant influence on the performance of organic solar cells, as they lower the mobility, disturb the internal field distribution and affect the recombination dynamics. We investigated the trap states in the polymer P3HT as well as in fullerene derivatives commonly used as electron acceptors in organic bulk-heterojunction solar cells, namely PC<sub>61</sub>BM, PC<sub>71</sub>BM and bisPC<sub>61</sub>BM, by thermally stimulated current measurements. Hereby, broad trap distributions were revealed for all investigated materials. In addition to the pure materials also polymer-fullerene blends were studied, revealing even deeper trap states, which were not detected in the single materials, with the amount of these deeper traps depending on the preparation conditions of the solar cells. The investigations are complemented by current-based deep level transient spectroscopy yielding additional information about the emission rates of the traps, which is of fundamental importance to describe charge carrier dynamics, e.g. in transient experiments

CPP 6.19 Mon 17:30 Poster A

**Structured Interfaces in Organic Photovoltaic Devices —**

•CLAUDIA MARIA PALUMBINY<sup>1</sup>, ROBERT MEIER<sup>1</sup>, HOLGER CHRISTIAN HESSE<sup>2</sup>, RICKY DUNBAR<sup>2</sup>, LUKAS SCHMIDT-MENDE<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik -Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — <sup>2</sup>LMU München, Center for NanoScience (CeNS), Hybrid Nanostructures, Amalienstr.45, 80799 München, Germany

Precise control of the heterojunction morphology in thin films is one of the key issues for the improvement of organic photovoltaic (OPV) devices. Interdigitated interfaces of the organic material on the nanoscale provide ideal charge extraction pathways for separated charge carriers. Structured surfaces of the selective electrode on the lower microscale further allow to enhance the optical absorption of the thin film components due to light trapping. Two different ways of artificial structuring are under investigation: Using anodized aluminum oxide hard templates as stamps with controlled dimensions, nanostructured organic layers can be realized on ITO support. As shown recently, a sufficient replica of the template structure can be transferred into the organic compound[1]. Alternatively, master molds with nanoscale channels are used for the imprinting routine of the PEDOT:PSS layer. The shape of the imprinted structures is easily tunable by the concentration of an additional plasticizer. Depending on the structure dimensions the device efficiency of OPVs can be increased this way[2].

[1] Hesse et al., Nanotechnology, 22, 055303 (2011)

[2] Meier et al., DOI: 10.1039/C1JM13766B

CPP 6.20 Mon 17:30 Poster A

**Influence of Nongeminate Recombination on the Field-Dependence of the Photocurrent in Organic Solar Cells —**

•IAN HOWARD, RALF MAUER, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer Research, Mainz

The role of interfacial charge-transfer (CT) states in determining the bias dependence of the photocurrent in Organic Solar Cells is debated. Understanding the bias dependence of the photocurrent is necessary to optimize device fill factors, and therefore resolution of this debate is important. In this contribution we directly determine the field dependence of bimolecular recombination at the charge densities relevant to photovoltaic devices using a novel optical pump electrical probe experiment that enables the ultra fast time resolution of optical spectroscopy to be combined with high signal to noise achievable in current measurements.[1] We relate these results to temperature dependent transient absorption (pump-probe) spectroscopy over the entire relevant timescale from femtoseconds to milliseconds [2] We conclude that in the benchmark polythiophene:methanofullerene system nongeminate recombination plays a dominant role in determining the bias dependence of the photocurrent.

[1] R. Mauer, I.A. Howard, F. Laquai, J. Phys. Chem. Lett. 2011, 2 (14), 1736-1741.

[2] R. Mauer, I.A. Howard, F. Laquai, J. Phys. Chem. Lett. 2010, 1 (24), 3500-3505.

CPP 6.21 Mon 17:30 Poster A

**Immobilization of quantum dots via conjugated SAMs and their application as a light-controlled sensor for the detection of hydrogen peroxide —**

•WAQAS KHALID<sup>1</sup>, MIRA EL HELOU<sup>1</sup>, TOBIAS MURBÖCK<sup>1</sup>, ZHAO YUE<sup>1</sup>, JOSE-MARIA MONTENEGRO<sup>1</sup>, KIRSTEN SCHUBERT<sup>2</sup>, GERO GÖBEL<sup>2</sup>, FRED LISDAT<sup>2</sup>, GREGOR WITTE<sup>1</sup>, and WOLFGANG PARAK<sup>1</sup> — <sup>1</sup>Fachbereich Physik und WZMW, Philipps-Universität Marburg, Marburg, Germany — <sup>2</sup>Biosystems Technology, Technical University of Applied Sciences Wildau, Germany

A light-addressable gold electrode modified with CdS and FePt or with CdS@FePt nanoparticles (NPs) via an interfacial dithiol layer is presented. High-resolution synchrotron-based XPS measurements reveal that trans-stilbenedithiol (StDT) provides high quality self-assembled monolayers compared to benzenedithiol, biphenyldithiol (capped, uncapped) and capped StDT, in case they are formed at elevated temperatures. This alternative preparation evokes a discernible enhancement of lateral dithiol packing. The CdS NPs well immobilized on the dithiol layer allow for current generation under illumination and appropriate polarization. High quality of SAMs and the enhanced conductivity of their fully conjugated backbones impair a refinement in photocurrents and device performance by an order of magnitude. Moreover, FePt NPs serve as catalytic sites for the reduction of hydrogen peroxide to water. Advantageously, both NP properties can be combined by the use of hybrid NPs fixed on the electrode by means of the optimized StDT layer. This allows a light controlled analysis of different peroxide concentrations.[1] [1] W. Khalid et al. ACS Nano, 2011 (in print).

CPP 6.22 Mon 17:30 Poster A

**Determination of the mobility and lifetime of charge carriers in organic solar cells under operating conditions —**

•ANDREAS BAUMANN<sup>1</sup>, JENS LORRMANN<sup>2</sup>, DANIEL RAUH<sup>1</sup>, CARSTEN DEIBEL<sup>2</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Experimental Physics VI, Physical Institute, Julius Maximilian University of Würzburg, Am Hubland, D-97074 Würzburg

The field of organic photovoltaics (OPV) is rapidly raising the last years with power conversion efficiency values exceeding 7%. For a better understanding of the performance and especially the limitations of these solar cells, it is, however, still essential to study the fundamental processes like the transport and the recombination dynamics of photogenerated charge carriers. A prominent experimental technique, which is more and more applied in the field of OPV, is the charge extraction technique CELIV studying both the mobility and lifetime of light induced charge carriers, simultaneously. However, there are several drawbacks, such as charge carrier injection causing large RC or inhomogeneous charge carrier profiles (non-steady-state conditions) resulted by the laser flash, which prevent a direct correlation to the solar cell working conditions. With our newly developed charge extraction technique OTRACE, it is now feasible to get new insights into the transport and the recombination dynamics in organic BHJ solar cells under operating conditions. Results are shown for the highly efficient solar cells of PTB7 and PCDTBT blended with [70]PCBM, whereas the I-V characteristics are correlated to the mobility and lifetime.

CPP 6.23 Mon 17:30 Poster A

**Increasing the performance of vacuum-processed organic light-emitting pin diodes by inserting an solution-processed hole-transport layer —**

•THORSTEN UMBACH, STEFAN SCHNEIDER, HEIKE KLESER, and KLAUS MEERHOLZ — Universität zu Köln, Department Chemie, Luxemburgerstr. 116, 50939 Köln, Germany

High ohmic losses and a poor charge injection are the main obstacles on the way to stable organic light emitting diodes (OLED's) with high-power efficiencies and low driving voltages. A promising technique to get rid of these drawbacks is a molecular doping of charge transport layers. Throughout the last decade this has been successfully applied in vacuum processed devices leading to pin OLED architecture with internal efficiencies approaching unity.

However, major improvements in the field of OLED technology can be made by improving the light out-coupling. In conventional device architectures around 80% of the generated light is lost within the layers due to total internal reflection, wave guiding, and absorption.

By inserting an additional nanoporous hole-transport layer (HTL) into an OLED system we gain a strongly enhanced light output. The external quantum efficiency is increased up to 20%. This enhancement is due to a lower film density and the resulting lower refractive index of the HTL.

Here, we demonstrate the combination of both techniques. By optimizing the light out-coupling-properties by the HTL and the electronic structure by doping, the resulting hybrid devices have great potential to overcome most of the drawbacks OLED devices still suffer from.

CPP 6.24 Mon 17:30 Poster A

**Towards Highly Efficient Vacuum-processed Merocyanine Tandem Solar Cells —**

•VERA STEINMANN<sup>1</sup>, NILS KRONENBERG<sup>1</sup>, HANNAH BÜCKSTÜMMER<sup>2</sup>, DIRK HERTEL<sup>1</sup>, MARTIN LENZE<sup>1</sup>, STEVEN GRAF<sup>1</sup>, FRANK WÜRTHNER<sup>2</sup>, and KLAUS MEERHOLZ<sup>1</sup> — <sup>1</sup>Department für Chemie, Universität Köln, Luxemburger Straße 116, 50939 Köln (Germany) — <sup>2</sup>Institut für Organische Chemie und Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg (Germany)

In the last decade, high demand for low-cost, renewable energy spurred strong developments in the research of organic photovoltaics (OPV). To date, the highest power conversion efficiency (PCE) of 8.4% is reported for polymer solar cells. However, small molecules (SM) have recently gained increased interest, reaching PCEs around 6%. Admittedly, most efficient SM solar cells still require rather sophisticated multilayer device configurations. In the past, we successfully introduced merocyanine (MC) dyes in vacuum-processed (VAC) single solar cells with PCEs up to 4.9%. Further device optimization led to high PCEs beyond 6%, while maintaining a simple device setup. Impressive performances motivated the implementation of MCs in VAC tandem cells. We present a "proof of concept" MC tandem cell, consisting of two identical subcells. A high PCE of 4.7% is obtained, closely

approaching the comparable single cell PCE of 5.0%. The optimized open-circuit voltage is as large as 2.1 V. Moreover, we introduce a novel tandem cell configuration, combining a planar- and bulk heterojunction. First MC tandem cells with different subcells are already highly promising.

CPP 6.25 Mon 17:30 Poster A

**Structure and properties of reduced graphene oxide** —

•MICHAEL ENZELBERGER<sup>1</sup>, SIEGFRIED EIGLER<sup>2</sup>, PHILIPP HOFMANN<sup>1</sup>, CHRISTOPH DOTZER<sup>2</sup>, ANDREAS HIRSCH<sup>2</sup>, and PAUL MÜLLER<sup>1</sup> — <sup>1</sup>Department of Physics and Interdisciplinary Center of Molecular Materials, Universität Erlangen-Nürnberg, Germany — <sup>2</sup>Department of Chemistry and Pharmacy, Universität Erlangen-Nürnberg and Institute of Advanced Materials and Processes (ZMP), Germany

Reducing graphene oxide is an economic method for the large scale production of graphene. However, the reduction process causes a large number of defects. During thermal annealing of graphene oxide,  $CO_2$  becomes mobile at around 50°C and a  $CO_2$  intercalated compound is formed. This intermediate decomposes by the release of water and  $CO_2$  at around 150°C as shown by thermogravimetric analysis and mass spectroscopy. Single flakes as well as sheets of flakes of the reduced graphene oxide were investigated. We characterize the quality of the samples by combining Raman spectroscopy and Hall mobility measurements. For high quality samples we find a Raman D/G ratio of 3 and Hall mobilities exceeding 10  $Vs/cm^2$ .

CPP 6.26 Mon 17:30 Poster A

**Modelling charge carrier dynamics in disordered semiconducting materials** —

•JENS LORRMANN<sup>1</sup>, JULIEN GORENFLOT<sup>1</sup>, VLADIMIR DYAKONOV<sup>1,2</sup>, and CARSTEN DEIBEL<sup>1</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — <sup>2</sup>Bavarian Center for Applied Energy Research e.V. (ZAE Bayern e.V.), Würzburg

Organic semiconductors are promising candidates for low cost electronic applications, i.e. organic solar cells or organic light emitting diodes. Their performance is now approaching market maturity. But still there is little known about the impact of energetic and spatial disorder present in these materials, on the charge carrier dynamics and thus on the performance. To gain further insight, we developed a time dependent multiple trapping and release model to track the fate of electrons and holes hopping in a gaussian or exponential density of states (DOS). The tail states of the DOS act as trap-states, where as the charge carriers move freely above the transport energy with a temperature dependent mobility. We show how disorder influence thermalization, non-geminate recombination and transport. For instance the recombination rate strongly increases with increasing energetic disorder or decreasing temperature, which reproduces the experimentally observed deviations from the Langevin theory [1]. Furthermore, the model is capable to describe temperature dependent transient absorption measurements on poly(3-hexyl thiophene-2,5-diyl) (P3HT) blended with [6,6]-phenyl-C<sub>61</sub> butyric acid methyl ester (PCBM).

[1] P. Langevin, Ann. Chim. Phys. 28, 433, 1903.

CPP 6.27 Mon 17:30 Poster A

**Influence of Polarization on the Energy Landscape for Charge Transport in Organic Electronic Materials** —

•FALK MAY<sup>1</sup>, BJÖRN BAUMEIER<sup>1</sup>, DENIS ANDRIENKO<sup>1</sup>, and CHRISTIAN LENNARTZ<sup>2</sup> — <sup>1</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>2</sup>BASF SE, GVC/E - B009, Ludwigshafen, Germany

Design of organic semiconductors for particular applications requires

knowledge of the distribution of energy levels participating in charge transport. These levels are often approximated by EA/IP of single molecules in vacuum, while effects of the environment (broadening, shifts) are taken into account phenomenologically, using simple dielectric cavity or lattice models. Using a representative host-guest system of the active layer of an organic light emitting diode, we show that these approximations can be incompatible with the microscopic evaluation of site energy disorder in realistic morphologies. In a particular case of electron transport, microscopic polarization effects do not reduce the energetic disorder arising from static Coulomb interactions, in contradiction to the predictions of lattice models. Inclusion of polarization effects also leads to a relative shift of the guest and host distributions, which again cannot be rationalized within mesoscopic descriptions. Both effects lead to a strong overlap of site energy distributions and hence affect electron transport dynamics and the current distribution in the host-guest mixture.

CPP 6.28 Mon 17:30 Poster A

**Controlled polymerization of electron-deficient monomers: controlled preparation of n-type semiconducting polymers for organic electronics** —

•ANTON KIRIY and VOLODYMYR SENKOVSKYY — Leibniz Institut für Polymerforschung Dresden

Electron-conducting (n-type) main-chain pi-conjugated polymers are commonly prepared via well-established step-growth polycondensation protocols which enable limited control over polymerization. Chain-growth catalyst-transfer polycondensations were recently developed for controlled preparation of only hole-conducting (p-type) semiconducting polymers and block copolymers. In this contribution we present a new synthetic protocols that allows preparation of well-defined n-type semiconducting polymers. Specifically, we report on controlled polymerization of naphthalene-diimide based monomer resulting into corresponding n-type conjugated polymer (PNDIT2) with controlled molecular weight, relatively narrow polydispersities, and specific end-functions. Electron mobility of this polymer will be also presented (Senkovskyy, Kiriya, et al. J. Am. Chem. Soc. 2011, ASAP, ja-2011-08710x).

CPP 6.29 Mon 17:30 Poster A

**Built-in potential and validity of Mott-Schottky analysis in organic bulk heterojunction solar cells** —

•MARKUS MINGEBACH<sup>1</sup>, CARSTEN DEIBEL<sup>1</sup>, and VLADIMIR DYAKONOV<sup>1,2</sup> — <sup>1</sup>Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — <sup>2</sup>ZAE Bayern, D-97074 Würzburg

The built-in potential is an important key parameter of organic bulk heterojunction (BHJ) solar cells since it determines the internal electric field profile in the device but also gives an estimate for the open circuit voltage and hence the solar cell efficiency. The correct determination of the built-in potential is a nontrivial task, since zero field inside the BHJ device is not easy to achieve. We investigated poly(3-hexylthiophene-2,5-diyl):[6,6]-phenyl-C<sub>61</sub> butyric acid methyl ester BHJ solar cells by means of temperature dependent measurements of the open circuit voltage and compared the results with the Mott-Schottky analysis of capacitance-voltage characteristics, which is a well-established tool to determine the built-in potential in inorganic devices. By applying the Mott-Schottky analysis to our solar cells we found considerably lower built-in voltages than expected from the difference of the electrode work functions. Moreover, a dependence of the built-in voltage, determined this way, on the active layer thickness of the devices was observed. We conclude that Mott-Schottky analysis seems not to be generally appropriate for the determination of the built-in potential in organic BHJ solar cells.