CPP 24: Poster: Organic Semiconductors

Time: Wednesday 11:00–13:00 Location: Poster A

CPP 24.1 Wed 11:00 Poster A

Plasmonics in nanostructured organic solar cells — •Thomas Pfadler[1], Ricky Dunbar[1], and Lukas Schmidt-Mende[2] — [1]LMU Munich — [2]University of Konstanz

Organic solar cells have the potential to become an important low-cost alternative to conventional solar cells. However, before this can happen, the energy harvesting potential of organic solar cells must become more comparable with that of the pervading technology. This research is based upon the construction of organic solar cells that demonstrate highly favourable light-plasmonic coupling at a nanostructured silver electrode. These nanostructured silver electrodes are prepared via nanoimprint lithography (NIL) and optimised to improve the light harvesting and efficiency of organic thin-film solar cells. Given appropriate control of loss mechanisms such as interfacial recombination, the absorption enhancement will correspond to an increase in the solar cell efficiency.

CPP 24.2 Wed 11:00 Poster A

Ortho- and Terminal-substituted Perylene Diimides as Acceptor Materials for Organic Solar Cells — •Valentin Kamm, Glauco Battagliarin, Ian A. Howard, Michael Hansen, Hans W. Spiess, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institute for Polymer Research, Mainz, Germany

Perylene diimide (PDI) is a promising electron acceptor material for high open circuit voltage bulk heterojunction organic solar cells. However, many PDI molecules have the tendency to strongly aggregate leading to intermolecular excited state formation that can result in exciton trapping.[1] Recently, a method for substitution at the ortho-position of the PDI core was introduced giving access to novel acceptor molecules.[2] The substitution affects the stacking and therefore the charge carrier mobility and excited state energies and dynamics. In this contribution we present the excited state and intermolecular packing of a series of PDI molecules with different substitution patterns at the terminal- and ortho-position investigated by time-resolved photoluminescence and solid-state NMR techniques.

[1] I. A. Howard, F. Laquai, P. E. Keivanidis, R. H. Friend, N. C. Greenham, J. Phys. Chem. C, 2009,113, 21225-21232. [2] Glauco Battagliarin, Chen Li, Volker Enkelmann, and Klaus Müllen, Organic Letters, 2011,13,3012-3015.

CPP 24.3 Wed 11:00 Poster A

Photophysical Characterisation of Novel Polymeric Absorber Materials for Organic Solar Cells — •Hannah Mangold[1], Ian A. Howard[1], Ralf Mauer[1], Silvia Janietz[2], and Frédéric Laquai[1] — [1]MPI for Polymer Research, Mainz, Germany — [2]Fraunhofer IAP, Potsdam, Germany

The power conversion efficiency of organic solar cells has significantly increased in the last year as the old benchmark poly(3-hexylthiophene) (P3HT) has been surpassed by novel donor-acceptor polymers with enhanced absorption in the near-infrared region of the solar spectrum. We investigate terpolymers synthesized with different contents of dialkyl substituted diphenyl-benzopyrazine or diphenyl-thienopyrazine, which determine the optical properties of the materials, and triphenylamine units that should determine the charge transport properties of the material by acting as the hole conductor. Using ultrafast transient absorption we see that the hole indeed transfers to the triphenylamine unit, validating the approach of simplifying material property optimization by decoupling the role of light absorption and hole transport within a single polymer backbone. We achieve open circuit voltages approaching 1V and power conversion efficiencies of 3%, demonstrating the potential of this class of terpolymer. However, the inclusion of the triphenylamine unit does not enhance device performance, and based on light intensity dependent measurements, we attribute this observation to an increase in carrier trapping. Therefore, we demonstrate that it is possible to achieve independent control of light absorption and transport properties with the three monomers of a terpolymer.

CPP 24.4 Wed 11:00 Poster A

Photophysical investigation of core-enlarged rylene dyes for solid state dye-sensitized solar cells — •Yoojin Kim, Michael Meister, Ian A. Howard, Belinda Nölscher, Glauco Battagliarin, Denis Andrienko, Chen Li, Klaus Müllen, and Frédéric Laquai — MPI for Polymer Research Mainz

Perylene derivatives used as sensitizers in solid state dye-sensitized solar cells have attracted a lot of interest owing to their high molar extinction coefficients and broad absorption spectra. However, their absorbance is limited to the visible spectral region. By enlarging the perylene core with additional naphthalene units, the absorption can be extended to the near infrared region. However, devices employing such core-enlarged rylene dyes and an anhydride as anchoring group do not necessarily show higher efficiencies. In this study, the photophysical properties of rylene films in device structures are examined using quasi steady-state photoinduced absorption (PIA) and time-resolved photoluminescence spectroscopy. In presence of the hole transporter Spiro-MeOTAD, we observe a Stark effect in the PIA that suggests a change in the direction of the dipole moment unfavorable for charge separation. This change most probably originates from ring opening of the anhydride group during adsorption to the metal oxide, which is also supported by first-principles (TD-DFT, B3LYP) calculations. However, we note that moderate charge generation and regeneration of the dyes are still observed. By relating our results to solar cell performance we point out the factors which reduce the performance after the spectral response is extended to the infrared region.

CPP 24.5 Wed 11:00 Poster A

Impedance measurements on organic solar cells based on DIP and C_{60} — •Theresa Linderl, Stefan Grob, Julia Wagner, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Impedance spectroscopy (IS) has turned out to be a powerful tool to study organic semiconductor devices by measuring differential resistances and capacitances. Recently, it was shown that a connection can be established between recombination and series resistances extracted from IS and current-voltage (j-V) curves of polymer solar cells [1]. IS bypasses the influence of the photocurrent, which is assumed to be constant and measures directly the recombination current, that in turn can be used to understand the shape of the j-V curve of a solar cell. In this contribution we apply this method to describe organic solar cells based on diindenoperylene (DIP) and the fullerene C_{60}. By comparing results of IS measurements of planar- and bulk-heterojunction solar cells we investigate the effect of charge carrier recombination on organic solar cell performance.

[1] P. P. Boix et al., Adv. Eng. Mater. 1 (2011) 1073.

CPP 24.6 Wed 11:00 Poster A

Structural, morphological and electrical characterization of organic donor-acceptor photovoltaic cells based on diindenoperylene (DIP) and C_{60} — •Mark Gruber[1], Monika Rawolle[2], Julia Wagner[1], Alexander Hinderhofer[3], Andreas Opitz[4], David Magerl[2], Jan Perlich[5], Stephan V. Roth[5], Frank Schreiber[3], Peter Müller-Buschbaum[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg — [2]TU München, Physik Department, Garching — [3]Fakultät für Physik, Universität Tübingen — [4]Institute of Physics, Humboldt University, Berlin — [5]HASYLAB at DESY, Hamburg

Due to a variation of the substrate temperature during film deposition, the structure and morphology of DIP and C_{60} layers are changed perceptibly. Atomic force microscopy (AFM) images reveal larger lateral grains of both materials for elevated substrate temperatures. With grazing incidence small angle X-ray scattering (GISAXS) measurements we can show that the mean lateral domain distance within the volume of the DIP film increases in the same way as the surface grain size. The vertical domain size of DIP is determined by X-ray diffraction (XRD) measurements, pointing towards coherently ordered domains with a height corresponding to the whole DIP layer thickness. C_{60} on top of DIP forms domains which are twice as large for an increase of substrate temperature during evaporation from room temperature to 100 °C. To demonstrate the effect of enhanced crystallization on planar and planar-mixed organic solar cells, we characterized comparable devices utilizing DIP as donor and C_{60} as acceptor.

CPP 24.7 Wed 11:00 Poster A

Contact and injection properties of organic planar heterojunction solar cells studied by transient current methods —

•Lena Reichardt, Ulrich Hörmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Contact properties and charge carrier injection behavior of organic planar heterojunction solar cells have been investigated by means of complementary transient current methods. Charge extraction by linearly increasing voltage (CELIV) at different initial DC bias and impedance spectroscopy (IS) reveal that, depending on the contact properties, injection either of both charge carrier types at the same time or of one type prior to the other one may occur. This corresponds to the injection behavior of poly(3-hexylthiophene)/fullerene (P3HT/C_{60}) and P3HT/diindenoperylene (P3HT/DIP), respectively with PEDOT:PSS and BCP/Al as contacts. Both CELIV and steady state measurements on P3HT/C_{60} directly indicate injection currents in forward direction. By contrast, measurements on P3HT/DIP result in transient current signals of CELIV measurements at bias voltages where no injection current is seen in steady state measurements. The presence of injected charges in both cases is confirmed by IS which exhibits a change in device capacitance with bias voltage. The ability to deliberately influence the presence of injected charges by contact modification might be helpful to determine the mobility of a specific charge carrier type by (dark) CELIV or to prevent unfavorable injection under forward bias in photo-CELIV measurements.

CPP 24.8 Wed 11:00 Poster A

Characteristics of the excitonic processes in molecular donor/acceptor bilayers

— •A.K. Topczak[1], A. Steindamm[1,2], M. Brendel[1], P. Schütz[1], and J. Pflaum[1,2] — [1]Exp. Phys. VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — [2]ZAE Bayern e.V., D-97074 Würzburg

Knowledge of the exciton transport in molecular thin films is of great importance for organic photovoltaic (OPV) applications. We address this issue by Photoluminescence (PL)-Quenching measurements on the molecular semiconductor Diindenoperylene (DIP) in combination with different acceptor (C_{60}, Phthalocyanine) and excitonic blocking (BPhen) materials both of relevance for OPV devices. This technique yields detailed information on the exciton diffusion length, which can be significantly enhanced for highly crystalline materials, and on the exciton dissociation probability at suited donor/acceptor interfaces. As will be demonstrated the latter strongly depends on the respective material combination in correlation with interface morphology and trap states. Furthermore, DIP-PL variation can be attributed to exciton dissociation, recombination or reflection at the respective interfaces. For the case of DIP/C_{60} bilayers, the dissociation efficiency amounts to 90% rendering recombination losses in this bilayer structure almost negligible. To further enhance charge carrier generation in DIP/C_{60} bilayer cells the impact of a BPhen exciton blocking layer was analysed via PL-measurements. By this approach effects by metal penetration and exciton reflection on exciton harvesting and therefore on the macroscopic device performance can be discriminated.

CPP 24.9 Wed 11:00 Poster A

Femtosecond Transient Absorption Spectroscopy of PTB7/PCBM Blend Systems

— •Benjamin Müller[1], Björn Gieseking[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Due to their low fabrication costs bulk heterojunction organic solar cells show great potential for photovoltaic applications. The actual certified well working solar cell comprised of the copolymer PTB7 and $PC_{71}BM$ acceptor reaches an efficiency of more than 7% reflecting the remarkable progress in this field [1]. However, recent studies indicate that the device performance strongly depends on the morphology of the active layer and is very sensitive to sample preparation [2].

In this work we investigate the influence of solvent additive on the photophysical properties of PTB7:$PC_{71}BM$ blend films by applying picosecond timeresolved photoluminescence spectroscopy and femtosecond transient absorption spectroscopy. The experimental results are discussed in terms of the influence of the morphology on exciton diffusion and charge carrier photogeneration.

[1] Liang et al., Advanced Energy Materials 2010, 22 [2] Chen et al., Nano Letters 2011, 11, 3707-3713

CPP 24.10 Wed 11:00 Poster A

Open-Source-Code for Numerical Drift-Diffusion Simulations of Organic Solar Cells

— •Janine Fischer, Wolfgang Tress, Karl Leo, and Moritz Riede — IAPP, TU Dresden

Organic photovoltaics have recently made impressive progress by reaching efficiencies up to 10%. The versatility of the accessible materials demands for simulation tools explaining and predicting material properties that allow for a specific donator/acceptor synthesis. Numerical drift-diffusion-simulations have repeatedly shown to well reproduce experimental data and provide a powerful tool for the interpretation of measured J-V-curves. Here, we present an open-source-code for device-simulations of multilayer - bulk as well as planar heterojunction - organic solar cells. Our C++-based algorithm iteratively solves the discretized differential equation system comprising the continuity equations for electrons and holes, drift and diffusion currents, as well as the Poisson equation for space-charges caused by free charge-carriers and localized ionized dopants. In particular it also deals with non-linearities introduced by effects such as the field and/or temperature dependence of the mobility, different recombination mechanisms, or various trap distributions which can each be selected individually according to the device design. Additionally, automated parameter variations are enabled.

CPP 24.11 Wed 11:00 Poster A

Polyethylene induced structural modification in polymer blends used in photovoltaic cells

— •Ammara Akhtar, Eva M. Herzig, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Photovoltaic cells consisting of organic semiconducting polymer poly(3-hexylthiophene) (P3HT): fullerene derivative PCBM blends have attracted much interest over the last two decades. In order to improve the morphology of organic materials in solar cells, a third component such as the commodity polymer polyethylene can be introduced. It is reported that among different commodity polymers, high density polyethylene (HDPE) is a promising material for organic solar cells because of an observed improvement in the photocurrent generation efficiency of the system [1]. Furthermore, it is also expected that, the use of HDPE instead of low density polyethylene (LDPE) provides a better control to the microstructure in the final photovoltaic cell because of its highly crystalline nature [2]. In order to improve the interfacial morphology of the P3HT:PCBM blend by adding HDPE spin coating at elevated temperature is necessary. A structural analysis of the ternary system is being carried out with the aid of spectroscopy and scattering experiments. [1] Ferenczi et al., Adv. Mater. 23, 4093 (2011) [2] Goffri et al., Nat.Mater. 5, 950 (2006)

CPP 24.12 Wed 11:00 Poster A

The morphology of flexible all polymer solar cells

— •Weijia Wang[1], Matthias A. Ruderer[1], Ezzeldin Metwalli[1], Shuai Guo[1], Kai Scherer[1], Stephan V. Roth[2], Jan Perlich[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany — [2]HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

The interest in photoactive polymers and its applications in organic photovoltaics increased in the last decades dramatically due to promising properties such as mechanical stability, light weight, easy processibility and low cost compared to traditional inorganic solar cells. There have been already many studies on organic solar cells, but only little attention has been focused on fully flexible organic solar cells so far. Carbon nanotubes (CNT) are among the most promising candidates of flexible electrode materials, which can be deposited on flexible PET substrates. In this work, CNT/PET substrates are used as electrodes for solar cells. The CNT/PET substrates are characterized with transmission and resistance measurements. The substrates are coated with an electron blocking layer PEDOT:PSS which is modified by methanol to better wet the substrate. The morphology of the PEDOT:PSS layer is investigated with grazing incidence small angle X-ray scattering and atomic force microscopy methods and its thickness is measured with X-ray reflectivity.

CPP 24.13 Wed 11:00 Poster A

Influence of PSS on the Morphology of P3HT:PCBM Solar Cells

— •Anna Naumann, Eva M. Herzig, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

In organic photovoltaics the combination of poly(3-hexylthiophene) (P3HT) and PCBM for the active layer is very promising, but there are still many attempts for further improvement of device efficiency. One approach is to add a third component, like in this case polystyrenesulfonate (PSS), which can increase the performance by almost 30% compared to the reference P3HT:PCBM-cell [1]. PSS is an ionomer, which is neither conductive nor absorbent, hence it has to influence the morphology of the P3HT:PCBM-blend. In our study we analyze the film surface and the crystallization behavior of spin-coated thin films with different mixing ratios with the aid of optical microscopy, atomic force microscopy and x-ray diffraction, respectively. Furthermore, the interaction between substrate and film is of great interest, so an investigation of accumulation layers in the blend is made with reflectivity measurements.

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

CPP 24.14 Wed 11:00 Poster A

Comparing the device performance of organic light-emitting diodes processed from solution — •Benedikt Stender[1], Maximilian Nothaft[2], Jörg Wrachtrup[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius-Maximilian-University of Würzburg, D-97074 Würzburg — [2]3rd Physics Institute and Research Center SCoPE, University of Stuttgart, D-70550 Stuttgart — [3]ZAE Bayern, D-97074 Würzburg

The feasibility of inkjet-printing offers great advantageous in terms of reduced recombination losses and controlled positioning of solution processed organic light-emitting-diodes (OLEDs). However, due to inherent effects of droplet formation and the sensitivity on printing conditions, it still remains challenging to obtain films of similar quality as from spin-coating. For this purpose, the device performance of poly(para-phenylene-vinylene) OLEDs prepared by spin-casting and inkjet printing is compared with respect to structural and opto-electronic characteristics. As we will demonstrate, by choosing suited sets of preparation parameters, inkjet printed PPV-OLEDs of similar performance can be achieved, thereby paving the way towards innovative devices based on local doping of the emission layer with single molecules.

CPP 24.15 Wed 11:00 Poster A

Excitonic lifetime changes in organic light-emitting diodes induced by triplet-polaron-quenching — •Sebastian Wehrmeister, Tobias Daniel Schmidt, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Although organic light emitting diodes (OLEDs) have matured in technical applications in recent years they still have not reached high efficiencies. The external quantum efficiency (EQE) and thereby the luminous efficacy is limited by multiple effects, such as low outcoupling efficiency, energy dissipation to surface plasmons and waveguided modes, unbalanced charge carrier ratio and quenching induced non-radiative energy losses especially at high brightness. However, to distinguish between triplet-triplet-annihilation and triplet-polaron-quenching, the two major quenching processes at high brightness, time-resolved measurements under combined electrical and optical excitation have been performed [1]. In our experiments we examine the effect of triplet-polaron quenching on excitonic lifetimes in a phosphorescent OLED with fac-tris(2-phenylpyridine)iridium(III) (Ir(ppy)$_3$) as emitter. We probe exciton lifetime in the steady-state region of a rectangular electric pulse by a short laser pulse on top. In order to achieve reliable data we have continuously increased the current density of the electrical pulse resulting in an exponential decrease of the excitonic lifetime and thus a decrease in the EQE.

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

CPP 24.16 Wed 11:00 Poster A

Microscopic charge transport simulations in P3HT lamellae and P3HT:PCBM blends — •Carl Poelking and Denis Andrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Atomistic force fields for poly(3-hexylthiophene) (P3HT) and phenyl-C61-butyric acid methyl ester (PCBM) are parametrized using first-principles calculations. Lamellae of regioregular and regiorandom P3HT are then simulated using atomistic molecular dynamics. Microscopic simulations of charge transport in the resulting morphologies help to identify origins of energetic disorder leading to a different Poole-Frenkel behavior of regiorandom and regioregular P3HT. The role of polarization effects on the relative energy level alignment is then assessed for a P3HT:PCBM blend. Finally, we discuss the impact of energetic disorder on formation of a charge transfer state and efficiency of a P3HT:PCBM bulk heterojunction solar cell.

CPP 24.17 Wed 11:00 Poster A

In situ structural and electrical studies of P3HT droplet solidification — Linda Grodd, •Eduard Mikayelyan, Ullrich Pietsch, and Souren Grigorian — Solid State Physics, University of Siegen, Siegen, Germany

Due to it's good semiconducting properties poly(3-hexylthiophene) (P3HT) is a promising candidate for organic field effect transistors (OFETs). Thus, there is a lot of effort to understand a conduction mechanism and to tune the material properties to receive optimal performance of the final device.

In our studies we investigated the structural and electrical properties of P3HT during the solidification process from the solution to the thin film formation stage. P3HT/chloroform solution was dropped onto Si/SiO$_2$ substrates with source/drain electrodes to which a fixed voltage was applied. During solidification the structure was investigated by monitoring the (100) reflection and (020) reflection, respectively, using grazing incidence x-ray diffraction (GIXD). Simultaneously, the source/drain current was recorded.

Interestingly, the measurements revealed that the current was peaking just before the Bragg peak intensity had reached its final maximum at the constant level. This fact leads to the conclusion that not only crystalline order, represented by Bragg peak intensity, but the overall network connection is a key parameter for high conductivity.

We gratefully acknowledge the BMBF, Germany for financial support.

CPP 24.18 Wed 11:00 Poster A

Change of unit cell during the growth of Diindenoperylene (DIP) on polycrystalline gold followed by Grazing Incidence X-ray Diffraction — •Sebastian Bommel[1,2], Christopher Weber[2], Peter Schäfer[2], and Stefan Kowarik[2] — [1]HASYLAB at DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

Organic-inorganic semiconductor hybrid-structures are promising candidates for applications in opto-electronics, photovoltaics and sensing. The molecular structure at the organic-inorganic interface is crucial for the effectiveness of such devices. Here we report results of real-time and in situ grazing incidence X-Ray diffraction (GIXD) measurements for growth of the organic semiconductor diindenoperylene (DIP) on polycrystalline gold. By monitoring the evolution of unit cell we find that the cell parameters a, b, c and the angle beta change during growth. These unit cell changes are a strong indication of a change in molecular tilt for the molecular layers adjacent to the gold surface.

CPP 24.19 Wed 11:00 Poster A

Organic Heteroepitaxy of RGB Nanoneedles — •Martin Oehzelt[1], Clemens Simbrunner[2], Günther Schwabegger[2], Francesco Quochi[3], Ingo Salzmann[4], Antje Vollmer[1], Norbert Koch[1,4], and Helmut Sitter[2] — [1]HZB-BESSY II, Berlin, Germany — [2]Inst. Semincond. and Solid State Physics, JKU Linz, Austria — [3]Dipartimento di Fisica, Universita di Calgiary, Italy — [4]Institut für Physik, HU-Berlin, Germany

Self-assembly processes and organic-organic heteroepitaxy are powerful techniques to obtain highly ordered molecular aggregates. Here we demonstrate that combining both methods allows not only to fabricate highly crystalline and uniaxially oriented self-assembled nanofibers but also to tune their polarized emission. We show that submonolayer coverage of sexithiophene on top of para-sexiphenyl nanofibers is sufficient to change their emission color from blue to green. Triband emission in the red, green, and blue is generated in nanofibers with thicker sexithiophene coverage, where layers of co-oriented crystals are separated by green-emitting molecular sheets. The nanofibers were grown on a dielectric substrate mica and therefore the study of the electronic structure with photoemission is hampered due to sample charging. To solve this problem the same organic heterostructures were grown on HOPG (highly oriented pyrolytic graphite), as evidenced by x-ray diffraction as well as fluorescence measurements. The main difference, however, is that the fibers are not uniaxially oriented any more. Nevertheless, the color-tuning ability and also the crystal plane that makes contact to the substrate surface are preserved on HOPG when compared to mica.

CPP 24.20 Wed 11:00 Poster A

The influence of meso-phenyl torsion on the chemical properties of porphyrine — •Michal Wojdyr, Wichard Beenken, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Extension of the porphyrin π-system due to meso-substitution [1] leads to significant changes in the chemical behaviour of porphyrine: porphyrine as well as tetra-mesity-porphyrine can be protonated in a two-step mechanism, while only a one-step mechanism is observed if the meso-positions are bearing phenyl substituents rather than hydrogens or mesityl-groups. Only in case of phenyl substitution the π-system is extended. Therefore, the observed change in basicity may be attributed to electronic effects. However, the torsion of the phenyl against the porphyrine macrocycle induces torsion in the macrocycle too, which also might raise basicity of the porphyrine. To get deeper insights into the dependence of porphyrine basicity on π-conjugation and steric effects, various molecular properties were studied in dependence of the phenyl torsion of mono-protonated porphyrine bearing the phenyl group at one meso-position.

CPP 24.21 Wed 11:00 Poster A

Tuning the light induced charge separation in Ru(II) terpyridine complexes: a quantum chemical study — •Jakob Kreismann, Lars Winterfeld, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Ru(II) poly-pyridine complexes have proven their ability to act as photocatalysts, e.g., for the production of molecular hydrogen. One of the essential steps there is the initial charge transfer (CT) transition oxidizing Ru and reducing the ligand sphere, while recombination to the initial ground state should be minimized to maximize the efficiency of further charge transfer to a catalytic active site. In our study, we focus on the dependence of the initial CT on the electronic properties of the terpyridine ligands, which are bearing differently functionalized phenylens at the 4*-position. Using resonance Raman spectroscopy and density functional theory, we found that the CT extends to the functionalized phenylens even at the Franck-Condon point.

CPP 24.22 Wed 11:00 Poster A

Optics and electronic excitations in organic copper complexes from first-principles theory — •Martin Rohrmüller and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33098 Paderborn, 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 experimentally well characterised model systems μ-η^2:η^2-peroxodicopper(II) species (P) and the bis-μ-oxodicopper(III) species (O) [2].

We calculate the ground state as well as the optical response and electronic excitations of $[\mathrm{Cu_2(dbdmed)_2(O_2)}]^{2+}$ using (Time Dependent) Density Functional Theory and Many Body Perturbation Theory [3]. Particular attention is paid to the influence of the physical and numerical approximations (basis set, exchange-correlation functionals, spin structure) as well as the impact of environment (ligands, solvents).

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

[2] Mahadevan *et al.*, J. Am. Chem. Soc. 2000, **122**, 10249

[3] Onida *et al.*, Rev. Mod. Phys. 2002, **74** , 601

CPP 24.23 Wed 11:00 Poster A

Vibronic spectra of Frenkel excitons in a 2-dimensional polyacene lattice — •Peter Reineker[1], Ivan J. Lalov[1,2], and Thomas Hartmann[1] — [1]Institute for Theoretical Physics, Ulm University, 89069 Uln, Germany — [2]Faculty of Physics, Sofia University, Sofia 1164, Bulgaria

The vibronic spectra of Frenkel excitons (FEs) in a 2-dimensional lattice which models the (ab)-plane of polyacenes have been studied. The linear optical susceptibilities of the 2-dimensional crystal have been calculated using the Green functions method and the vibronic approach for the spectral ranges of FEs and their vibronic replicas. In the simulations of the vibronic spectra we use the excitonic and vibrational parameters of the crystals anthracene, tetracene and pentacene and obtain the linear absorption spectra in the excitonic and vibronic regions (FE plus one or several intramolecular vibrational quanta). The linear FE-phonon coupling is strong enough to create a bound or quasi-bound state of FE and one phonon, but it is not sufficient to bind the FE and more than one phonon. A hypothetical quadratic FE-phonon coupling makes the bound FE-phonon states more pronounced in the vibronic spectra. The strong transfer of the FE between two sublattices of the polyacene crystals widens the vibronic absorption lines.

CPP 24.24 Wed 11:00 Poster A

A quantum chemical study of the dependency of absorption properties on meso-substituent conformations of two different corrole NH-tautomers — •Philipp Keck, Wichard J. D. Beenken, Erich Runge, and Martin Presselt — TU Ilmenau, Ilmenau, Germany

Corroles, contracted tetrapyrrolic macrocycles lacking one meso-carbon atom, have emerged as attractive porphyrinoid materials for novel catalysts, antitumor treatment and imaging agents as well as active materials in the design of new sensors and optoelectronic devices. We are focussing on the dependency of the optical properties on meso-substituent conformations of two different tautomers, which were spectroscopically distinguished recently. Therefore, extensive density functional theory studies were performed employing the functional BP86 in conjunction with the "multipole accelerated resolution of the identity" approximation to achieve a linear scaling of the computational effort on the system size.

CPP 24.25 Wed 11:00 Poster A

Influence of the treatment of organic films on the blinking dynamics of embedded inorganic QDots — •Ines Trenkmann[1], Harald Graaf[2], and Christian von Borczyskowski[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]Kassel University, Institute of Chemistry and Center for Interdisciplinary Nanostructure Science and Technology, Germany

The possibility of tailoring properties of hybrid optoelectronic devices, such as light-emitting devices, by embedding inorganic quantum dots (QDots) in organic materials arouse more and more interest in the last years. Mainly the modification of optical properties of QDots due to interactions with the surrounding organic matrix is studied at the ensemble level.

At the same time, single particle studies of QDots reveal fluctuations of the emission intensity. This fluorescence intermittency, mostly denoted as blinking, is commonly explained by trapping of generated charges in the QDots shell and/or surrounding [1]. Only a few studies have analyzed the influence of an organic matrix on the optical properties of single inorganic QDots [2].

In this contribution, we show the variation of the optical properties of CdSe/ZnS-QDots embedded in thin TPD films. Thereby the focus lies on the influence of the film treatment on the blinking dynamics of single QDots and possible effects on the analytics of hybrid optoelectronic devices.

[1] C. Krasselt, et al. PCCP 2011, 13, 17084.

[2] H. Huang, et al. Nano Letters 2007, 7, 3781.

CPP 24.26 Wed 11:00 Poster A

The influence of voltage bias on charge carrier generation and recombination processes in oligothiophene-based organic solar cells — •Christian Koerner[1], Hannah Ziehlke[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany — [2]Institute of Organic Chemistry II and Advanced Materials, University of Ulm, Ulm, Germany

Dicyanovinyl end-capped oligothiophenes (DCVnT) have demonstrated their ability of achieving high power conversion efficiencies of up to 7.0% in a bulk heterojunction solar cell. Additionally, they act as an excellent model system to investigate the influence of systematical changes to the molecular structure on the thin film properties.

We use a sexithiophene derivative to investigate the influence of voltage bias on the charge generation and recombination processes in bulk heterojunction solar cells. Therefore, we combine the normal IV measurement with photoinduced absorption (PIA) spectroscopy. Using this method, we can investigate the long-living (μs-ms) excited species present after photoexcitation of DCV6T:C60 blends acting as photo-active layers in complete and working devices. With PIA, the generation and recombination behaviour of charged molecular states (polarons) are subsequently investigated for various voltage bias and illumination intensities.

CPP 24.27 Wed 11:00 Poster A

Influence of intermolecular gap and film morphology on the open circuit voltage of organic heterojunction solar cells — •Ulrich Hörmann[1], Julia Wagner[1], Mark Gruber[1], Andreas Opitz[2], and Wolfgang Brütting[1] — [1]Institute of Physics, University of Augsburg, Germany — [2]Institute of Physics, Humboldt University of Berlin, Germany

The efficiency of a photovoltaic cell is directly proportional to its open circuit voltage. This in turn is eventually set by the intermolecular gap, i.e. the energy of the donor-acceptor charge-transfer state in organic solar cells. In this contribution we introduce diindenoperylene (DIP) as a new molecular acceptor and compare it to C_{60} in planar heterojunction cells. Being able to deliberately change the morphology of the molecular films by varying the substrate temperature during the growth process, we demonstrate that the V_{oc} not only scales with the intermolecular gap but also strongly depends on the morphology of the organic films. We show that planar heterojunctions of thiophene derivatives and DIP yield extraordinarily high open circuit voltages of approximately 1.2 V for poly(3-hexylthiophene) and almost 1.4 V for heat treated α-sexithiophene [1]. Those values are close to the maximum V_{oc} attainable for these material systems.

[1] U. Hörmann *et al.*, phys. stat. sol. RRL 5 (2011) 241

CPP 24.28 Wed 11:00 Poster A

Triplet Exciton Formation and Electron Back Transfer in High-Efficiency Conjugated Polymer-Fullerene Blends studied by Optically Detected Magnetic Resonance — •Hannes Kraus[1], Stefan Väth[1], Andreas Sperlich[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg, Germany — [2]ZAE Bayern, D-97074 Würzburg, Germany

The properties of forward and backward electron transfer between (D)onor and (A)cceptor moieties of polymer-fullerene BHJ solar cells, are vital to the photovoltaic performance. The forward electron transfer is the essential part of efficient charge generation, while its backward counterpart can lead to formation of excitonic states with lower energy (e.g. triplet excitons, TE), culminating in complete loss of the excitation for power generation. We investigated the TE formation attributes of P3HT:PC_{60}BM and P3HT:Lu_3N@PCBEH, finding no triplets in the former, while the latter shows a distinct TE yield. This is conclusive with the relative positions of the energy levels of triplet excitons located on the polymer and the fullerene LUMO. To generalize this assumption, we investigated the D-A blends with different donor polymers and acceptor fullerenes using the optically detected magnetic resonance (ODMR), a method sensitive to the spin state and orientation of quasi-particles. The highly performing PTB7:PC_{70}BM was found to also exhibit both CT and triplet states, whereas P3HT:PC_{70}BM shows only CT state generation. We discuss these findings regarding the morphology and energy level driven electron back transfer.

CPP 24.29 Wed 11:00 Poster A

Charge transport and recombination dynamics in low-bandgap polymer:fullerene solar cells — •Andreas Zusan[1], Andreas Baumann[2], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

In the class of low-bandgap conjugated polymers PCPDTBT blended with PC_{70}BM is a promising candidate on the route towards highly efficient organic photovoltaics. The substitution of the bridging carbon atom by silicon (Si-PCPDTBT) is known to cause the formation of separated donor and acceptor phases and an enhanced power conversion efficiency. In this context the transport and recombination dynamics in PCPDTBT:PC_{70}BM and Si-PCPDTBT:PC_{70}BM bulk heterojunction solar cells were studied by the use of charge extraction by linearly increasing voltage (CELIV) under working conditions. We found an enhanced density of photogenerated charges as well as an increased effective charge carrier lifetime for Si-PCPDTBT:PC_{70}BM. The results are explained by the changes in morphology and can be directly linked to the raised device performance bridging the gap between nanoscale and application.

CPP 24.30 Wed 11:00 Poster A

Triplet excimer emission in CBP-derivatives — •Alexander Rudnick[1], Sebastian Hoffmann[1], Pamela Schrögel[2], Peter Strohriegel[2], and Anna Köhler[1] — [1]Uni Bayreuth, Experimentalphysik II — [2]Uni Bayreuth, Makromolekulare Chemie I

Carbazole-biphenyl-derivatives (CBP) are widely used as host matrix materials for efficient phosphorescent organic light-emitting diodes (OLEDs). For blue phosphorescence, a key requirement is a high energy of the triplet excited state, and no other decay channels. Here we have investigated the electronic and optical properties of two series of CBP derivatives using time-resolved fluorescence and phosphorescence measurements in combination with density functional calculations. We show that such materials form sandwich-type triplet excimer states at 2.5 eV that compete with the monomer triplet state at 3.0 eV and that are detrimental to OLED performance.[1] The broad excimer emission can be suppressed using three approaches, (i) by adding sterically demanding outer groups, (ii) by enforcing torsion of the central biphenyl group and (iii) by changing the position where the pendant carbazole is attached to the biphenyl moiety from a para- to a meta-connection.[2,3]

[1]ST Hoffmann et al, J. Phys. Chem. B, 2011, 115, 414-421

[2]P. Schrögel et al, J. Mater. Chem., 2011, 21, 2266-2273

[3]P. Schrögel et al, Organic Electronics, 2011, 12, 2047-2055

CPP 24.31 Wed 11:00 Poster A

Correlation between polymer architecture, mesoscale structure and photovoltaic performance in PAE-PAV:fullerene bulk-heterojunction solar cells — •S. Rathgeber[1], F. Kühnlenz[2], H. Hoppe[2], D.A.M. Egbe[3], S. Türk[4], J. Perlich[5], and R. Gehrke[5] — [1]University Koblenz-Landau — [2]Ilmenau University of Technology — [3]Johannes Kepler-University Linz, Austria — [4]Chemnitz University of Technology — [5]DESY.

A poly(arylene-ethynylene)-alt-poly(arylene-vinylene) (PAE-PAV) statistical copolymer carrying linear and branched alkoxy side chains along the conjugated backbone in a random manner, yields, compared to its regular substituted counterparts, an improved performance in polymer:PCBM bulk-heterojunction solar cells. GiWAXS experiments show that the improved performance of the statistical copolymer may be attributed to the following structural features: 1. Well, ordered stacked domains that promote backbone planarization and thus $\pi\pi$-overlap. 2. Partly face-on alignment of domains relative to the electrodes for an improved active layer electrode charge transfer. Branched side chains seem to promote face-on domain orientation. They might minimize their unfavorable contact with the interface by just bringing the CH_3 groups of the branches into direct contact with the surface so that favorable phenylene-substrate interaction can promote face-on orientation. 3. A more isotropic domain orientation throughout the active layer i.e. the backbone alignment direction has components perpendicular and parallel to the electrodes compromises between light absorption and intra-chain charge transport.

CPP 24.32 Wed 11:00 Poster A

Optical characterisation of highly ordered donor-acceptor films as fabricated by means of the Langmuir Blodgett technique — •Felix Herrmann[1], Sviatoslav Shokhovets[1], Harald Hoppe[1], Uwe Ritter[1], Rainer Beckert[3], Karl-Heinz Feller[2], Gerhard Gobsch[1], Erich Runge[1], and Martin Presselt[1] — [1]TU Ilmenau, Ilmenau, Germany — [2]University of Applied Sciences Jena, Jena, Germany — [3]Friedrich Schiller Universität, Jena, Germany

In organic solar cells the interface between electron donor and acceptor molecules is of crucial importance for charge separation, but is rather inhomogeneous and difficult to characterize in bulk-heterojunction organic solar cells. Therefore, we applied the Langmuir-Blodgett technique to tune the molecular ordering at the heterointerface of donor-acceptor bilayers up to more or less crystalline phases. The applied substances need to possess an amphiphilic structure to realize high surface pressures. As donor we used [6,6]-phenylC61-butyric acid and as donor a highly photostable thiazole derivative. The optical properties of these devices are characterizes by means of photothermal deflection and photoluminescence spectroscopy.

CPP 24.33 Wed 11:00 Poster A

Effect of doping on bias stress behavior of organic thin-film transistors — •Moritz Hein, Alexander Zakhidov, Moritz Riede, and Karl Leo — IAPP, TU Dresden

During the last few years, organic thin-film transistors have taken many important steps on their way into the market. By now they already reached a performance level that allows contributions in first applications such as backplanes for E-Ink-displays. An important problem regarding is the stability of the transistors during permanent gate bias stress. If the transistor operates on constant voltages for a longer period of time, the current flow between source and drain electrode is continuously reduced. This reversible degradation is found to be caused by a transport of charge carriers from the accumulation channel into the dielectric of the transistor and depends on the energy levels of both the dielectric and semiconductor. Hence, we compare the bias-stress effect for different organic semiconductors with given transistor geometry and silicon dioxide as dielectric material. Also we investigate the behavior of the characteristic transistor parameters before and after the bias-stress treatment. For the example of the system MeO-TPD on silicon dioxide, we show how the amplitude of the bias-stress effects can be reduced by weak doping of the semiconductor and a thereby induced shift of the Fermi energy.