

CPP 19: Poster Session 1 (joint session with BP)

Organic Electronics and Photovoltaics, Biomaterials and Biopolymers, Ionic Liquids, Glasses

Time: Tuesday 9:30–13:00

Location: P1

CPP 19.1 Tue 9:30 P1

The solid-liquid interface of ionic liquid solutions – Interfacial layering and solvent-induced screening — ●MARKUS MEZGER^{1,4}, HEIKO SCHRÖDER¹, PETER REICHERT^{1,4}, ROLAND ROTH², HARALD REICHERT³, and DIEGO PONTONI³ — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²Eberhard Karls Universität, 72076 Tübingen, Germany — ³European Synchrotron Radiation Facility, 38043 Grenoble, France — ⁴Johannes Gutenberg Universität, 55128 Mainz, Germany

The influence of the polar, aprotic solvent propylene carbonate on the interfacial structure of the ionic liquid 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphat ([bmpy⁺][FAP⁻]) on sapphire was investigated by high-energy x-ray reflectivity. Analysis of our experimental data revealed interfacial profiles comprised of alternating anion and cation enriched regions decaying gradually into the bulk liquid. With increasing solvent concentration, a decrease in the decay length of the interfacial layering structure was observed. Solvent molecules were found to accumulate laterally within the layers, hence screening the charges between like ions. The results are compared with the bulk structure of IL-solvent mixtures.

CPP 19.2 Tue 9:30 P1

Molecular Scale Structure of Ionic Liquid-Aqueous Solution Interfaces — ●XILIN WU¹, JULIAN MARS¹, BINYANG HOU^{1,2}, VEIJO HONKIMÄKI², and MARKUS MEZGER^{1,3} — ¹Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany — ²European Synchrotron Radiation Facility, 38043 Grenoble, France — ³Johannes Guttenberg-Universität, 55128 Mainz, Germany

Ionic liquids (ILs) are widely used as environmental friendly solvents for liquid-liquid extraction processes. However only little is known on their molecular scale structure near fluid interfaces. We employed high energy x-ray reflectivity (XRR) to study the free surface and the buried IL-water interface of 1-butyl-1-methylpyrrolidinium tris(pentafluoroethyl)trifluorophosphat ([bmpy⁺][FAP⁻]). The influence of metal cations on the interfacial structure was probed by adding cobalt ions ([Co²⁺][Cl₂⁻]) to the aqueous phase. The Electron density profile across the IL-aqueous solution interface was extracted from the experimental XRR data. Its dependence on the interfacial potential was studied by time-resolved XRR measurements recorded during cyclic voltammetry. The data shows clear correlations between the applied voltage and the XRR intensity, indicating potential induced ion rearrangement at the liquid-liquid interface.

CPP 19.3 Tue 9:30 P1

Photoelectron Spectroscopy on Ionic Liquid Surfaces – Theory and Experiment — ●WICHARD J. D. BEENKEN¹, ANGELA ULBRICH¹, MARKUS REINMÖLLER², and STEFAN KRISCHOK¹ — ¹Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — ²TU Bergakademie Freiberg, Institut für Energieverfahrenstechnik und Chemieingenieurwesen, Freiberg, Germany

We have studied various ionic liquids by photoemission spectroscopy. For a more in depth interpretation of the experimental results, in particular of valence spectra, a theoretical reconstruction of these spectra by means of density functional theory is desired. In order to obtain correct binding energies and peak intensities a simple calculation of the density of states is not sufficient. A self-developed method, which bases on known elementary cross sections for the photoeffect and adjustments of the kinetic energy of emitted electrons is applied. Particular attention is paid to the necessary relative shift for cation and anion due to their different Madelung potentials. In order to study this effect, we have varied the cations and the anions of the ionic liquids under investigation, systematically.

CPP 19.4 Tue 9:30 P1

Influence of cation on lithium transport in ionic liquid/Li-salt electrolyte: A molecular dynamics study — ●VOLKER LESCH¹, ANDREAS HEUER¹, ZHE LI², and DMITRY BEDROV² — ¹Westfälische Wilhelms-Universität Münster — ²University of Utah

Molecular Dynamics (MD) simulations is a powerful tool to get atomic scale understanding of different systems. Room temperature ionic li-

uids have been considered as new alternative materials for variety of applications, including as electrolytes for Li-ion batteries and supercapacitors. Addition of lithium salt to an ionic liquid results in strong interactions between anions with the small lithium ion and significantly alters electrolyte properties. However the details of the chemical structure of the ionic liquid cation and its influence on the lithium ion coordination and overall electrolyte properties are not well understood. Here we compare MD simulations of ionic liquids comprised of 1-Ethyl-3-methylimidazolium or N-methyl-N-propylpyrrolidinium cations paired with tri-(bis-fluorosulfonyl)-imide (TFSI) anion and mixed with LiTFSI salt. We performed MD-simulations of both ionic liquids with lithium salts at different temperatures and salt concentrations and examined the influence of cation properties (chemical structure, size, charge distribution) on electrolyte transport properties such as self-diffusion coefficients, ionic conductivity, and viscosity. These transport properties and the mechanisms of Li ion mobility were correlated with Li-ion local coordination structure and anion exchange rates inside the Li-ion first coordination shell.

CPP 19.5 Tue 9:30 P1

Layer Formation of Alkylimidazolium Ionic Liquids at the Sapphire/Liquid Interface — ●MICHAEL KLIMCZAK¹, NICOLA TACCARDI², and ANDREAS MAGERL¹ — ¹Lehrstuhl für Kristallographie und Strukturphysik, Universität Erlangen-Nürnberg — ²Lehrstuhl für Chemische Reaktionstechnik, Universität Erlangen-Nürnberg

Alkylimidazolium-based room temperature ionic liquids (RTILs) – among others – are known to form well-ordered structures in contact with smooth metal or oxide interfaces [1]. By means of specular X-ray reflectivity (XRR) interface normal electron density profiles are obtained with submolecular resolution giving detailed insight of structures at the interface [2]. 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide [EMIM][NTf₂] is shown to form a stack of alternating cation/anion monolayers at the (0001) sapphire/liquid interface. The first layer is confirmed to be composed of cations with their imidazolium rings parallel to the interface, followed by about five clearly distinguishable double layers.

With longer alkyl chains – replacing [EMIM] cations by [HMIM] (1-Hexyl-3-Methylimidazolium) or [DMIM] (1-Decyl-3-Methylimidazolium) – alternating cation/anion structures are still observed with the length and orientation of the alkyl chains significantly influencing the layering properties.

[1] H. Li, F. Endres, and R. Atkin, *Physical Chemistry Chemical Physics*: PCCP 15, 14624 (2013).

[2] M. Mezger, H. Schröder, and H. Reichert, *Science* 322, 424 (2008).

CPP 19.6 Tue 9:30 P1

New method for volatility determination of ionic liquids at the nanoscale by means of ultra-fast scanning calorimetry — ●MATHIAS AHRENBERG¹, MARCEL BRINCKMANN¹, JÜRGEN W.P. SCHMELZER¹, MARTIN BECK², CHRISTIN SCHMIDT³, OLAF KESSLER², UDO KRAGL³, SERGEY P. VEREVKIN³, and CHRISTOPH SCHICK¹ — ¹Institute of Physics, University of Rostock, Wismarsche Str. 43-45, 18051 Rostock, Germany — ²Faculty of Mechanical Engineering and Marine Technology, University of Rostock, Albert-Einstein-Str. 2, 18059 Rostock, Germany — ³Institute of Chemistry, University of Rostock, Albert-Einstein-Str. 3a, 18059 Rostock, Germany

Here we present a new method for the determination of vaporization enthalpies of Ionic Liquids using differential fast scanning calorimetry. We have developed and proven this method using [EMIm][NTf₂] at temperatures up to 750 K and in different atmospheres. This method allows very high heating rates (up to 100000 K/s) and thus much higher temperatures can be reached in the measurement of the mass loss rate as compared to common devices without significant decomposition of the ionic liquid.

CPP 19.7 Tue 9:30 P1

Polymeric nanoparticles for drug delivery, stability and pH response — ●NATALYA VISHNEVETSKAYA¹, MARGARITA DYAKONOVA¹, ANNA BOGOMOLOVA², SERGEY FILIPPOV², and CHRISTINE PAPADAKIS¹ — ¹TU München, Physikdepartment, Physik weicher Materie — ²Institute of Macromolecular Chemistry, Prague, Czech Republic

Polymer-drug conjugates based on the copolymer N-(2-hydroxypropyl) methacrylamide (HPMA) bearing the anticancer drug doxorubicin and a defined amount of hydrophobic moieties (cholesterol and its derivatives) are therapeutically highly potent. The structures of the pH cleavable cholesterol-HPMA linkage and of cholesterol itself influence on the nanoparticle formation and behavior in solution [1].

The micelle formation of various copolymers in phosphate buffer solution and their size was investigated using fluorescence correlation spectroscopy (FCS) by adding the fluorescence dye rhodamine 6G. We have compared the values of the hydrodynamic radii of the micelles and the critical micelle concentrations in very dilute solutions (as in blood) of the copolymers as well as the kinetics during time and pH changes. Using dynamic light scattering, the average size of the nanoparticles and their stability in various environments are studied, and (time-resolved) small-angle neutron scattering provides detailed information on the micellar core-shell structures.

[1] S.K. Filippov et al., *Biomacromolecules* 14, 4061 (2013)

CPP 19.8 Tue 9:30 P1

Energetics, optical response and spin structure of μ - η^2 : η^2 -peroxo and bis- μ -oxo dicopper model complexes calculated within (TD)DFT and MBPT — ●MARTIN ROHRMÜLLER¹, SONJA HERRES-PAWLIS², and WOLF GERO SCHMIDT¹ — ¹Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany — ²Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany

Binuclear Cu complexes play an important role in the enzymatic oxidation and are of potential interest for industrial redox processes [1]. However, the physics and chemistry of the corresponding charge transfer mechanism are not yet fully understood. In order to contribute to a microscopic understanding of the charge and structural dynamics in such complexes we focus on the characterisation of the transition of model systems from bis- μ -oxodicopper(III) species (O) to μ - η^2 : η^2 -peroxodicopper(II) species (P).

We investigate ground-state as well as excited-state potential energy surfaces, with particular emphasis on the influence of the spin structure. Optical response and electronic excitations are calculated using (Time Dependent) Density Functional Theory and Many Body Perturbation Theory [2]. Based on these findings we use non-adiabatic trajectory surface hopping [3] to tackle the pico second dynamics.

[1] Solomon *et al.*, *Chem. Rev.* 1996, **96**, 2563

[2] M. Rohrmüller *et al.*, *J. Comp. Chem.* 2013, **34**, 1035-1045

[3] M. Barbatti, *WIREs Comput Mole Sci*, 2011, **1**, 620-633

CPP 19.9 Tue 9:30 P1

Femtosecond dynamics of optically excited dicopper complexes — ●ANDREAS LÜCKE, MARTIN ROHRMÜLLER, and WOLF GERO SCHMIDT — Universität Paderborn, Lehrstuhl für Theoretische Physik, Germany

Copper proteins are of particular interest as they are crucial for biological functions like oxygen transport or cellular respiration [1]. Here we focus on bis-(μ -oxo)dicopper model complexes that contain a $[Cu_2O_2]^{2+}$ core. By means of comparison to results of many-body perturbation theory, i.e. quasiparticle calculations within the GW approximation and subsequent solution of the Bethe-Salpeter equation, it is shown that time-dependent density-functional theory (TDDFT) within the adiabatic approximation reliably describes the molecular optical response of the molecules [2]. Based on this finding, real-time TDDFT is used to explore the molecular electron dynamics in response to the optical excitation. Thereby the time-dependent Kohn Sham equations are solved to describe the electron relaxation on the femtosecond timescale.

[1] E. A. Lewis and W. B. Tolman, *Chem. Rev.* 2004, 104, 1047-1076

[2] M. Rohrmüller, S. Herres-Pawlis, M. Witte, and W. G. Schmidt, *J. Comp. Chem.* 2013, 34, 1035-1045

CPP 19.10 Tue 9:30 P1

Excited state proton transfer reaction pathways: Ab-initio study of solvated 7-Hydroxyquinoline — ●GÜL BEKÇIOĞLU, CHRISTOPH ALLOLIO und DANIEL SEBASTIANI — Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Deutschland

Biophysical processes often take place based on proton relay along a hydrogen bonded chain [1]. Such proton transfer reactions along water wires are difficult to observe directly inside a protein. Photosensitive acid/base systems provide a method to control and study ultrafast proton transport via infrared spectroscopy [2]. Upon excitation, Hy-

droxyquinolones (HQ) are simultaneously photoacids and photobases. We study the ground and excited state solvation of 7HQ, focussing on the identification of water wires and excited state protonation dynamics. Additionally, we characterize a novel pathway which has not been discussed in literature so far, namely the transfer of an anionic hydroxide ion species through a short water wire, initiated by proton donation to the photobasic site of 7HQ.

[1] F. Garczarek and K. Gerwert, *Nature* 439 (2006), 109-112. [2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., *Science* 310 (2005), 5745.

CPP 19.11 Tue 9:30 P1

Excited state proton transfer reaction pathways: Ab-initio study of solvated 7-Hydroxyquinoline — ●GÜL BEKÇIOĞLU, CHRISTOPH ALLOLIO und DANIEL SEBASTIANI — Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Deutschland

Biophysical processes often take place based on proton relay along a hydrogen bonded chain [1]. Such proton transfer reactions along water wires are difficult to observe directly inside a protein. Photosensitive acid/base systems provide a method to control and study ultrafast proton transport via infrared spectroscopy [2]. Upon excitation, Hydroxyquinolones (HQ) are simultaneously photoacids and photobases. We study the ground and excited state solvation of 7HQ, focussing on the identification of water wires and excited state protonation dynamics. Additionally, we characterize a novel pathway which has not been discussed in literature so far, namely the transfer of an anionic hydroxide ion species through a short water wire, initiated by proton donation to the photobasic site of 7HQ.

[1] F. Garczarek and K. Gerwert, *Nature* 439 (2006), 109-112.

[2] O. F. Mohammed, D. Pines, J. Dreyer, E. Pines and E. T. J. Nibbering., *Science* 310 (2005), 5745.

CPP 19.12 Tue 9:30 P1

FTIR-spectroscopy reveals the pressure-dependent interplay between internal and external constraints in spider silk — ●ARTHUR MARKUS ANTON¹, ROXANA FIGULI², PERIKLIS PAPADOPOULOS³, and FRIEDRICH KREMER¹ — ¹Institut für Experimentelle Physik I, Universität Leipzig, Germany — ²Institut für Technische Chemie und Polymerchemie, Karlsruher Institut für Technologie, Germany — ³Max Planck Institut für Polymerforschung, Germany

Due to its unique mechanical properties, namely high tensile strength combined with great elasticity, spider silk surpasses modern synthetic fibers [S. Kubik, *Angew. Chem. Int. Ed.* **41** (2002)]. Until recently, one was incapable of manufacturing materials with similar properties on a large scale [M. Heim et al., *Angew. Chem. Int. Ed.* **48** (2009)], because of an incomplete understanding of spider silk's microscopic structure. Its mechanical properties are based on a refined architecture at the molecular and mesoscopic scale. β -sheet nanocrystals are interconnected through *prestrained* amorphous regions offering an internal force counterbalanced by the fiber's outer skin. Due to that structure, external stress is directly transferred to the nanocrystals evident in a shift of an Alanine-specific IR absorption band [P. Papadopoulos et al., *Eur. Phys. J. E* **24** (2007); R. Ene et al., *Soft Matter* **5** (2009)]. To unravel this interplay between internal and external constraints a pressure-dependent analysis of this Alanine-specific band by means of hydrostatic pressure provided by a diamond anvil cell (DAC) was carried out [A. M. Anton et al., *Macromol.* **46** (2013)].

CPP 19.13 Tue 9:30 P1

Bundling of grafted, reversibly crosslinked biopolymers — ●DANIEL WILKIN, RICHARD VINK, and ANNETTE ZIPPELIUS — Institute for Theoretical Physics, Georg-August University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

In this poster, we present a Monte Carlo simulation of a system consisting of parallel aligned polymers which are grafted perpendicularly on a flat surface. The polymers are described as weakly-bending chains (persistence length much larger than the polymer length) and neighboring chains can be reversibly crosslinked (the crosslinks being modeled as harmonic springs which induces an attractive force between the polymers). Upon increasing the number of crosslinks, our simulations reveal a transition from a homogeneous state to a state where the polymers have grouped themselves into bundles. When the polymers are grafted on the surface randomly, the bundles appear to be frozen in space (i.e. once they have formed, they never dissolve). In contrast, by grafting the polymers regularly on a lattice, the resulting bundles are mobile, i.e. they form and disappear again at any spatial location

on the surface.

CPP 19.14 Tue 9:30 P1

Mapping nanomechanical properties of hydrated type-I collagen fibrils with MUSIC mode AFM — JULIA HANN¹, DIANA VOIGT¹, EIKE-CHRISTIAN SPITZNER¹, ANKE BERNSTEIN², and ROBERT MAGERLE¹ — ¹Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — ²Muskuloskelettales Forschungslabor, Department Orthopädie und Traumatologie, Universitätsklinikum Freiburg, Freiburg i. Br., Germany

Type-I collagen forms fibrils with water embedded between the tropocollagen molecules. The amount and distribution of structural, free, and adsorbed water has a large impact on the fibril's mechanical properties. We study native type-I collagen fibrils using multi-setpoint intermittent contact (MUSIC) mode atomic force microscopy (AFM) in air and in phosphate buffered saline (PBS) solution with different salt concentrations. MUSIC mode AFM is based on point-wise recording amplitude and phase of an oscillating AFM cantilever as the tip-sample distance is reduced. In this way, the unperturbed surface, the tip indentation as well as a quantitative and depth-resolved information about the tip-sample interaction is obtained. Our measurements aim at a better understanding of the tip-sample interaction in liquids as well as the structural and nanomechanical properties of native collagen fibrils under physiological conditions. We find that the fibril's shape and its nanomechanical properties in PBS solution differ distinctly from the fibril's properties in air and we discuss the physical origin of these differences.

CPP 19.15 Tue 9:30 P1

Multivalency in the binding of the viral transmembrane protein hemagglutinin with the cellular receptor sialic acid studied by single molecule force spectroscopy — VALENTIN REITER¹, SUMATI BHATIA², MANUEL GENSLER¹, CHRISTIAN SIEBEN¹, DANIEL LAUSTER¹, SUSANNE LIESE², ANDREAS HERRMANN¹, RAINER HAAG², ROLAND NETZ², and JÜRGEN P. RABE¹ — ¹Humboldt-Universität zu Berlin — ²Freie Universität Berlin

We use force spectroscopy techniques based on the scanning force microscope (SFM) to gain insight into the multivalent interactions between the viral transmembrane protein hemagglutinin (HA) and sialic acid (SA), a part of the cellular glyco-proteins. The binding of a virion to its host in order to induce the endocytosis is the first step in the reproduction of the virus and therefore the inhibition of this attachment is a good approach to prevent infection of cells. Custom designed nano particles outfitted with SA can be used as decoy particles to prevent the virion from attaching itself to a cell membrane [1],[2]. In order to increase the probability and efficiency of the binding of the nano particle to the virus the process of binding and unbinding of the HA to the SA has to be well understood, so that scaffolds suitable to fit the HA binding pockets can be designed. In order to obtain insight into the binding affinities, single molecule force spectroscopy (SMFS) can be used by functionalizing the SFM cantilever with receptor molecules and creating structured arrays of the ligand HA using poly histidine tags. [1] I. Papp et al., *small* 2010, 6, No. 24, 2900-2906; [2] I. Papp et al., *ChemBioChem* 2011, 12, 887-895;

CPP 19.16 Tue 9:30 P1

Amino Acid-Sequence Dependent Interactions between Receptors and Ligands Studied with Optical Tweezers — TIM STANGNER¹, CAROLIN WAGNER¹, DAVID SINGER², STEFANO ANGIOLETTI-UBERTI³, CHRISTOF GUTSCHE¹, JOACHIM DZUBIELLA³, RALF HOFFMANN², and FRIEDRICH KREMER¹ — ¹University of Leipzig, Department of Experimental Physics I, D-04103 Leipzig, Germany — ²University of Leipzig, BBZ, D-04103 Leipzig, Germany — ³Humboldt University Berlin, Department of Physics, Berlin 12489, Germany

For diagnostic procedures that rely on monoclonal antibodies (mAbs), it is imperative to know whether the antibody recognizes the epitope of its target peptide/protein specific or whether possible cross-reactions to other forms of the protein may occur. In a previous study non-specific interactions of the phosphorylation-specific mAb HPT-101 to tau-peptides with similar epitopes, differing only by a single isolated phosphorylation site, were detected. Based on this result, it is obvious that the specificity of this mAb refers not exclusively to the phosphorylation pattern but also to the amino acid sequence in the tau peptide. Here, we investigate with the help of optical tweezers assisted dynamic force spectroscopy the influence of single amino acids on the binding of mAb HPT-101 to the peptide tau[pThr231/Ser235]. For this purpose,

we characterize the unbinding process by analyzing the measured rupture force distributions. Furthermore, the binding process is specified by means of the relative binding frequency. Using these parameters, it is possible to identify essential as well as secondary amino acids for the interaction of this receptor-ligand system.

CPP 19.17 Tue 9:30 P1

Quantification of DNA Damage by ROS using AFM Tapping Mode — FLORIAN BERG¹, JANINE WILKEN¹, STEPHAN BLOCK², and CHRISTIANE A. HELM¹ — ¹Inst. f. Physik, Uni Greifswald, 17487 Greifswald, Germany — ²Chalmers University of Technology, Gothenburg, Sweden

During times of environmental stress (e.g., UV or heat exposure), levels of reactive oxygen species (ROS) can increase dramatically. This may result in significant damage to cell structures. Here we focus on the effects of ROS on DNA.

The plasmid pBR322 (E. coli cloning vector) is attacked by free hydroxyl radicals in liquid surroundings. ROS are produced by Fenton's reaction. DNA damage is assessed by AFM Tapping Mode imaging of the plasmids in air (after adsorption onto PAH-functionalized mica). As damaged DNA strands (height 0.1 nm) are much smaller than intact DNA strands (height 0.35 nm), DNA damage can be quantified based on height distribution histograms. The amount of damaged DNA strands increases with increasing strength of radical attack, and decreases if ROS scavengers like sodium acetate are added.

CPP 19.18 Tue 9:30 P1

Direct evidence of the CT-state in organic small molecule solar cells by electroluminescence measurements — THERESA LINDERL, JULIA KRAUS, STEFAN GROB, and WOLFGANG BRÜTTING — Institut of Physics, University of Augsburg, 86135 Augsburg, Germany

The open-circuit voltage of organic solar cells is limited by the formation of a charge-transfer (CT) state at the donor-acceptor interface. Direct spectroscopic evidence of the CT-state of organic solar cells can be obtained from electroluminescence measurements.

For single layer devices the electroluminescence signal is expected to reflect the fluorescence spectra of the respective material, whereas in heterojunction devices charge carrier recombination can either occur on one of the constituents or from the CT-state. We compare spectroscopic signatures of planar and bulk heterojunction organic solar cells based on small molecules to the signal of single layer devices of the individual components.

For voltages just above the open-circuit voltage V_{oc} an additional feature in the low energy part of the spectrum can be detected, that can not be attributed to any of the used materials. We interpret this additional feature as the transition from the interfacial CT-state to the ground state and relate its energy to the open-circuit voltage of solar cells.

CPP 19.19 Tue 9:30 P1

Analysis of higher recombination orders in organic bulk heterojunction solar cells — JĘDRZEJ SZMYTKOWSKI — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Recently, it has been experimentally demonstrated that an order of nongeminate recombination exceeds two in some types of organic bulk heterojunction donor-acceptor structures. This result is different than for the case of bimolecular recombination described by Langevin theory. Although several theoretical explanations of this effect have been presented, the origin of higher recombination orders is still questionable. In this work, we analyze the process of interaction between an exciton and a polaron and its role in the increasing of recombination order. The influence of a charge concentration effect on mobility is discussed.

CPP 19.20 Tue 9:30 P1

Performance of P3HT:PCBM solar cells modified with iron oxide nanoparticles — DANIEL MOSEGUÍ GONZÁLEZ and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department - LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Among the different systems studied in organic solar cells, the combination of P3HT:PCBM has received the highest attention. Recently, the performance of such devices under magnetic stress has been investigated. In the case of organic electronic devices, the addition of magnetic fields can be achieved via the incorporation of iron oxide nanoparticles, which has been reported as a factor influencing the de-

vice performance [1]. Magnetic fields, amongst other effects, alter the position of the molecular energy levels, allowing "a priori" forbidden spin transitions. Moreover, the presence of heavy metals increases the L-S coupling in the system, increasing the rate of intersystem crossing. The aim of the present investigation is to characterize through which channels the presence of iron oxide nanoparticles affects the performance of P3HT:PCBM based solar cells. The morphology evolution is tracked with scattering techniques. Spectral behavior and electrical response of devices are also investigated.

[1] Zhang et al., Sol. Energ. Mat. Sol. Cells, 95 (2011) 2880-2885

CPP 19.21 Tue 9:30 P1

Investigation on enhanced efficiency introduced by solvent treatment in PTB7:PC71BM bulk heterojunction organic photovoltaics — ●SHUAI GUO¹, BIYE CAO¹, WEIJIA WANG¹, JEAN-FRANÇOIS MOULIN², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748, Garching — ²Helmholtz Zentrum Geesthacht, MLZ, Lichtenbergstr. 1, 85747 Garching

Organic photovoltaics have become of major interest in fundamental researches as well as in applications. Among all the parameters governing the device performance, the morphology of active layers in organic solar cells is of highest importance. In this work the most efficient bulk heterojunction (BHJ) system PTB7:PC71BM with and without solvent treatment is thoroughly investigated. The surface structure of each film is accessed via AFM, and the depth profile of the inner film morphology is revealed by the advanced neutron scattering technique GISANS. Consequently, the complete active layer is probed. The different morphologies formed from solvent treatment are determined and compared with the corresponding performance of each system.

CPP 19.22 Tue 9:30 P1

Synthesis of porous anatase titania nanostructures by block-copolymer assisted sol-gel method — ●LIN SONG, MARTIN A. NIEDERMEIER, VOLKER KÖRSTGENS, DANIEL MOSEGUÍ GONZÁLEZ, YUAN YAO, WEIJIA WANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells, consisting of conjugated polymers and n-type inorganic nanocrystals (such as titania), have received great attention due to the combination of advantages such as low cost, high electron mobility, and good chemical and physical stability. To obtain high efficiency, a large surface-to-volume ratio of the inorganic semiconductor is desirable, since the excitation dissociation occurs at the interface of the inorganic and the organic parts. We prepare titanium dioxide nanostructures from sol-gel synthesis assisted with a diblock copolymer templating approach. With GISAXS the inner film morphology is probed and compared with results from SEM and AFM. The nanocrystals size and phase are confirmed by XRD and GIWAXS.

CPP 19.23 Tue 9:30 P1

Hierarchically structured titania films for efficient light harvesting in dye-sensitized solar cells — ●BO SU, YICHUAN RUI, MARTIN A. NIEDERMEIER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Due to high surface to volume ratio and their bicontinuous morphology, foam-like nanostructures are becoming more interesting in photovoltaics. To improve the power conversion efficiency, the light-trapping strategy is widely used in dye-sensitized solar cells (DSSCs) and organic photovoltaics (OPVs). In our study, we demonstrate hierarchically structured titania films, which are made by sol-gel chemistry and soft-molding method, with an additional superstructure in the sub-micrometer range. The master is prepared by photolithography. Then replica molds are made from the master with poly(dimethyl siloxane) (PDMS). Finally, the structured titania films are prepared by PDMS molds. A fairly high level of control over the final morphology is reached via this route. The morphology of these films is characterized with SEM and AFM. The optical properties are determined by UV/Vis spectroscopy and the photocurrent-voltage characteristics of DSSCs are measured.

CPP 19.24 Tue 9:30 P1

Effect of a third component addition on high efficiency organic solar cells — ●ROSA MARIA TORRADEMÉ, SHUAI GUO, BIYE CAO, WEIJIA WANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-

Franck-Str. 1, 85748 Garching, Germany

Rapid progress has been envisioned on the solution-processed organic bulk heterojunction (BHJ) solar cells in the past decade, and the efficiency has exceeded the threshold for commercial application of 10%. In this work the record-setting system PTB7:PC71BM is investigated regarding the influence of addition of a third component. The aim to introduce this new component is to improve the conductivity of the active layer using polymers with relatively higher crystallinity than that of the host polymer PTB7. Photophysical properties are probed with UVvis spectroscopy and PL measurements. The inner film morphology is revealed by GISAXS and the film crystallinity is probed with GIWAXS. Surface structures are probed with AFM. The device performance is probed by measuring IV-characteristics. Therefore, the influence of the third component on the performance of the solar cells as well as the structure of the active film is addressed.

CPP 19.25 Tue 9:30 P1

The influence of solvent atmosphere on bulk heterojunction solar cells — ●WEIJIA WANG¹, SHUAI GUO¹, Kuhu SARKAR¹, MARKUS SCHINDLER¹, DAVID MAGERL¹, MARTINE PHILIPP¹, JAN PERLICH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — ²DESY, Notkestrasse 85, 22603 Hamburg

Organic solar cells have attracted tremendous attention in the last decades. Among different architectures of solar cell, the morphology called bulk heterojunction (BHJ) plays an important role as it yields high device efficiencies. Annealing or solvent additive processing is a way to optimize the morphology of BHJ films. However, if a solar cell encapsulation is taken into account, it is also crucial to figure out how solvent atmosphere, evaporated from residual solvent, affects the solar cells, especially for the one treated with solvent. Therefore, in this work, BHJ solar cells are stored in solvent atmosphere to accelerate the related aging. In order to gain the fundamental understanding of the solar cell degradation, the final structure of BHJ films is investigated with AFM and GISAXS. Additionally, the crystalline structure is investigated with GIWAXS and compared to the absorption in the visible regime.

CPP 19.26 Tue 9:30 P1

Novel structuring of organic thin films for improved absorption and performance in organic solar cells — ●JOHANNES SCHLIPF, CLAUDIA PALUMBINY, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic solar cells (OSC) have recently broken the 10% efficiency barrier hence they will soon become competitive with their inorganic counterparts. In addition, OSC still have huge advantages over (the commonly used) silicon solar cells, e.g. low production costs, possible fabrication on flexible substrates, as well as their good performance under diffuse and indirect light. The latter two are addressed in this work. Nano-imprint lithography is used to form novel, artificially structured organic thin films of high aspect ratio. Applying this structure in a solar cell provokes enhanced light scattering and induced light trapping in the photo-active layer for an overall better absorption particularly under oblique incident light. Furthermore, the conductivity of the commonly used PEDOT:PSS is improved by a combination of previously established methods: the addition of a fluorosurfactant (Zonyl FS-300)[1] and subsequent post-treatment with ethylene glycol [2, 3]. Thus PEDOT:PSS becomes applicable as a stand-alone transparent electrode. In total, this provides the possibility for high-performance, flexible and ITO-free devices based on already well-established materials in the field of organic electronics. [1] Vosguerichtian et al., Adv. Funct. Mater. 2012, 22, 421-428; [2] Kim et al., Adv. Funct. Mater. 2011, 21, 1076-1081; [3] Palumbiny et al. (submitted)

CPP 19.27 Tue 9:30 P1

Trap-assisted recombination in PCDTBT:PC₇₁BM blend films investigated by transient absorption — ●JEREMIAS WEINRICH¹, ANDREAS FRITZE¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius-Maximilian University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), D-97074 Würzburg

Organic photovoltaic cells have the potential to be a key technology in the field of renewable energies. They are comparatively cheap and compatible to mass production, yet have a lower power conversion efficiency (PCE) compared to silicon solar cells. The low-bandgap

polymer PCDTBT, blended with PC₇₁BM as acceptor, is a promising electron donor in organic bulk heterojunction solar cells, with PCE's yielding above 6%.

Charge carrier recombination is the dominant loss mechanism in these devices, reducing the number of charge carriers before extraction at the electrodes. We performed transient absorption spectroscopy to probe the laser-pulse induced charge carrier concentration and its decay on a time scale of 10 ns to 1 ms at different pump intensities and temperatures. We discuss the charge carrier dynamics and activation energies as well as the origin of nongeminate losses in PCDTBT-based solar cells.

CPP 19.28 Tue 9:30 P1

Hybrid solar cells based on aqueous processed titania nanoparticles — ●CHRISTOPH MAYR¹, VOLKER KÖRSTGENS¹, HRISTO IGLEV², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching — ²TU München, Physik Department, LS Laser- und Röntgenphysik, James-Frank-Str. 1, 85748 Garching

One way towards 'green' solar cells is using aqueous-processed hybrid solar cells, because they require only a low energy amount in fabrication and furthermore a production without toxic organic solvents is possible. For the electron donor and acceptor we use a water soluble P3HT analogon and TiO₂ nanoparticles, respectively. The advantage of these particles is their size tuneability, their high absorption coefficient and the high surface area. Therefore a large interfacial area with the polymer is facilitated. The active layer is applied via solution casting. The final solar cells work with a decent efficiency, which we determined under AM 1.5 conditions. Moreover we investigate the thin films of the active layer with XRD and SEM measurements to characterize the crystalline structure and the surface structure, respectively.

CPP 19.29 Tue 9:30 P1

Bottom-up parametrization of macroscopic charge transport models — ●PASCAL KORDT¹, OLE STENZEL², BJÖRN BAUMEIER¹, VOLKER SCHMIDT², and DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Institute of Stochastics, Ulm University, Helmholtzstr. 18, 89069 Ulm, Germany

Computer simulations help to rationalize the link between macroscopic system properties and the underlying chemical structure of the material. This requires model development at different length scales, starting from microscopic, first-principles-based simulations, to lattice-based Gaussian disorder models (GDM), to drift-diffusion equations. Here we show how one can link the microscopic, mesoscopic off-lattice (stochastic), and finally the lattice-based GDM models and examine the parameters extracted from simulations at different length scales. The approach is tested on an amorphous mesophase of a dicyanovinyl-substituted quaterthiophene (DCV4T), which belongs to a family of efficient donors used in small-molecule organic solar cells.

CPP 19.30 Tue 9:30 P1

Characterization of quenching processes on the external quantum efficiency of phosphorescent organic light-emitting diodes — ●SEBASTIAN WEHRMEISTER¹, TOBIAS D. SCHMIDT¹, WOLFGANG BRÜTTING¹, DANIEL S. SETZ², THOMAS WEHLUS², ANDREAS F. RAUSCH², and THILO C. G. REUSCH² — ¹Institute of Physics, University of Augsburg, Germany — ²OSRAM Opto Semiconductors GmbH, Regensburg, Germany

Efficiency roll-off in organic light-emitting diodes (OLEDs) as result of high current densities represents a substantial drawback for technical applications. However, since high brightness is a major request for lighting purposes, high current densities are unavoidable. To identify and analyse the impact of quenching processes on the efficiency, time-resolved spectral measurements on a red phosphorescent OLED with Iridium(III)bis(2-methylidibenzo-[h]quinoxaline)(acetylacetonate) (Ir(MDQ)₂(acac)) as emitter have been performed. We probe the excited states lifetime after a short laser pulse on top of the steady-state region of a rectangular electrical pulse [1]. By continuously increasing the current density of the electrical pulse, the non-radiative decay becomes more likely and the excited states lifetime decreases. A comparison of the calculated external quantum efficiency (EQE) based on these data with direct EQE measurements reveals the influence and the origin of quenching processes on the efficiency roll-off of the device.

[1] N. C. Giebink, S. R. Forrest, Phys. Rev. B, 235215-1 (2008)

CPP 19.31 Tue 9:30 P1

Calculation of electronic transport properties through polymers — ●FLORIAN GÜNTHER¹, SIBYLLE GEMMING¹, and GOTTHARD SEIFERT² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany

Organic thin-film transistors producible by low-cost roll-to-roll manufacturing processes seem to be highly promising for flexible electronics. Therefore, high mobility semiconducting polymers with ambient stability, good solubility and film-forming properties are needed. Our study is turned to the calculation of the electronic transport properties through polymers consisting of conjugated thiophene based donor units and di-ketopyrrolo-pyrrol based acceptor units. Therefore, we use empirical hopping equations such as Marcus transfer theory in order to determine the mobility of holes and electrons. The parameters required for this are taken from first-principles calculations such as density functional theory and Hartree-Fock approaches.

CPP 19.32 Tue 9:30 P1

Detailed study of the charge carriers mobility in organic bulk heterojunction solar cells — ●KATRIN ANNESER¹, ANDREAS ZUSAN¹, VLADIMIR DYAKONOV^{1,2}, and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²Bavarian Centre for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg

Organic solar cells provide a good alternative to conventional, silicon based photovoltaics, since they are cheaper and easy to produce. A key issue for further optimization of the power conversion efficiency is to understand fundamental loss mechanisms such as charge carrier recombination. One important parameter influencing the nongeminate recombination is the charge carrier mobility. In this work we studied the mobility in bulk heterojunction solar cells based on P3HT:PC₆₀BM and low-bandgap:PC₇₀BM by different charge extraction techniques. We discuss impact of carrier concentration, field and temperature dependence of the mobility on the recombination losses.

CPP 19.33 Tue 9:30 P1

Non-adiabatic molecular dynamics of [2+2] addition reaction of C60 driven by the electron excitation. — ●ZOBAC VLADIMIR¹, HAPALA PROKOP¹, JOSE ORTEGA², JAMES LEWIS³, and PAVEL JELINEK¹ — ¹Institute of Physics, Academy of Sciences of the Czech Republic — ²Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center Universidad Autónoma de Madrid — ³Department of Physics, West Virginia University

Co-crystallizations and supramolecular assemblies are giving rise to an explosion of new crystal structures. Here we report theoretical study of [2+2] addition mechanism of C₆₀ molecules induced by the electron excitation. These phenomena need to describe not only ground state potential energy surface (PES), but also the excited one. Therefore we employ an efficient non-adiabatic molecular dynamics with electronic transitions using DFT local orbital formalism, which evolves simultaneously the ions and electrons. We will discuss the mechanism of the [2+2] addition and the yield as function of distance and fullerenes orientations.

CPP 19.34 Tue 9:30 P1

Electronic excitations in push-pull oligomers and their complexes with fullerene — ●BJÖRN BAUMEIER¹, MICHAEL ROHLFING², and DENIS ANDRIENKO¹ — ¹Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz — ²Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present a comparative study of excited states in push-pull oligomers of PCPDTBT and PSBTBT and prototypical complexes with a C₆₀ acceptor using GW-BSE. We analyze oligomers up to a length of 5 nm and find that, for both materials, the absorption energy saturates for structures larger than two repeat units due to the localized nature of the excitation. In the bimolecular complexes with C₆₀, the Frenkel to CT transition is exothermic and we observe a strong influence of the acceptor's position and orientation on the CT energy. Their binding energy is still of the order of 2 eV resulting from the lack of an explicit molecular environment. Embedding the the donor-acceptor complex into a polarizable lattice leads to an energetic stabilization of the CT exciton by about 0.5 eV, while its binding energy is reduced to about 0.3 eV. We also identify a CT state with a more delocalized hole at higher energy, which opens another potential pathway for charge sep-

ation. For both polymers, the absorption and the driving force to form intermediate CT excitations are largely similar. These results confirm that the higher power conversion efficiency observed for solar cells using PSBTBT as donor material is rather a result of molecular packing than of the electronic structure of the polymer.

CPP 19.35 Tue 9:30 P1

Structure and performance of water soluble solar cells functionalized with non-magnetic nanoparticles — ●NURI HOHN, DANIEL MOSEGUÍ GONZÁLEZ, and PETER MÜLLER BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic solar cells (OSCs) offer a great potential due to low cost, large scale production and flexible design. For preparation of OSCs the hole conducting polymer Poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) is employed. For comparability reasons with the broadly studied P3HT:PCBM system, P3P6T is combined with an also water-soluble C60 fullerene derivative. With respect to environment protection, the manufacturing process of the active layer tends towards a more friendly approach compared to common OSCs based on harmful organic solvents. Additionally, inclusion of non-magnetic nanoparticles in the above mentioned system is carried out, which is found to have a strong impact on the efficiency of organic, electronic devices. We pursue to characterize the influence of these nanoparticles on the rate of intersystem crossing, as this effect eventually leads to extended exciton lifetimes. Primary investigations address the electrical, spectral and morphological characterization.

CPP 19.36 Tue 9:30 P1

Flexibility investigations on low-temperature processed nanostructured polymer/titania hybrid films — ●TOBIAS WIDMANN, WELJIA WANG, LIN SONG, and PETER MÜLLER BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

On the way to green energy, hybrid solar cells show great potential. They combine a conducting polymer with an inorganic semiconductor and therefore have advantages of both materials. The flexibility is one of the most promising properties of hybrid solar cells, which ensures the production by a roll-to-roll process and in large scale. Hence, in this work the flexibility of low temperature processed hybrid thin films is investigated. A porous film structure is synthesized by incorporating a titania precursor into a diblock copolymer which functions as the template. Thereafter it is deposited on a flexible substrate and a bending test is implemented by a custom made machine. The alteration of the bare titania structure and the hybrid film structure due to bending is investigated with optical microscopy and SEM and correlated with photophysical properties probed with UVvis and PL.

CPP 19.37 Tue 9:30 P1

Aggregation Control in Organic Photovoltaic Blends — ●JUAN FELIPE MARTÍNEZ GRISALES^{1,2}, EVA M. HERZIG¹, and PETER MÜLLER-BUSCHBAUM² — ¹TU München, MSE, Lichtenbergstr. 4, 85748 Garching — ²TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Since the discovery of conductive polymers, organic photovoltaics has turned into a very active field of research. This is owed to the potential of the inexpensive and widely available energy of the sun and the wide range of possible applications [1]. To fully exploit organic photovoltaics for efficient energy conversion processes the morphology of the active layer is a crucial parameter [2]. For example, the charge transport properties closely depend on the aggregation state, i.e. the nanomorphology of the polymers. Exploiting the properties of selective solvents we present a method to control the aggregation of a binary photovoltaic blend via the addition of a co-solvent. The system is thoroughly investigated using microscopy, spectroscopy and scattering to gain fundamental understanding on the processes involved and to relate these to solar cell performance. [1] E. M. Herzig, P. Müller-Buschbaum, *Acta Futura*, 2013, 6, 17-24 [2] M. A. Ruderer, et al., *Soft Matter*, 2011,7, 5482-5493

CPP 19.38 Tue 9:30 P1

Surface morphology of P3HT, PCBM and blends of both — ●MARTIN DEHNERT¹, MARIO ZERSON¹, ALESSANDRO SEPE², SVEN HÜTTNER², ZHUXIA RONG², ULLRICH STEINER², and ROBERT MAGERLE² — ¹Chemische Physik, Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany — ²Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K

We investigate the surface morphology and the nanomechanical properties of thin films of pure regioregular poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methyl ester (PCBM) and blends of both using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) mode. This allows for depth-resolved mapping of the mechanical properties of the top surface layer of the specimen. AFM images of pure P3HT and PCBM before and after annealing at 175°C show the morphology at the film surface. Both materials form a nanocrystalline texture with 10 * 30 nm large domains, but with different nanomechanical properties and different surface roughness. The P3HT surface is covered with a 3-nm-thick, compliant surface layer whereas the PCBM surface is stiff and shows less tip indentation. The small needlelike crystals of PCBM are only visible in the attractive regime of the tip-sample-interaction. Thin films of blends of P3HT:PCBM were treated with 1,8-diiodooctane, a selective solvent for PCBM. This allows us to identify the contribution of PCBM to the microstructure at the blend-air-surface.

CPP 19.39 Tue 9:30 P1

Influence of electrochemical grown thiophenes at the anode interface of bulk hetero structure organic solar cells studied by photo-CELIV. — ●ARNE HENDEL, SIDHANT BOM, and VEIT WAGNER — Jacobs University Bremen, 28759 Bremen, Germany

The charge carrier mobility and the charge carrier density in the active layer play a crucial role in organic solar cells for the device performance. The need for long lasting and stable solar cells requires an understanding of the transport and degradation processes of the cell. By the technique of charge carrier extraction by linearly increasing voltage with an additional light source (photo-CELIV) the charge transport, the lifetime and recombination dynamics in the organic BHJ is studied, which gives insight into the charge carrier creation and extraction. An additional layer of thiophenes at the interface of PDOT-PSS and P3HT-PCBM grown by electropolymerization is beneficial to the solar cell performance. The effect of such layers is studied by photo-CELIV analysis and the reason for improvements is discussed.

CPP 19.40 Tue 9:30 P1

Combination of Raman spectroscopy and GIWAXS for the investigation of the morphology of organic solar cell materials — ●SIMON SCHMITT¹, EVA HERZIG², FRANZISKA FUCHS¹, VLADIMIR DYAKONOV^{1,3}, PETER MÜLLER-BUSCHBAUM², and CARSTEN DEIBEL¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²MSE & Physik-Department, LS Funktionelle Materialien, Technische Universität München, 85747 Garching — ³ZAE Bayern, 97074 Würzburg

The efficiency of organic solar cells crucially depends on their active layer morphology and donor:acceptor phase separation. Therefore a more thorough understanding of the impact of varying preparation parameters on morphology changes is important to improve solar cell performance. In this study we combine the two complementary non-destructive scattering techniques of Raman spectroscopy and GIWAXS (grazing incidence wide-angle X-ray scattering) for the investigation of the PCDTBT:PC70BM blend system. GIWAXS provides information about the molecular order whereas the Raman spectra reveal the vibrational modes of the conjugated polymer and fullerene. We discuss our experimental findings for different donor:acceptor blend ratios in view of the high degree of disorder in the polymer PCDTBT and the implications for the morphology-performance relation.

CPP 19.41 Tue 9:30 P1

Exciton quenching in inverted bilayer all polymer solar cells — ●KARL-PHILIPP STRUNK, THOMAS PFADLER, MIHAEL CORIC, JONAS WEICKERT, and LUKAS SCHMIDT-MENDE — University of Konstanz

All polymer solar cells are a promising type of emerging solar cells. As the current generating layer consists only of polymers it offers a great versatility and a potential for low cost fabrication. Here we combine the n-type polymer N2200 (also called P(NDI2OD-T2)) with different hole conducting p-type polymers to bilayered solar cells.

Absorption measurements and data about the band structure give an idea about good matching polymer combinations. Three different electron donors, namely P3HT, MDMO-PPV and F8TBT, are investigated in depth as they show a favourable band structure and a complementary absorption to N2200. As P3HT is one of the most investigated p-type polymers, bulk heterojunction solar cells from N2200:P3HT are optimized by improving the fabrication parameters and compared with bilayer solar cells of N2200:P3HT, MDMO-PPV and F8TBT.

Quantitative studies of photoluminescence in bulk heterojunction

and bilayers from all polymer combinations have been performed in order to calculate the exciton quenching rate. Quenching is strongest for the internal charge transfer (CT) state in N2200 which is an indication for a high diffusion length of the internal CT state.

CPP 19.42 Tue 9:30 P1

Cryogenic Break-Junction Measurements for the Characterization of Organic Molecules — •THOMAS GRELLMANN and ROGER WÖRDENWEBER — PGI-8, Forschungszentrum Jülich, Deutschland

A cryogenic setup was developed to characterize single organic molecules via the lithographical prepared break-junction technique. Measurements are performed in a helium-flow cryostat, with temperatures ranging from 20K to room temperature. Additionally, a magnetic field up to 0.5T can be applied. The break-junction sample consists of a coated metal substrate with a lithographical prepared gold nanobridge. Repeated bending of the substrate via a piezo crystal opens and closes the gold-bridge and molecules are trapped between the tips. This allows measuring the conductance and subsequently the IV-spectra of a single molecule. Due to the temperature range from cryogenic to room temperature the conduction mechanisms of molecules can be obtained. Conductance and nonlinear IV-curves of 1,4-Benzenedithiol at different temperatures were measured, and more complex porphyrine molecules are in examination.

CPP 19.43 Tue 9:30 P1

Control and Analysis of the interface trap density in MIS structures by surface treatments and impedance spectroscopy — •HIPPOLYTE HIRWA, STEVE PITNER, and VEIT WAGNER — Jacobs University Bremen, Germany

For high performance electronic devices, reliability and stability are crucial parameters. Reliability and stability issues in field effect transistors are mainly related to their interface properties. MIS capacitors are very useful tools for investigations of interface traps. Hence, they can be used to evaluate the effect of different surface treatments on the interface traps distribution. In order to improve interface properties in field effect transistors various surface treatments are in use. Octadecyltrichlorosilan (OTS) and Hexamethyldisilazan (HMDS) treatment of SiO₂ surfaces are commonly used. Their effects in terms of interface trap density of states and the corresponding time constants are investigated. Impedance measurements have been carried on MIS capacitors fabricated using silicon oxide as insulator with 3 different surface treatments and poly(3-hexylthiophene) as the semiconductor. With a proper equivalent circuit of our MIS structure, the interface trap density was extracted from a fit of the obtained impedance in dependence of frequency and applied DC voltage. A good agreement between the experimental results and the MIS structure model can be obtained upon taking into account the dispersive transport of the bulk and the surface potential fluctuations at the interface. The results reveal that the interface states density and energy distribution can be strongly modified by the surface treatment.

CPP 19.44 Tue 9:30 P1

The influence of co-evaporated polydimethylsiloxane oil on small molecule bulk heterojunction solar cells — •FELIX HOLZMUELLER¹, LUTZ WILDE², CHRISTIAN KOERNER¹, and KARL LEO¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany — ²Fraunhofer Institute for Photonic Microsystems, 01069 Dresden, Germany

For efficient organic solar cells (OSC), the morphology of donor-acceptor (DA) heterojunctions is of great importance. It can be influenced by methods like post-annealing or substrate heating during the evaporation. Furthermore Kaji et al. recently proposed a new method called "co-evaporant induced crystallization" [1]. An additive is co-evaporated during the vacuum deposition of the donor and acceptor materials. At the same time, the substrate is heated to a certain temperature to ensure that the incoming additive molecules desorb from the substrate surface after their arrival. A vapor of additive molecules forms above the substrate surface and supports the crystallization of the bulk phases. In this contribution we use this method to test the influence of co-evaporated polydimethylsiloxanes on different DA-combinations like e.g. zinc-phthalocyanine (ZnPc) and C₆₀. Grazing incidence X-Ray diffraction and X-ray reflection measurements are performed on co-evaporated bulk layers showing a significant increase of crystallinity for the C₆₀ phase in ZnPc:C₆₀ blends. Additionally, the influence of the co-evaporation method on the device efficiency is investigated. [1] Kaji, T. et al. (2011). Adv. Mater., 23, 3320

CPP 19.45 Tue 9:30 P1

Toolkit for microscopic charge/energy transport simulations in disordered organic semiconductors — CARL POELKING, BJORN BAUMEIER, PASCAL KORDT, JEROEN VAN DER HOLST, ANTON MELNYK, JENS WEHNER, and •DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz 55128, Germany

We present recent developments in the toolkit for charge and energy transport simulations in amorphous organic materials (VOTCA, www.votca.org) [1]. These include (i) interfaces to the GAUSSIAN, TURBOMOLE and NWCHEM packages to compute electronic couplings, internal energies and electrostatic multipoles (ii) the QM/MM scheme combined with the polarizable Thole model for evaluating energies of charged clusters embedded in a molecular environment (iii) the kinetic Monte Carlo algorithm for finite charge densities. The methods are illustrated by studying processes at a donor-acceptor interface of dicyanovinyl-substituted quaterthiophene/C60, a typical donor-acceptor pair used in small molecule organic solar cells [2].

[1] V. Rühle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, D. Andrienko, J. Chem. Theory Comput., 7, 3335, 2011

[2] M. Schrader, R. Fitzner, M. Hein, C. Elschner, B. Baumeier, M. Riede, K. Leo, P. Baeuerle, D. Andrienko, J. Am. Chem. Soc., 134, 6052, 2012

CPP 19.46 Tue 9:30 P1

AFM, STXM, and TEM studies of DCV-5T:C60 absorber layers for highly efficient organic solar cells — •TOBIAS MÖNCH¹, PETER WARNICKE³, PETER FORMANEK², CHRISTIAN KÖRNER¹, and KARL LEO¹ — ¹TU Dresden, IAPP, Dresden — ²Leibniz-Institut für Polymerforschung Dresden e.V., Dresden — ³Paul Scherrer Institut, Villigen, Schweiz

The optoelectronic properties of organic thin film solar cells are closely related to the microstructure of the self-organized, nanostructured network of donor and acceptor molecules. Hence, the microstructure plays a crucial role in the understanding and optimization of organic solar cells. Here we use multiple high-resolution (<40 nm) techniques to study the relationship between the microstructure and electronic properties of the device: scanning transmission X-ray microscopy (STXM), photoconductive atomic force microscopy (pcAFM), and transmission electron microscopy (TEM) were used to study local chemical composition, local charge transport, and local crystallinity, respectively. Utilizing these techniques we study the impact of in-vacuo substrate heating on the phase separation of DCV-5T:C60 (2:1 by volume) blends, used in highly efficient organic solar cells.

CPP 19.47 Tue 9:30 P1

The impact of a varying C₆₀:C₇₀-acceptor mixing ratio on the opto-electronic properties of planar bilayer cells — •JOHANNES MAHR¹, MICHAEL BRENDEL¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Many small molecule organic photovoltaic cells (OPVCs) are based on the electron acceptor C₆₀. We discuss the effect of employing C₇₀ instead of C₆₀ in prototypical diindenoperylene (DIP) based planar bilayer cells. As a result the short circuit current density (j_{sc}) is increased by 25 %, whereas the other solar cell parameters such as the fill factor and the open circuit voltage remain almost unaffected. By comparison of complementary optical and electrical measurements, the gain in j_{sc} is predominantly attributed to an enhanced absorption of the higher order fullerene C₇₀. Both acceptor molecules under investigation, are created simultaneously in common fullerene synthesis procedures. The cost extensive step to obtain pure C₆₀ and C₇₀ is the separation process of the different sizes, rendering pristine mixtures of both materials much cheaper. Therefore the effect of a varying C₆₀:C₇₀-acceptor mixing ratio, realized by co-evaporation of the two fullerenes, on the opto-electronic properties of planar bilayer cells will be elucidated in the course of this study. The occurring changes in the devices performance will be discussed in relation with structural data obtained by AFM and X-Ray diffraction. Financial support by the DFG focus program SPP1355 is gratefully acknowledged.

CPP 19.48 Tue 9:30 P1

Hierarchy of stochastic pure state wavefunctions for open quantum systems — DANIEL SÜSS¹, WALTER T. STRUNZ¹, and •ALEXANDER EISFELD² — ¹TU Dresden — ²MPI-PKS

A method is presented to efficiently solve open quantum system prob-

lems with a non-Markovian structured environment. The approach is based on the Non-Markovian quantum state diffusion (NMQSD). We derive a hierarchy of stochastic differential equations, which can be solved numerically efficient and which converges rapidly to the exact reduced density matrix. We demonstrate the usefulness of the method by considering the spin-boson problem, electronic excitation transfer in the light-harvesting Fenna-Matthews-Olson (FMO) complex and the calculation of absorption spectra of molecular aggregates.

CPP 19.49 Tue 9:30 P1

Spatially resolved defect investigation of pinholes in metal electrodes of organic photovoltaic cells — ●DANIEL FLUHR, ROLAND RÖSCH, BURHAN MUHSIN, MARCO SEELAND, and HARALD HOPPE — Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

To date long operation lifetime remains a major problem of organic photovoltaic (OPV) devices, even though considerable improvements were achieved over the last few years. Among the reasons for solar cell degradation are impurity induced shunts, photobleaching of the organic semiconductors via oxygen and water as well as corrosion and delamination of the metal contacts due to the same reagents. In this study we focus on so-called pinholes occurring through the metal back electrode of typical devices. These pinholes provide pathways for the ingress of water and oxygen, which locally attack the metal organic interface, resulting in contact delamination. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion is reduced and hence the overall efficiency suffers. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements provide information on location and size of inactive areas induced by pinholes in the metal back contact. Periodically applied non-invasive measurements during degradation of the devices reveal the dynamics and rate of growth of these defects. By looking at different device structures we find important conclusions for increasing the lifetime of organic photovoltaic devices.

CPP 19.50 Tue 9:30 P1

Optimization of Transient Photocurrent measurements for organic solar cell characterization — ●DANIEL FLUHR¹, SHAHIDUL ALAM¹, CHETAN RAJ SINGH², and HARALD HOPPE¹ — ¹Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²Department of Macromolecular Chemistry I, Universität Bayreuth, 95440 Bayreuth, Germany

We report on the extension of transient photocurrent measurements for increasing the characterization range in current and time domain. The challenge is to trace the transient photocurrent over several orders of magnitude. We compare results from using various ohmic resistors with those done via a current amplifier for tracing smaller photocurrents. Here the specific resistor capacitor discharge time is a critical value, which may yield changes in the discharging dynamics. By application of the current amplifier we are able to trace the photocurrent down by several orders of magnitude. However, slight differences in the internal resistor within the current amplifier -present at different amplifier settings- complicate the quantitative analysis of the photocurrent decay. As the presence of deep traps could not be verified, further efforts are to be invested for tracing photocurrent decays over even larger current ranges. Models describing the solar cell discharge are discussed in addition.

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Influencing optical properties and the morphology in thin polymer films consisting of P3HT, PFO und MEH-PPV by adding small amounts of high-boiling solvent additives — ●MARKUS REICHENBERGER — Universität Bayreuth, Lehrstuhl EP2

If admixing a few volume percent of higher boiling point additives to a solution with constant polymer concentration and solvent, impact on optical transitions, electronic properties and film morphology is resulting. It is shown how this modification of the polymer solution affects thin films of P3HT. The investigation is carried out by different spectroscopical methods and various techniques of surface analysis. Diiodooctane, dichlorobenzene and octanedithiols are used as exemplary high-boiling additives. The effect of incorporating diiodooctane on films made of PFO and MEH-PPV gives approximately equivalent results as in P3HT films: By admixing a small amount of an arbitrary high boiling point additive to the polymer solution, one can control the fraction of amorphous and aggregated phase, hence potentially the charge transport, in the spin-coated polymer film.

Many a time in the literature one observes an high energetic peak at 2.12 eV, respectively 585 nm, in the photoluminescence spectrum of thin P3HT films. Recent results are able to clarify the origin of this peak.

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Understanding exciton dissociation at different donor-acceptor interfacial morphologies using field dependent photocurrent measurements — ●TOBIAS HAHN¹, MARLENE SCHUBERTH², PETER STROHRIEGL², and ANNA KÖHLER¹ — ¹University of Bayreuth, Exp. Physics 2 — ²Bayreuth Institute of Macromol. Research (BIMF)

Photocurrent measurements up to high electric fields may be employed to assess whether exciton dissociation prevails at an extended donor-acceptor interface with interfacial dipoles, or whether it takes place by dopant-assisted dissociation at individual donor sites. Here we have investigated the influence of acceptor diffusion into the donor layer on the contribution between these two processes, and on the impact this has on the overall solar cell efficiency. We used a donor polymer that can be cross-linked by various degrees such as to control the thermally activated diffusion of the acceptor C60 molecule into the film. Future work will focus on replacing acceptor C60 molecule by inorganic materials including an amorphous silicon layer or, eventually, silicon nanoparticles. The aim of these studies will be to understand the mechanism underlying the dissociation process at the organic / inorganic interface in hybrid solar cells.

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Simulations of morphology, charge transport, and optical absorption in PCPDTBT derivatives — ●ANTON MELNYK^{1,2}, BJÖRN BAUMEIER¹, DENIS ANDRIENKO¹, FLORIAN FISCHER³, SABINE LUDWIG³, MARTIN BRINKMANN⁴, and NAVAPHUN KAYUNKID⁴ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²Graduate School Materials Science in Mainz, Staudinger Weg 9, 55128, Germany — ³Institut für Polymerchemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart — ⁴Institut Charles Sadron, CNRS-Universität de Strasbourg, 23 rue du Loess, 67034 Strasbourg Cedex, France

Crystalline molecular arrangements in unit cells of PCPDTBT derivatives are probed using molecular dynamic simulations. Scattering patterns are calculated and compared to TEM measurements. The morphologies are then used to evaluate electronic coupling elements, energetic disorder, and finally simulate charge transport in crystalline cells. Optical excitation spectra in solid state are calculated using a QM/MM scheme based on many-body Green's function formalism, which accounts for electrostatic embedment. A link between electronic structure, morphology, and charge transport properties is established.

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Molecular Dynamics of Perylene Bisimide and its Conformational States — ●MANUEL HOLLFELDER and STEPHAN GEKLE — Biofluid Simulation and Modeling, Nachwuchsgruppe Theoretische Physik, Universität Bayreuth, Germany

Perylene bisimide dimers are a promising material for organic solar cells. Recent fluorescence experiments (Spreitler et al. *Phys. Chem. Chem. Phys.* (2012)) have shown evidence of three molecular states in the fluorescence spectrum. Here we use Molecular Dynamics to simulate perylene bisimide solvated in toluene and relate these three states to their three geometric conformations: A non stacked state "open" and two stacked states, where the aromatic rings are located on top of each other, which we call "para" and "anti". The stacked states are distinguished by the orientation of the perylene molecules with respect to the connection point of the alkane chain. We further investigate the stability of the three states and their transition dynamics. We find that the transition dynamics is strongly influenced by the surrounding solvent.

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Temperature induced conformational changes in P3HT — ●FABIAN PANZER¹, RUTH LOHWASSER², MUKUNDAN THELAKKAT², and ANNA KÖHLER¹ — ¹Experimental Physics II, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth — ²Macromolecular Chemistry I, University of Bayreuth, Universitätsstraße30, 95447 Bayreuth

P3HT is known to exist in two distinct conformations, associated with different film morphologies. These conformations consist of coiled higher-energy phase and aggregated red phase implying a more ex-

tended, planarized and better ordered conformation. These two conformations show different behaviors in absorption and fluorescence, leading to a strong impact on device performance such as OLEDs or solar-cells. We show here that the transition from one phase to the other is a phenomenon that can also be induced by temperature and occurs at a critical temperature in the polymer P3HT. We have investigated how these conformational changes depend on various material parameters such as molecular weight and polydispersity.

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Polarity Effects in Organic Solar Cells: The Importance of Being Long-Range — ●CARL POELKING¹, MAX TIETZE², CHRIS ELSCHNER², KARL LEO², BJÖRN BAUMEIER¹, and DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, 55128 Mainz, Germany — ²Institute for Applied Photophysics, 01062 Dresden, Germany

We highlight the staggering importance of long-range interactions in predicting energy levels in organic semiconductors. Our simulation method addresses selectively charged, polarizable systems with broken 2D periodicity. We show that the resulting polarity effects are strong enough to easily reverse the role of donor and acceptor in organic solar cells as conditioned by gas-phase energy levels. Comparing atomistic simulations to experiments, we address implications for the empirical link between molecular energy levels and open-circuit voltage and account for why the acceptor-donor-acceptor architecture is particularly suited for solar-cell applications.

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Surface structure of organic solar cells based on PBDTTT-C and PC71BM — ●MARIO ZERSON¹, ANDREAS ZUSAN², BJÖRN GIESEKING², CARSTEN DEIBEL², and ROBERT MAGERLE¹ — ¹Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany, — ²Experimental Physics VI, Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of organic heterojunction solar cells based on blends of poly[4,8-bis-(2-ethylhexyloxy)-benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-(4-(2-ethylhexanoyl)-thio-no[3,4-b]thiophene))-2,6-diyl] (PBDTTT-C) and PC71BM with a weight ratio of 1:1.5. The co-solvent diiodooctane (DIO) was used with ratios between 0% and 10% to increase the solubility of PC71BM. Thin films spun cast with different amounts of DIO exhibit different power conversion efficiencies and surface morphologies. We investigate the latter with amplitude modulation atomic force microscopy (AFM). Conventional AFM height and phase images are complemented with data obtained from maps of amplitude-phase-distance (APD) curves. This allows us to determine the unperturbed (true) surface and the mechanical properties of the top surface layer of the specimens. For describing and quantifying the surface morphology we use different morphological measures. We discuss the structure formation process of the blends in terms of intermixing and demixing of the donor and acceptor material during spin casting, the size of the interfacial area between donor and acceptor components, and the formation of percolation pathways for the charge carriers.

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Preparation and (magneto-) optical characterisation of thin film organic transition metal complexes — ●FRANK LUNGWITZ¹, MICHAEL FRONK², CAROLA MENDE³, HEINRICH LANG³, DIETRICH R.T. ZAHN², and GEORGETA SALVAN² — ¹Physics Department, Chemnitz University of Technology, Chemnitz, Germany, now at HZDR, Dresden-Rossendorf, Germany — ²Physics Department, Chemnitz

University of Technology, Chemnitz, Germany — ³Chemistry Department, Chemnitz University of Technology, Chemnitz, Germany

Characterisation of thin films of organic materials is an important step in the development of novel electronic and spintronic devices. A class of molecules which have promising perspective for application in such devices are the porphyrins. Due to their thermal stability they are evaporable in vacuum and their optical properties can be tuned by applying different sidegroups. In this work Tetra(methoxyphenyl)Porphyrins were deposited onto silicon substrates via organic molecular beam deposition (OMBD) and characterised by variable angle spectroscopic ellipsometry (VASE) and magneto-optical Kerr effect spectroscopy (MOKE) in polar geometry. The VASE data were subsequently modelled to recursively calculate the films optical constants, thickness, roughness and the molecules tilt angle with respect to the substrate. Under knowledge of the optical constants the MOKE data were used to obtain the Voigt constant which, as a conversion factor between magneto-optical effects, was employed to determine the magnetic circular dichroism (MCD) spectra of these molecules.

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Theoretical Investigations of Surface Relief Gratings Based on Azobenzene-Containing Polymers — ●MARCUS BÖCKMANN and NIKOS L. DOLTSINIS — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Münster, Germany

Polymers containing the azobenzene (AB) chromophore are known to exhibit photo-fluidity when exposed to inhomogeneous light fields [1]. This phenomenon results in effective mass transport and can be utilized to, e.g., create surface relief structures of distinguished shape. Recently, it has been demonstrated that specific surface relief gratings (SRGs) imprinted on the rear panel of organic photovoltaic solar cells contribute to enhanced efficiency due to trapping of incident light [2].

We investigate the photoinduced behaviour of such an active layer based on the PDO3M azo-polymer by means of multiscale molecular dynamics simulation techniques [3] making use of a molecular mechanics switch for AB photoisomerisation that we designed recently [4].

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Charge transport and energetics in merocyanine-C60 organic solar cells — ●JENS WEHNER, CARL POELKING, and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Solar cells with efficiencies of more than 10% have recently been reported for a number of small-molecule-based organic solar cells. Among these, cells based on merocyanine dyes (easy to mass-produce and purify colorants with high absorption coefficients) offer an opportunity to make both solution and vacuum-processed devices. Due to the donor-acceptor architecture of the molecule, these compounds have large dipole moments, which in principle should impede charge mobility and change the transport levels at the donor-acceptor interface. By combining molecular dynamics simulations and quantum chemical methods we study charge transport as well as energetics at these interfaces and show why merocyanines are efficient donors in combination with C60 as an acceptor.