

CPP 8: Poster: Organic Semiconductors

Time: Monday 17:30–19:30

Location: P2

CPP 8.1 Mon 17:30 P2
Spectroscopic Signatures of Anions on C60, C70 and C80 — ●MORITZ LIEDTKE^{1,2}, CARSTEN DEIBEL², and VLADIMIR DYAKONOV^{1,2} — ¹Energy Technology, Bavarian Centre for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany — ²Experimental Physics VI, Julius-Maximilian University of Würzburg, 97074 Würzburg, Germany

We applied photo-induced absorption technique to find the signatures of electrons on fullerenes in polymer:fullerene blends used for organic photovoltaic and pure fullerene layers. These negative charge carriers show different excitation energies into higher states which seem to depend only on the fullerene size and not on the sidechains of the fullerenes or the polymer used. The knowledge of these signatures might offer new insights in the process of charge carrier generation by exciting only the polymer in the blend while probing the electron on the fullerene.

CPP 8.2 Mon 17:30 P2
Temperature dependant investigation of charge-transfer states in P3HT:PC60BM studied by time resolved ESR — ●MAGDALENA ZAWADZKI¹, ANDREAS SPERLICH¹, HANNES KRAUS¹, CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — ²ZAE Bayern, D-97074 Würzburg

The time resolved ESR-technique (trESR) is a powerful tool to study the temporal evolution of charge-transfer states (CTS) photogenerated at the donor-acceptor interface. Right after the photoexcitation, spin-polarized radical pairs are formed in the system, showing themselves as an alternating pattern of microwave absorption and stimulated microwave emission (A/E/A/E). At longer timescales the pattern converts into pure absorption one (A/A) due to free charges in the blend. The separation dynamics within the pair as well as the thermalization are assumed to be dependent on the temperature. In this contribution, we report on temperature dependent trESR studies performed on thin films of P3HT:PCBM bulk-heterojunction.

CPP 8.3 Mon 17:30 P2
Morphology and electronic triplet states of regioregular P3HT and PCPDTBT ultrathin films — ●STEFAN VÁTH¹, HANNES KRAUS¹, ANDREAS SPERLICH¹, MARIO ZERSON², ROBERT MAGERLE², CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University Würzburg, D-97074 Würzburg — ²Chemische Physik, TU Chemnitz, D-09107 Chemnitz — ³ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg

The intensively studied donor polythiophene P3HT and the novel low band-gap donor-acceptor copolymer PCPDTBT are used in very well performing solution processed organic solar cells. Therefore, understanding the materials' electronic properties and in particular the influence of morphology on them is crucial for optimizing the device preparation as well as the synthesis of novel organic semiconductors. We gain access to the morphological bearing on the triplet state employing angle resolved optically detected magnetic resonance (ODMR) on very thin ordered films, a technique sensitive to the alignment of exciton triplet states. Furthermore we attempt to link these results with high resolution Nanotomography images of the film morphology.

CPP 8.4 Mon 17:30 P2
Multifrequency LESR of P3HT:C70 blends — ●JOHANNES RÖMER¹, ANDREAS SPERLICH¹, HANNES KRAUS¹, OLEG POLUEKTOV², CARSTEN DEIBEL¹, and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, D-97074 Würzburg — ²Chemical Sciences and Engineering Division, Argonne National Laboratory, Argonne, IL 60439, USA — ³ZAE Bayern, D-97074 Würzburg

For application in polymer bulk heterojunction solar cells, the blend of the polythiophene P3HT and the PC₇₀BM fullerene electron acceptor material is a promising model system, as C₇₀-derivatives are used in the most efficient organic solar cells.

Using high-frequency electron spin resonance (ESR), we were able to separate the signals of the positive polaron from the negative anion localized on the C₇₀-cage, and the involved g-tensor components could

be obtained. The focus of this work is the analysis of the main parameters of light induced ESR spectra obtained at different microwave frequencies, namely 9, 36, and 130 GHz.

CPP 8.5 Mon 17:30 P2
Investigation of recombination process in organic bulk heterojunction solar cells — ●JĘDRZEJ SZMYTKOWSKI — University of Saskatchewan, Saskatoon, Canada — Gdańsk University of Technology, Gdańsk, Poland

The mechanism of charge carrier recombination in organic solar cells is still under debate. Although Langevin model of bimolecular recombination is usually used with success, the experimental deviations from this theory have been observed. Recently, several different scenarios have been proposed for explanation. To make further progress, we have analyzed recombination coefficient as a function of several physical parameters. The obtained good agreement between theoretical and experimental results is promising.

CPP 8.6 Mon 17:30 P2
Effect of Nongeminate Recombination on Fill Factor in Polythiophene:Methanofullerene Organic Solar Cells — ●RALF MAUER, IAN A. HOWARD, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer Research, Mainz, Germany

A key factor in solar cell efficiency is the dependence of the photocurrent on applied bias. With respect to organic solar cells, it is often suggested that this factor is governed by the field dependence of charge-transfer state separation. Here we demonstrate that this is not the case in benchmark polythiophene:methanofullerene solar cells. By examining the temperature and light intensity dependence of the current voltage characteristics we determine that: 1) the majority of free charge generation is not dependent on temperature, and 2) the competition between extraction and recombination of free charges principally determines the dependence of photocurrent on bias. These results are confirmed by direct observation of the temperature dependence of charge separation and recombination using transient absorption spectroscopy and highlight that in order to achieve optimal fill factors in organic solar cells minimizing free carrier recombination is an important consideration.

CPP 8.7 Mon 17:30 P2
Charge Generation and Recombination in PCDTBT:PCBM Photovoltaic Blends — ●FABIAN ETZOLD, IAN HOWARD, RALF MAUER, MICHAEL MEISTER, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer Research, Mainz, Germany

Low-bandgap donor-acceptor copolymers have recently demonstrated their potential in bulk heterojunction organic solar cells. Among them, poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) blended with fullerene derivatives proved to be very efficient, yielding power conversion efficiencies in excess of 3 % even without postproduction annealing, which is typically applied to polythiophene:fullerene blends. We investigate exciton dynamics in pristine PCDTBT and charge carrier dynamics in as-cast and annealed blends with [6,6]-phenyl C₆₁ butyric acid methyl ester (PCBM) by transient absorption and time-resolved photoluminescence spectroscopy. We find that in PCDTBT:PCBM blends a large fraction of excitons undergoes ultrafast generation of free charge carriers as previously observed for other material systems including P3HT:PCBM. However, a fraction of interfacial charge transfer states is also created, which recombine geminately with a lifetime of 2.5 ns. By monitoring the recombination dynamics over the previously unobserved time range from 1 ns to 1 ms, we conclude that the device efficiency must be limited by geminate recombination and charge extraction.

CPP 8.8 Mon 17:30 P2
Morphological and Photophysical Characterisation of Novel Absorber Materials for Organic Solar Cells — ●HANNAH MANGOLD¹, SILVIA JANIEZ², INGO LIEBERWIRTH¹, MICHAEL MEISTER¹, IAN H. HOWARD¹, and FRÉDÉRIC LAQUAI¹ — ¹Max-Planck-Institut für Polymerforschung, Mainz, Germany — ²Fraunhofer Institut für Angewandte Polymerforschung, Potsdam, Germany

In this contribution new tailor-made fluorene based terpolymers are

investigated as absorber materials in organic solar cells. These terpolymers contain different contents of dialkyl-substituted diphenylbenzopyrazine or diphenyl-thienopyrazine and triphenylamine units and possess bandgaps between 1.3 and 1.8 eV. Power conversion efficiencies up to 3% with open circuit voltages close to 1 V are obtained in blends with [6,6]-phenyl C61 butyric acid methyl ester (PCBM) even without prior thermal treatment. The morphology of the blends is investigated by atomic force microscopy (AFM) and transmission electron microscopy (TEM) and correlated with the results obtained from I-V-measurements under simulated sunlight. Photophysical experiments such as steady-state photoinduced absorption (PIA) and transient absorption (TA) spectroscopy are employed to understand the effect of variation of the polymer structure on exciton dissociation and charge recombination. Using a combination of these methods the understanding of the structure-property-relationship of these materials is extended towards the molecular scale and the impact of molecular structure and processing conditions on charge generation, transport and recombination processes can be elucidated.

CPP 8.9 Mon 17:30 P2

Effects of 1,8-Diiodooctane and 1,8-Octanedithiol on the performance of low bandgap devices — ●VIDA TURKOVIC², SEBASTIAN ENGMANN², MIGUEL CARRASCO-OROZCO¹, HARALD HOPPE², and GERHARD GOBSCH² — ¹Merck Chemicals Ltd. Chilworth Technical Centre, University Parkway, Southampton SO16 7QD, UK — ²Technisches Universitaet Ilmenau, Fakultae fuer Mathematik und Naturwissenschaften, Institut fuer Physik, Experimentalphysik I, Weimarer Strasse 32, 98693 Ilmenau

We have tested the role of octanedithiol (ODT) and diiodooctane (DIO) on the performance of organic solar cells. They are known to contribute in improving the performance of the lowbandgap polymer PCPDTBT devices. We investigated their influence on the performance of other novel low bandgap polymers. Different amounts of ODT and DIO were added to different low bandgap polymer/PC70BM blend systems. Optical, morphological and electrical properties of solar cells are reported.

CPP 8.10 Mon 17:30 P2

Targeted Side Chain Substitution for Tuning the Photovoltaic Performance of Conjugated Polymers — ●S. RATHGEBER¹, D. BASTOS DE TOLEDO², F. KÜHNLENZ³, R. JADHAV³, G. ADAM⁴, H. HOPPE³, and D.A.M. EGBE⁴ — ¹Johannes-Gutenberg-University Mainz, Institute for Physics, Mainz — ²MPI Mainz, Polymer Physics, Mainz — ³TU Ilmenau, Institute for Physics, Ilmenau — ⁴Linz Institute for Organic Solar Cells, Johannes-Kepler-University Linz, Austria

We used targeted side chain (SC) substitution for tuning the performance of poly(arylene-ethynylene)-alt-poly(arylene-vinylene) (PAE-PAV) copolymers in polymer:PCBM bulk heterojunction (BHJ) solar cells. The layered structure (degree of order, inter-layer- and pi-pi-stacking distance) was systematically modified by linear alkyloxy- and/or branched 2-ethylhexyloxy SC substitution. We identified a correlation between polymer architecture, structural properties as investigated by x-ray scattering techniques, photophysical characteristics and photovoltaic performance in the device. Optimization led to a statistical copolymer, comprising linear and branched SC statistically distributed along the backbone. This material combines the benefits of linear- and branched-substituted polymers i.e. high supramolecular order in combination with good solubility at low volume fraction of isolating SC. It exhibits high charge carrier mobilities and high power conversion efficiencies of 3.8% in BHJ solar cells - the present state-of-the-art value for PAV-based materials. We consider this approach to be transferable to other material classes. (Macromolecules 2010, 43, 306; Macromolecules 2010, 43, 1261; J. Mater. Chem. 2010, 20, 9726)

CPP 8.11 Mon 17:30 P2

Effect of annealing processes on morphology of photoactive polymer layers for solar cell applications — ●WEIJIA WANG, MATTHIAS A. RUDERER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funkt. Mat., James-Frank-Str. 1, 85748 Garching, Germany

The interest in photoactive polymers and its applications in organic photovoltaics increased in the last decades dramatically. The promise of these materials for production of mechanical stable, light weight and easy processible organic solar cells at low cost make them especially interesting. Currently the major drawback is still the low efficiencies compared to standard inorganic solar cells and the short lifetime. It was found that morphology plays an important role in both areas.

Therefore the importance of structure control is crucial. We investigated the influence of different control parameters such as annealing and blending ratio on a bulk heterojunction systems based on a polythiophene derivative. The changes in structure were monitored with imaging methods such as AFM. The effect on molecular level is investigated by absorption and photoluminescence measurements.

CPP 8.12 Mon 17:30 P2

Solution Processed Organic Bulk Heterojunction Tandem Solar Cells — ●STEVE ALBRECHT and DIETER NEHER — Soft matter Physics, University of Potsdam, D-14476 Potsdam, Germany

One of the critical issues regarding the preparation of organic tandem solar cells from solution is the central recombination contact. This contact should be highly transparent and conductive to provide high recombination currents. Moreover it should protect the 1st subcell from the solution processing of the 2nd subcell. Here, we present a systematic study of various recombination contacts in organic bulk heterojunction tandem solar cells made from blends of different polymers with PCBM. We compare solution processed recombination contacts fabricated from metal-oxides (TiO₂ and ZnO) and PEDOT:PSS with evaporated recombination contacts made from thin metal layers and molybdenum-oxide. The solar cell characteristics as well as the morphology of the contacts measured by AFM and SEM are illustrated. To compare the electrical properties of the varying contacts we show measurements on single carrier devices for different contact-structures. Alongside we present the results of optical modeling of the subcells and the complete tandem device and relate these results to experimental absorption and reflection spectra of the same structures. Based on these studies, layer thicknesses were adjusted for optimum current matching and device performance.

CPP 8.13 Mon 17:30 P2

Charge Transfer Processes in Hybrid Solar Cells Composed of Amorphous Silicon and Organic Materials — ●SEBASTIAN SCHAEFER¹, TIM SCHULZE², LARS KORTE², and DIETER NEHER¹ — ¹Universität Potsdam, Inst. Physik u. Astronomie, Karl-Liebknecht-Strasse 24/25, 14467 Potsdam-Golm, Germany — ²Helmholtz Zentrum Berlin, Inst. für Silizium Photovoltaik, Kekuléstrasse 5, 12489 Berlin, Germany

The efficiency of hybrid solar cells composed of organic materials and amorphous hydrogenated silicon (a-Si:H) strongly depends upon the efficiency of charge transfer processes at the inorganic-organic interface. We investigated the performance of devices comprising an ITO/a-Si:H(n-type)/a-Si:H(intrinsic)/organic/metal multilayer structure and using two different organic components: zinc phthalocyanine (ZnPc) and poly(3-hexylthiophene) (P3HT). The results show higher power conversion- and quantum efficiencies for the P3HT based cells, compared to ZnPc. This can be explained by larger energy-level offset at the interface between the organic layer and a-Si:H, which facilitates hole transfer from occupied states in the valence band tail to the HOMO of the organic material and additionally promotes exciton splitting. The performance of the a-Si:H/P3HT cells can be further improved by treatment of the amorphous silicon surface with hydrofluoric acid (HF) and p-type doping of P3HT with F4TCNQ. The improved cells reached maximum power conversion efficiencies of 1%.

CPP 8.14 Mon 17:30 P2

Photophysical Study on Core-Enlarged-Rylendiimides and -Anhydrides for Dye Sensitized Solar Cells — ●BELINDA NÖLSCHER, MICHAEL MEISTER, IAN HOWARD, GLAUCO BATTAGLIARIN, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer Research, Mainz, Germany

Dye Sensitized Solar Cells (DSSCs) are promising devices for lightweight and cheap photovoltaic energy conversion. Up to now many different dyes have been synthesized to improve the efficiency of these solar cells. Investigation of the relation between the photophysical properties of the dyes and their performance in solar cells is required for a better understanding of the working principle of DSSCs.

In this contribution we present a photophysical study on novel core-enlarged-rylendiimides and -anhydrides [1]. By changing the core size or expanding the bay-position the absorption maximum can be tuned and further shifted into the red part of the solar spectrum. We employ transient and steady-state photoinduced absorption as well as time-resolved photoluminescence spectroscopy to investigate the dynamics of charge generation and recombination of these dyes in solid-state DSSCs. Theoretically a higher efficiency of core-enlarged dyes due to increased photon harvesting can be expected, however, it appears that

these dyes follow a different trend. Based on our results we draw conclusions for future material development of higher efficiency all-organic dyes for DSSCs.

[1] Synthesis and application of core-enlarged perylene dyes, Y. Avlasevich, C. Li, K. Müllen, *Journal of Materials Chemistry*

CPP 8.15 Mon 17:30 P2

Charge Generation and Recombination in Perylene Dye-sensitized Solar Cells — ●MICHAEL MEISTER, BELINDA NÖLSCHER, IAN HOWARD, HENRIKE WONNEBERGER, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer Research, Mainz, Germany

All-organic sensitizer molecules are interesting alternatives to replace the commonly used expensive Ru-complex dyes in dye-sensitized solar cells (DSC). Dyes with large extinction coefficients are especially interesting for solid state DSCs, which work better with thinner mesoporous TiO₂ structures. Perylene derivatives have attracted strong interest, since they combine a strong absorption with reasonably good device efficiencies if used with Spiro-MeOTAD as solid state hole transporter [1]. Here we present a photophysical study of perylene monoimide dyes (PMI) for DSCs with different functional groups attached to the core that influence the position of the HOMO and LUMO. By employing quasi steady-state photoinduced absorption spectroscopy and transient absorption spectroscopy on device-like structures, we gain insight into the mechanisms of charge generation and recombination. For instance, we found that a rise of the LUMO energy, which should in principle facilitate electron injection into the TiO₂, does not necessarily lead to more efficient charge separation. Our investigations aim to a thorough understanding of the structure-property-relationship of these PMI-based organic dyes in solid state DSCs.

1. Cappel, U.B., et al., *J. Phys. Chem. C*, 2009. 113(33): p. 14595-14597.

CPP 8.16 Mon 17:30 P2

Influence of different exciton blocking layers on device characteristics and solar cell degradation in a planar heterojunction DIP/C₆₀ solar cell — ●CHRISTOPH SCHUHMAIR, JULIA WAGNER, MARK GRUBER, ANDREAS OPITZ, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The application of exciton blocking layers (EBLs) in organic solar cells has become a well-established method to prevent exciton quenching at the acceptor/cathode interface. One of the most common exciton blocking materials is the organic semiconducting material bathocuproine (BCP), yet its precise working mechanism is not fully understood.

In this contribution we show the impact of two different EBLs (BCP and 1,4,5,8-Naphthalene-tetracarboxylic-dianhydride (NTCDA)) on the performance of planar heterojunction organic solar cells based on the donor diindenoperylene (DIP) and the fullerene C₆₀ as acceptor. The studies cover the influence of the EBL thickness and its impact on device degradation. Moreover, it is shown how substrate heating during deposition of the donor material influences the growth morphology of the donor and subsequent layers leading to distinct differences in device degradation.

CPP 8.17 Mon 17:30 P2

Design of a chamber for production and *in-situ* characterization of small-molecule photovoltaic cells — ●GIOVANNI LIGORIO, SIMEON LANGE, CHRISTOPHER LORCH, JENS REINHARDT, ALEXANDER HINDERHOFER, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen

The design and construction of an integrated ultra-high vacuum system to produce and characterize organic small-molecule solar cells is presented. Through the new system, it is possible to produce several solar cells simultaneously on the same ITO substrate via organic molecular beam deposition under vacuum conditions. *In-situ* electric contact is achieved through aluminum deposition. With the sample holder the temperature can be systematically modified between 200 K and 700 K while liquid nitrogen cooling or resistive heating to control the deposition process and to permit temperature dependent measurements.

We present first results for OPV cells of diindenoperylene (DIP)/C₆₀ (see Ref. [1] for complementary results) and DIP/perfluoropentacene (PFP).

[1] Wagner, J., et al., *Adv. Funct. Mater.*, doi: 10.1002/adfm.201001028

CPP 8.18 Mon 17:30 P2

Automatisierte elektrische und spektrale Charakterisierung organischer Solarzellenproben — ●ANDRÉ MERTEN, RONNY TIMMRECK, MORITZ RIEDE and KARL LEO — IAPP/TU-Dresden, George-Bähr-Straße 1,01069 Dresden

Organische Solarzellen basierend auf kleinen Molekülen stellen eine vielversprechende Möglichkeit für eine künftige kostengünstige Versorgung mit elektrischer Energie dar. Dazu muss jedoch deren Effizienz, welche für die besten Laborzellen mittlerweile bei 8,3% liegt noch erheblich gesteigert werden. Dies geschieht vor allem durch die Suche nach neuen Absorber und Transportmaterialien sowie Untersuchung des Einflusses der Morphologie. Dies erfordert systematische Variation des Stackaufbaus hinsichtlich Material, Schichtdicke und Dotierung sowie der Prozessierungsparameter und führt zu einer hohen Zahl zu charakterisierender Proben. Hoher Durchsatz, Genauigkeit und Zuverlässigkeit erfordert eine Automatisierung der elektrischen und spektralen Charakterisierung. Die dazu am Institut für Angewandte Photophysik entwickelten und eingesetzten Instrumente zur automatischen Charakterisierung von bis zu 144 Proben werden vorgestellt und an Beispielen demonstriert. Besondere Schwerpunkt sind dabei die Korrektur des Spektralen Mismatches, die Messung der spektralen Response von Einfach- und Tandemzellen, sowie die Bestimmung der Internen Quanteneffizienz unter Berücksichtigung von gemessener EQE, Absorption sowie simulierter Absorption der aktiven Schichten.

CPP 8.19 Mon 17:30 P2

Structure and morphology of organic donor-acceptor photovoltaic cells based on DIP and C₆₀ — ●MONIKA RAWOLLE¹, DAVID MAGERL¹, JAN PERLICH², STEPHAN V. ROTH², ANDREAS OPITZ³, MARK GRUBER³, JULIA WAGNER³, WOLFGANG BRÜTTING³, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funkt. Mat., James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, 22603 Hamburg, Germany — ³Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

A promising candidate for energy conversion utilizing organic semiconductors in small-molecule photovoltaic cells is diindenoperylene (DIP) as a new donor material in combination with the fullerene C₆₀ as an electron acceptor [1].

In this contribution we investigate the influence of substrate temperature on the domain size of thermally evaporated DIP and C₆₀ molecules in planar as well as in bulk heterojunctions. With Grazing-Incidence Small-Angle X-ray Scattering (GISAXS) information on horizontal and vertical structures are obtained. The real space structure information is measured with atomic force microscopy and compared with the reciprocal space investigations. Higher substrate temperatures allow growing of DIP films with higher crystallinity and increasing lateral structure sizes up to several 100 nm which serves as template for crystalline growth of C₆₀ in planar heterojunctions. Even in co-evaporated films large lateral structure sizes are observed giving a large scale phase separation.

[1] J. Wagner et al. *Adv. Funct. Mater.* (2010), early view.

CPP 8.20 Mon 17:30 P2

Structural investigations of liquid crystalline Perylene-diester benzimidazole — ●GAURAV GUPTA¹, MATHIS MUTH², PETER KOHN¹, THOMAS THURN ALBRECHT¹, and MUKUNDAN THELAKKAT² — ¹Institute für Physik Martin Luther Universität Halle — ²Applied Functional Polymer University of Bayreuth

Discotic liquid crystals typically comprise a rigid aromatic core and flexible peripheral chains where the structure of the core determines the optical and intramolecular electronic properties, while the flexible side chains are decisive for self assembly and processibility from solution. As part of a side chain polymer the electro-optical properties of the discotic can be combined with the mechanical, film forming properties of a polymer. We here present the structural and optical characterization of a new liquid crystal model compound Perylene-di-ester benzimidazole (PDBI) and its polymer (PPDBI) based on XRD, DSC, UV/Vis spectroscopy. In comparison to a common Perylene Bisimide and its side chain polymer, PDBI shows an extended absorption spectrum and a less ordered, columnar liquid crystalline phase.

CPP 8.21 Mon 17:30 P2

XRD investigation of organic disordered oligothiophene films — ●CHRIS ELSCHNER, ALEXANDR LEVIN, CHRISTIAN KOERNER, MORITZ RIEDE, and KARL LEO — IAPP, TU Dresden

Organic small molecule semiconducting devices are well suited for optoelectronic applications like OLED (organic light emitting diode) or OSC (organic solar cell). Here, we focus on the arrangement of the molecules in the organic thin film layers, especially in the case of structurally disordered films like mixed layers. Single layers tend to show a higher degree of crystallinity in comparison to mixed layers which are often amorphous. The tool for our investigations is X-ray diffraction in grazing angle geometry combined with the pair distribution function analysis, which gives information about the short-range order of amorphous matter as well as the long-range order in the case of crystalline matter. In detail, we investigate in C60 and oligothiophene single-layers and correlate these results with a 1:1 mixed layer of these materials. As result we obtain information on the loss of crystallinity and show micro-structural information about the arrangement of the molecules in the disordered layer.

CPP 8.22 Mon 17:30 P2

The role of molecular design for optimized morphology in organic solar cells — ●CHRISTOPH SCHUENEMANN, JOERG ALEX, JAN MEISS, WOLFGANG TRESS, KARL LEO, and MORITZ RIEDE — IAPP, TU Dresden

Diindenoperylene (DIP) is a well known organic semiconductor which is also an attractive absorber material for applications in small molecule organic solar cells. We have synthesized Ph4-DIP, a new derivative, consisting of the DIP core and four phenyl rings attached to the two indeno-groups. To compare these two similar molecules, DIP and Ph4-DIP, we characterize the morphology of thermally evaporated thin films using x-ray diffraction and atomic force microscopy. Pristine films and mixed layers with C60 (1:1 by volume) relevant for bulk heterojunction solar cells are deposited at different substrate temperatures. Whereas DIP forms highly crystalline pristine and DIP:C60 blend layers, Ph4-DIP is found to grow amorphous even at substrate temperatures of 110°C in pristine and Ph4-DIP:C60 blend layers. These results highlight the strong influence of the molecular design on the molecular arrangement in organic thin films. The stacking of the Ph4-DIP molecules is disturbed by the four phenyl rings that are tilted with respect to the flat DIP core. The DIP molecules without these phenyl rings, however, are able to stack very densely and form large crystallites. These morphological differences can explain the diverse performance of organic solar cells made from DIP and Ph4-DIP due to different exciton diffusion length and charge carrier mobilities.

CPP 8.23 Mon 17:30 P2

Influence of substrate heating on excited state generation rates and lifetime in organic solar cells studied by photoinduced absorption spectroscopy — ●HANNAH ZIEHLKE¹, CHRISTIAN KOERNER¹, ROLAND FITZNER², EGON REINOLD², PETER BÄUERLE², KARL LEO¹, and MORITZ RIEDE¹ — ¹IAPP, TU Dresden — ²Institut für Organische Chemie II und Neue Materialien, Uni Ulm

The performance of organic solar cells crucially depends on the separation of photogenerated excitons into free charge carriers. The dissociation process is sensitively influenced by the nanomorphology of donor (D) and acceptor (A) phases in the photoactive blend layer. Closed percolation paths have to be present such that the created charges are able to leave the blend layer, but also the crystallinity of the D- and the A-phase influence exciton dissociation on a molecular scale. Substrate heating during the vacuum deposition of the active layer is a method to influence the thin film morphology that can lead to improved device performance. We here characterize dicyanovinyl capped quinquethiophenes (D) deposited on substrates at different temperatures (30 and 80°C). Photoinduced absorption spectroscopy (PIA) is used to determine excited state lifetimes and generation rates. We find that efficient charge separation occurs in blends with C₆₀ (A) and identify the observed excited states as donor cations and triplet excitons. Heating the substrate results in an increased lifetime of the donor cation on the one hand and a decrease in the generation rate of cations on the other hand. The PIA results are complemented by solar cell devices as well as morphological studies.

CPP 8.24 Mon 17:30 P2

Influence of the exciton generation profile within the active layer on organic solar cell performance — ●WOLFGANG TRESS, MAURO FURNO, ANDRÉ MERTEN, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

As the device thickness of an organic solar cell (50...200 nm) is below the coherence length of sunlight, interference effects play an important role. An optimization of the solar cell stack is commonly done with re-

spect to high photocurrents. Here, we go one step further and analyse not only the integral effect of sun light absorption, but additionally the effect of the spatial absorption profile within a 50 nm thick ZnPc:C₆₀ bulk heterojunction device. The absorption profile is manipulated by applying transparent spacer layers with varied thicknesses. We observe a significant change of fill factor (*FF*) and a slight change of the open circuit voltage (*V_{oc}*), depending on the position of the absorption maximum in the layer. Simulation data of optical (transfer-matrix) and electrical (drift-diffusion) modelling explain this behaviour, which is mainly caused by an imbalance in charge carrier mobilities, that is determined by the blend composition. The effect can be enhanced by using spectrally narrow illumination via monochromatic LEDs to obtain a sharper generation profile in the active layer. Hence, the spatial absorption profile also explains the dependence of *FF* and *V_{oc}* on illumination colour in these devices. As consequence, the spectral mismatch factor, which is very important when properly characterizing an organic solar cell under simulated sunlight, depends on the applied voltage.

CPP 8.25 Mon 17:30 P2

External and internal quantum efficiency determination of small molecule organic tandem solar cells — ●RONNY TIMMRECK, ANDRÉ MERTEN, DAVID WYNANDS, JAN MEISS, WOLFGANG TRESS, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany

Measuring external quantum efficiency (EQE) is an important method for characterizing solar cells. In addition to its relevance for the spectral mismatch correction of solar cells, it yields deep insight into different physical processes in solar cells because many different measurement parameters can be varied independently. Hence, especially for organic solar cells it is an important technique to get a better understanding of the underlying physics.

We perform systematic studies of the EQE of single and tandem heterojunction organic solar cells by varying the wavelength and intensity of the bias illumination. Furthermore, the bias voltage that is applied to the solar cell during measurement is varied such that for every working point of the solar cell IV-characteristics an EQE spectrum can be obtained. Both requires the use of lock-in techniques for detecting the current response of the solar cell to the chopped monochromatic light on top of the bias illumination.

Our results show a strong influence of the bias voltage on the EQE-spectrum implying that optimization of organic solar cells should be done considering EQE at maximum power point and not short-circuit. With our measurements, it is furthermore possible to independently determine the IV-characteristics of the subcells of a tandem solar cell.

CPP 8.26 Mon 17:30 P2

Water and oxygen induced degradation of small molecule organic solar cells — ●MARTIN HERMENAU¹, KION NORRMAN², FREDERIK KREBS², KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden, Deutschland — ²Risø National Laboratory for Sustainable Energy, Technical University of Denmark, Roskilde, Denmark

Small molecule organic solar cells are studied with respect to water and oxygen induced degradation by mapping the spatial distribution of reaction products to elucidate the degradation patterns and failure mechanisms.

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) and X-ray photoelectron spectroscopy (XPS) in conjunction with isotopic labeling using H₂¹⁸O and ¹⁸O₂ provides information on where and to what extent the atmosphere has reacted with the device. A comparison is made between the use of a humid (oxygen free) atmosphere, a dry oxygen atmosphere, and a dry (oxygen free) nitrogen atmosphere during testing of devices that are kept in the dark and devices that are subjected to illumination. It is found that water significantly causes the device to degrade. The two most significant degradation mechanisms are diffusion of water through the aluminum electrode resulting in massive formation of aluminum oxide at the Al/BPhen interface, and diffusion of water into the ZnPc:C₆₀ layer where ZnPc becomes oxidized. Finally, electrode diffusion is found to have no or a negligible effect on the device lifetime.

CPP 8.27 Mon 17:30 P2

Study of trap charge in bulk heterojunction organic solar cell structures using impedance spectroscopy — ●DEBDUTTA RAY, LORENZO BURTON, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062

Dresden, Germany

In this study we use impedance spectroscopy to directly observe and estimate the trap charge density in an operating organic solar cell. Since the carrier collection efficiency in an organic solar cell is directly proportional to the electric field present in the device, the electric field may undergo distortion in the presence of space/trap charge thereby affecting the short circuit current and the fill factor. Space charge formed by photogenerated carriers has been observed, albeit indirectly, from photocurrent-voltage (IV) characteristics until now. However, when using IV characteristics, the interpretation depends on the model used. Capacitance, on the other hand, is a direct measure of the spatial distribution of the electric field inside the device. In this work we measure the capacitance as a function of voltage and frequency in solar cells under illumination. The frequency dependence provides information regarding the energetic distribution of the trap charge. The voltage dependence yields estimation of the trap charge concentration. From experiments, we estimate the lower limit of the trap charge concentration to be approximately $6 \times 10^{16} \text{ cm}^{-3}$ in ZnPc/C60 bulk heterojunction solar cells. The photocurrent-voltage characteristics of the devices can be explained with the capacitance response and the data complements each other.

CPP 8.28 Mon 17:30 P2

Diindenoperylene derivatives as green donors for organic solar cells — ●FELIX HOLZMUELLER, JOERG ALEX, JAN MEISS, CHRISTOPH SCHUENEMANN, WOLFGANG TRESS, MARKUS HUMMERT, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

Clean energy production is one of the most challenging problems of this century. Organic solar cells (OSC) may contribute to a sustainable solution, providing a cost-efficient way to convert sunlight into electrical power. For high OSC performance, a full coverage of a broad part of the solar spectrum is necessary, which will require materials with blue, green, and red absorption.

Here, we present a series of diindenoperylene derivatives (DIPD) as green donors for OSC. We study the structure-property relationship by investigating their molecular properties and morphology of thin films, and then incorporating such materials into OSC.

Both type and size of DIPD sidegroups are found to significantly influence molecular stacking and absorption properties. We relate these results to OSC with C60 as acceptor with high open circuit voltages of around 1V and fill factors of up to 75%. The device efficiency is limited by the exciton diffusion length, which can be approximated from systematic thickness variations in flat heterojunction (FHJ) OSC. Bulk heterojunction and FHJ devices yield power conversion efficiencies of over 2% and are promising for application in tandem OSC with additional materials covering the red spectrum.

CPP 8.29 Mon 17:30 P2

Fluorinated hexaazatrinaphthylene (HATNA) derivatives as electron transport materials for organic solar cells — ●FRANZ SELZER¹, CHRISTIANE FALKENBERG¹, MARTIN BAUMGARTEN², MANUEL HAMBURGER², KLAUS MÜLLEN², KARL LEO¹, and MORITZ RIEDE¹ — ¹TU Dresden, Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01062 Dresden, Germany — ²Max Planck Institute for Polymer Research, 55128 Mainz, Germany

For optimizing small molecule organic solar cells the so-called p-i-n concept is a versatile approach. Here, the photoactive donor-acceptor heterojunction is sandwiched between a transparent p-doped hole transport layer and an n-doped electron transport layer. The transport layers not only facilitate the charge carrier extraction but also act as window layers shifting the maximum of the optical interference pattern to the absorbing layers. While there are a number of well suited hole transport materials, the choice of transparent electron transport materials (ETM) with high electron mobility and conductivity as well as thermal and morphological stability is very limited. Here, we present fluorinated hexaazatrinaphthylene (HATNA) derivatives as ETM in p-i-n type solar cells in comparison with the commonly used n-doped C60 or chlorinated HATNA. While C60 absorbs in the visible range of the sun spectrum, HATNA has an optical band gap of 2.9eV. Doping with either acridine orange base (AOB) or NDN1 (Novaled AG) leads to an increase of the conductivity by several orders of magnitude to $\sigma > 1 \cdot 10^{-6} \text{ S/cm}$. Finally, we show that it is possible to replace n-C60 in the solar cell stack by n-doped fluorinated HATNA.

CPP 8.30 Mon 17:30 P2

Infrared absorbing materials for organic solar cells —

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A contribution to the future power supply in the days of global warming and enhanced CO₂ emission might be the organic solar cells (OSC) as they provide a cost-efficient way to convert sunlight into electrical power. One way to improve OSC performance is to extend the absorption from the visible region of the solar spectrum (which can be harvested with current materials) into the infrared, a spectral region which is hardly used at the moment.

We incorporate a series of modified tin-phthalocyanines and different benz-annulated aza-bodipys as donor molecules into vacuum deposited SM-OSC, showing a thin film absorption above 700nm. We test different device configurations with C₆₀ as acceptor. To gain understanding of the structure-property relationships, we additionally investigate molecular donor layers using AFM and SEM, and we study the influence of substrate heating during evaporation. Despite low open circuit voltages of about 0.4 V, we believe that the materials may be good candidates for tandem devices with complementary absorption to enhance efficiency.

CPP 8.31 Mon 17:30 P2

Influence of the molecular structure of electron transport materials on the performance of organic solar cells — ●CHRISTIANE FALKENBERG, MARKUS HUMMERT, SELINA OLTHOF, CHRISTOPH SCHUENEMANN, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, TU Dresden, 01069 Dresden

The synthesis of new functional molecules is an important approach for improving the performance of organic electronic devices. Here, understanding the link between the molecular structure and the physical properties of the materials plays a key role. We present a series of small molecules with a naphthalenetetracarboxylic diimide core and different side groups. All materials are designed to be applicable as transparent electron transport materials (ETM) in p-i-n type organic solar cells. In particular, we investigate the influence of the side chain length on basic physical properties like absorption, energy level position, morphology, and the enhancement of lateral conductivity of vacuum deposited thin films by molecular n-type doping. The latter shows the largest variations ranging from $< 10^{-8} \text{ S/cm}$ (hexyl) to 10^{-4} S/cm (no side chains). Finally, we compare the performance of the synthesized materials as ETM in organic solar cells. Depending on the side chain length power conversion efficiencies of 0.01% to 2.1% are reached.

CPP 8.32 Mon 17:30 P2

Tetrapropyl-tetraphenyl-diindenoperylene derivative as new donor for organic solar cells — ●JAN MEISS, MARTIN HERMENAU, WOLFGANG TRESS, MARKUS HUMMERT, CHRISTOPH SCHUENEMANN, KARL LEO, and MORITZ RIEDE — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

We show a diindenoperylene derivative (P4-Ph4-DIP) as green donor for heterojunction organic solar cells (OSC). OSC are characterized by current voltage, EQE, and ageing measurements. Devices with C₆₀ as acceptor display very high fill factors FF of over 76% and open circuit voltages V_{OC} of 0.99V. A clear influence of donor thickness t_d on short circuit current density J_{SC} and FF is visible: with t_d = 9 nm, J_{SC} is enhanced from 1.8 mA/cm² (reference device with only C₆₀ as absorber) to 2.6 mA/cm², reaching FF = 75.7% with V_{OC} = 0.98 V ($\eta = 1.9 \pm 0.1\%$). At higher t_d of up to 63 nm, photocurrent and FF decrease, ultimately dropping below the characteristics of the reference device. We find an EQE of 23% at the position of the donor main absorption peaks (493 nm, 525 nm, and 568 nm), reaching highest efficiencies at t_d of 9-12 nm and then decreasing with higher t_d. We attribute this to a limited exciton diffusion length L_D in the donor: at high t_d, the material absorbs photons, but excitons do not reach the heterointerface for dissociation and thus cannot contribute to the photocurrent. By combining measured J(V) data with calculations, we show that L_D = (9±1) nm fits well to the experimental findings. Ageing experiments show that the resulting devices are highly stable when exposed to accelerated ageing.

CPP 8.33 Mon 17:30 P2

Nanowire Networks as a Transparent Electrode for Organic Solar Cells — ●CHRISTOPH SACHSE, YONG-HYUN KIM, LARS

MÜLLER-MESKAMP, and KARL LEO — Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, TU Dresden, 01062 Dresden, Germany

For a broad application of organic thin film solar cells, inexpensive roll-to-roll processing on flexible and lightweight substrates is desirable. On these flexible substrates, commonly used ITO electrodes do not show satisfying performance due to the brittle nature of anorganic oxides.

Among other alternatives, recently some promising results using silver-nanowires as a conductive layer were published [1]. Such close-meshed metal grids are capable of combining the high conductivity of metals with the transparency caused by low surface coverage. Ontop, the solution based process guarantees low manufacturing costs.

Here, we evaluate and improve this alternative electrode material for organic solar cells. We achieve suitable film homogeneities with a simple dip or spray-coating process on different substrates. After post-processing an ITO-like performance is obtained.

Apart from the optimization of the electrode parameters, the thin organic solar cell stack imposes special requirements on the electrode technology. Therefore, our established small molecule technology [3] is used to evaporate organic solar cells on the nanowire electrodes and measure their performance to find suitable combinations.

[1] J.-Y. Lee, et al., *Nano Lett.* 8, 689 (2008).

[2] M. Riede, et al., *Nanotechnology* 19, 424001 (2008).

CPP 8.34 Mon 17:30 P2

Alternative Electrode Concepts and Materials for Organic Solar Cells — •LARS MÜLLER-MESKAMP¹, CHRISTOPH SACHSE¹, YONG HYUN KIM¹, MICHAEL MACHALA¹, OLAF HILD², CHRISTIAN MAY², and KARL LEO^{1,2} — ¹Institut für Angewandte Photophysik, Dresdner Innovationszentrum Energieeffizienz, Technische Universität Dresden, George Bähr Straße 1, 01069 Dresden, Germany — ²Fraunhofer Institut für Photonische Mikrosysteme, Maria-Reiche Strasse 2 01109 Dresden, Germany

Organic photovoltaics, reaching efficiencies around 8% (Heliatek, Solarmer), have become a promising technology for future energy supply. It has the potential to be cost-effective, to use little material and to utilize advanced thin film production methods like roll to roll manufacturing. Requirements for producing such a low-cost and flexible product include a highly transparent, flexible electrode. Looking for alternatives to the dominant oxide electrodes, transparent, conductive electrodes were prepared by PEDOT:PSS deposited from solution, by deposition of metal nanowires, and by a combination thereof. As recently demonstrated by us, solvent treated PEDOT electrodes can be successfully integrated into OPV cells, showing similar performance than ITO. The application of conductive metal nanoparticles, e.g. silver nanowires as random mesh electrode is showing even better performance. Low sheet resistances and good transmission can be achieved in a percolation network of high aspect ratio nanowires with low space-fill ratios.

CPP 8.35 Mon 17:30 P2

Photolithography in the service of organic electronics — •ALEX ZAKHIDOV, HANS KLEEMANN, BJÖRN LÜSSEM, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Organic electronic materials have attracted interest due to their facile processing that creates tantalizing prospects for new fabrication techniques such as ink-jet printing to deliver materials only where needed. Photolithography, the gold standard process of the microelectronics industry, has received relatively little attention for the patterning of organics. The recent commercialization of organic light emitting diodes (OLEDs) in flat panel displays, however, involved their integration with silicon circuitry. Similar heterogeneous integration is envisioned in other emerging applications such as large area electronics. The ability to use photolithography to pattern all layers will enable simpler fabrication using already existing infrastructure, as well as the realization of device architectures currently not achievable using separate patterning techniques for organic and inorganic layers.

References:

1. Al.A. Zakhidov et al., *Adv. Mat.* 20, 3481 (2008)

2. J.-K. Lee et al., *J. Am. Chem. Soc.*, 130, 11564 (2008).

3. Y.-F. Lim et al., *J. Mater Chem.* 19, 5394 (2009).

4. P.G. Taylor et al., *Adv. Mat.* 21, 2314 (2009).

CPP 8.36 Mon 17:30 P2

White top-emitting OLEDs using organic colour-conversion

layers for improved colour-stability — •TOBIAS SCHWAB, SIMONE HOFMANN, MICHAEL THOMSCHKE, BJÖRN LÜSSEM, and KARL LEO — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01069 Dresden

In contrast to white organic light-emitting diodes (OLEDs) using several vertical stacked emitters [1], the principle of down-conversion gives the chance to achieve white light with a simplified layer structure and enhanced colour stability by preventing a colour shift over lifetime due to differential aging of dyes. We investigate an approach where the conversion material is integrated into a top-emitting OLED structure in a way, that only electrons can pass this layer. This assures optical excitation and avoids unwanted electrical recombination inside the conversion layer. The emission spectra, CIE-coordinates, efficiencies, and IV-characteristics depending on the conversion layer thickness have been determined and were compared to the non-emitting host-material with similar optical properties. Lifetime measurements show that these OLEDs have almost no colour change over an investigated period up to 2200 hours. It is shown that the external quantum efficiency of the OLED does not necessarily decrease with an increased conversion layer thickness, even if the photoluminescence quantum yield of these materials is below unity. This indicates that the efficiency is improved by out-coupling of isotropic re-emitted wave-guided modes.

[1] Reineke, S et al.: White organic light-emitting diodes with fluorescent tube efficiency, *Nature*, 2009, **459**: 234-238

CPP 8.37 Mon 17:30 P2

Determination of molecular dipole orientation in organic films — •CHRISTIAN MAYR, JÖRG FRISCHEISEN, and WOLFGANG BRÜTTING — University of Augsburg, Institute of Physics, Germany

Organic light-emitting diodes (OLEDs) have been investigated for 20 years standing now at the frontier to mass production. Current research focuses on the enhancement of light outcoupling efficiency which is reduced especially by the excitation of surface plasmons (SPs) at the interface to the cathode. The orientation of molecules in films used in OLEDs has a huge effect on the coupling to SPs. Numerical simulations show that a horizontal molecular orientation with respect to the substrate can enhance the efficiency by up to 50%.

An expeditious method to determine the orientation of the transition dipole moment of molecules has been developed using angular dependent photoluminescence spectroscopy. By comparing measurement with simulations, the orientation can be quantitatively determined. Although other methods to measure molecular orientation exist, the presented method makes it not only possible to study molecular orientation in neat thin films but also of small amounts of emitters doped into a matrix material without knowing any information of the optical properties of the dopant. Hence, this method is particularly useful for the investigation of newly developed materials. Measurements of the phosphorescent emitter Ir(ppy)₃ doped into a CBP-matrix and of other neat and doped organic materials have been performed. With this method a deeper understanding of OLEDs and possibilities to enhance light outcoupling can be gained.

CPP 8.38 Mon 17:30 P2

A High Gain and High Charge Carrier Mobility Indenofluorene-Phenanthrene Copolymer for Light Amplification and Organic Lasing — •HUN KIM¹, NIELS SCHULTE², GANG ZHOU¹, KLAUS MÜLLEN¹, and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²Merck KGaA - Dept. OLED PC/CP, Frankfurt am Main, Germany

The combination of excellent luminescence properties, high chromophore density and partially high charge carrier mobility makes conjugated polymers suitable candidates for optically and electrically pumped light amplifiers and organic lasers. In this contribution we introduce a novel class of copolymers based on the poly(indenofluorene) backbone and investigate their photophysical as well as optoelectronic device properties. In particular, we used time-resolved optical spectroscopy to study their excited state energies and lifetimes as well as amplified spontaneous emission (ASE) characteristics in slab waveguide structures. Charge carrier mobilities were investigated by the time of flight (TOF) technique. All materials were additionally tested in organic light emitting diodes to characterize their electroluminescence efficiencies. We demonstrate that copolymers based on the poly(indenofluorene) backbone can achieve previously unprecedented gain values of about 155 cm⁻¹ in combination with very high hole mobilities of up to 10⁻² cm²/Vs and very high electroluminescence efficiencies. This makes them ideal materials for organic lasing.

[1] H. Kim, N. Schulte, G. Zhou, K. Müllen, F. Laquai, *Adv. Mater.*,

2010, accepted

CPP 8.39 Mon 17:30 P2

Deep Insight into the Spectroscopic Properties of a High Mobility n-type conjugated Polymer with Implications on Morphology and Charge Transport — ●ROBERT STEYRLLEUTHNER¹, MARCEL SCHUBERT¹, ZHIHUA CHEN², ANTONIO FACCHETTI², and DIETER NEHER¹ — ¹Universität Potsdam, Germany — ²Polyera Corporation, USA

Electrical properties of conjugated polymers are severely influenced by the morphology of the semiconducting layer. Recently, Facchetti and coworkers reported a novel n-type polymer (Polyera ActivInk N2200) with an exceptionally high electron field-effect-mobility of up to 0.85 cm²/Vs. We could already show that the bulk mobility in this material is indeed high, though electron injection is contact limited for all used low work function cathodes. While it was initially believed that layers from N2200 are amorphous, X-ray studies by Rivnay et al. on N2200 showed an exceptional in-plane order with distinct "pi-stacking" of the naphthalene diimide cores. The purpose of our work was to study the morphology of N2200 layers prepared from different solvents and annealed at different temperatures. Information on the chain packing and layer structure was obtained by performing UV-Vis absorbance, photoluminescence, AFM and SNOM measurements on thin films and solutions. We could identify distinct absorbing species and assign them to intrachain charge-transfer excitons in the amorphous phase and to interchain excitations on aggregated chains. On this basis, conclusions regarding the morphology of the semicrystalline films are drawn and related to bulk charge transport properties.

CPP 8.40 Mon 17:30 P2

Excitonic coupling in poly(3-hexylthiophene)s - molecular weight and polydispersity effects. — CHRISTINA SCHARSICH¹, ANNA KÖHLER¹, ●RENÉ KALBITZ², DIETER NEHER², RUTH LOHWASSER³, MUKUNDAN THELAKKAT³, MICHAEL FORSTER⁴, SYBILLE ALLARD⁴, and ULLRICH SCHERF⁴ — ¹Universität Bayreuth, Experimentalphysik II, 95447 Bayreuth, Germany — ²Universität Potsdam, Physik weicher Materie, 14476 Potsdam-Golm, Germany — ³Universität Bayreuth, Makromolekulare Chemie I, 95447 Bayreuth, Germany — ⁴Universität Wuppertal, Makromolekulare Chemie, 42119 Wuppertal, Germany

The photophysical and electronic properties of regioregular poly(3-hexylthiophene) (P3HT) are of great interest for many applications in the field of organic semiconducting materials such as solar cells and field-effect transistors. Recent research has shown that the charge carrier mobility in P3HT depends not only on the molecular weight, but also on the conformation of the polymer backbone. This was attributed to differences in the intermolecular coupling that exists in weakly aggregated P3HT chains.

By means of absorption and photoluminescence measurements in solution in combination with a Franck-Condon analysis, we determine quantitatively how the coupling strength between the chains and the fraction of aggregated chains formed depend on molecular weight, polydispersity and solvent quality. We use these data to determine the chain conformation in solution. For thin films, we show that we can control the resulting film morphology by pre-aggregates formed in solution.

CPP 8.41 Mon 17:30 P2

Temperature and Molecular Weight Dependent Structures In Poly(3-hexyl thiophene) — ●JENS BALKO¹, PETER KOHN¹, RUTH LOHWASSER², MICHAEL SOMMER², MUKUNDAN THELAKKAT², and THOMAS THURN-ALBRECHT¹ — ¹Institute of Physics, Martin-Luther-University Halle-Wittenberg, 06120 Halle, Germany — ²Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. Despite of the extensive amount of work done on this material there are a number of important open questions concerning the structure and morphology. We performed temperature dependent scattering experiments on bulk samples of P3HT in order to elucidate the phase transitions taking place. We used chemically well-defined samples, i.e. with a very narrow distribution of molecular weights and a high degree of regiorregularity.

The measurements showed that all samples with molecular weights ranging from 5 to 34 kDa (GPC) exhibit a liquid-crystalline phase prior to melting during heating. The phase transitions also appear during

cooling from the isotropic melt. While for lower molecular weight crystallization leads to the formation of extended chain crystals, around a molecular weight of 20 kDa chain folded crystals form, with the number of folds depending on the cooling rate. Moreover the close analysis of WAXS patterns allows us to estimate the degree of crystallinity.

CPP 8.42 Mon 17:30 P2

In-situ GIXRD studies of current induced structural changes of P3HT thin films — ●LINDA GRODD, ANTON DAVYDOK, SOUREN GRIGORIAN, and ULLRICH PIETSCH — Solid State Physics, University of Siegen, Siegen, Germany

Conjugated polymers are of great interest for electronic applications. Especially, the poly(3-hexylthiophene) (P3HT) is a promising candidate for application in organic thin film transistors (OFETs). The correlation of electric and structural properties is essential for understanding the processes that are taking place inside the polymer, and in particular, charge transfer processes.

In-situ studies of P3HT OFETs were done by using synchrotron radiation in GIXRD geometry. The 100 reflection of a drop casted P3HT film was monitored while applying voltages between 0V and 100V to source and drain of the sample with top contacts geometry. A channel length of 2 mm ensured that the whole conducting area of polymer was illuminated by the synchrotron beam. Simultaneously to the structural studies, the current at the fixed voltage was also recorded.

The current-voltage characteristics were featuring a sudden increase of the current by several orders of magnitudes from μA range to mA range. For the latter one, a reversible change of the d(100) spacing of about 1.3% has been observed.

CPP 8.43 Mon 17:30 P2

Temperature dependent relaxation processes in MDMO-PPV films — ●HENRY ALBERTO MENDEZ PINZON¹, CLARA PATRICIA HERNANDEZ MORENO², and JUAN CARLOS SALCEDO REYES¹ — ¹Thin Films Group, Pontificia Universidad Javeriana, Bogotá (Kolumbien) — ²Electronics Engineering Department, Pontificia Universidad Javeriana, Bogotá (Kolumbien)

Thin films of the electroluminescent polymer MDMO-PPV were deposited on glass by means of the Doctor Blade technique. The behavior of radiative relaxation processes in MDMO-PPV films were characterized by a combination of photoluminescence and transmittance measurements in a wide range of temperatures (13K to 400K). From both types of optical measurements an unusual increase of the optical bandgap was observed. A further analysis of the spectra allows deducing structural changes in the organic film, involving segmentation of the polymeric chains, and giving rise to an improvement in the ordering of the electroluminescent layer as temperature increases. In this way, monochromatic emission from the polymer is favored after annealing.

CPP 8.44 Mon 17:30 P2

Correlation between sheet resistance and NIR-VIS absorption of PEDOT:PSS — ●FELIX HERRMANN, SEBASTIAN ENGMANN, SVIATOSLAV SHOKHOVETS, HARALD HOPPE, and GERHARD GOBSCH — TU-Ilmenau, Ilmenau, Germany

PEDOT:PSS is a widely used buffer and hole-collecting layer in organic photovoltaics. In the past years a constant improvement of the PEDOT:PSS conductivity has been shown. This make PEDOT:PSS a potential candidate to replace ITO electrodes. Although this material is widely used in optoelectronic devices like solar cells and light emitting diodes, only little is known about the optical properties. Especially the absorption in the NIR and VIS region contains some information about free carriers and trap states in the gap. Therefore a relation between the absorption of PEDOT:PSS and the conductivity can be expected. Typically the absorption coefficient in this region is below 10⁴ per cm and the film thickness reaches about 40 nm. For these small absorptions the sensitivity of standard measurement methods like transmission/reflection and ellipsometry is rather poor. Therefore ellipsometric measurements were complemented by photothermal deflection spectroscopy. The charge carrier density calculations on the basis of the absorption and dielectric function were compared with the experimentally determined sheet resistance of different films to prove that relation.

CPP 8.45 Mon 17:30 P2

Impedance spectroscopic investigations of molecularly doped conjugated polymers — ●PATRICK PINGEL and DIETER NEHER — Soft Matter Physics, University of Potsdam, Germany

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitry. Recently, doping of conjugated polymers with the strong molecular acceptor tetrafluorotetracyanoquinodimethane, F₄TCNQ, has been introduced [1]. It has been proposed that F₄TCNQ-doping leads to the formation of charge transfer complexes with hybrid supramolecular orbitals and a reduced band gap, and that free holes are generated via thermally-induced dissociation of these complexes. Here, thin layers of poly(2-methoxy-5-(2'-ethylhexyloxy)-*p*-phenylene vinylene), MEH-PPV, have been doped at various doping ratios. Investigation of these samples with impedance spectroscopy in a metal-insulator-semiconductor (MIS) geometry allowed us to determine both charge carrier density and mobility of the doped polymer layers. The free carrier density is found to be well below the dopant concentration, which is in full agreement to our model that free carrier formation proceeds via a charge transfer complex. Moreover, we observed the formation of an inversion layer upon depletion bias, which is absent in non-doped samples.

[1] E.F. Aziz et al., *Adv. Funct. Mater.* **2007**, 19, 3257.

CPP 8.46 Mon 17:30 P2

Near Infrared Spectroscopic Studies of Boundary Effects on n-doped Organic Semiconductor Layers — ●ANDRÉ MERTEN, MORITZ RIEDE, and KARL LEO — IAPP/TU-Dresden, George-Bähr-Straße 1, 01069 Dresden

Doping of organic semiconductors is a useful method to achieve well selected charge carrier transport properties and alignment of electronic energy levels. The efficacious p-i-n concept for small molecule organic light emitting diodes or solar cells is based on the doping of the electron- and the hole-transport layers in which the active layer is embedded. Besides providing appropriate conductivity, the doping reduces injection or extraction barriers between the organic layers or organic layers and the contacts, respectively, by adjusting energetic levels. Highly doped organic layers are also used as very efficient conversion contact in organic tandem solar cells. In this study we focus on the near infrared absorption properties of n-doped organic layers on ITO or in organic layers stack like solar cells. We found a considerable elevated near infrared absorbance if the n-doped organic materials were evaporated directly on ITO, which is in contradiction to the optical constants of the ITO and of the doped materials which were determined on glass substrate. This effect will allow an inside on the elevated charge carrier concentration and the shape of the energetic bands on the organic layer-ITO boundary. As example for the consequence of this effect on small molecule organic solar cells, the IV and spectral response characteristics of device in the inverted p-i-n design, using n-C60 as ETL is discussed.

CPP 8.47 Mon 17:30 P2

Investigating the effect of molecular doping on the energy levels using Seebeck measurements — ●TORBEN MENKE¹, PENG WEI², ZHENAN BAO², KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik (IAPP), TU Dresden, 01062 Dresden, Germany — ²Stanford University, CA 94305, USA

Molecular doping plays an essential role in small molecule based organic devices like solar cells or light-emitting diodes, because it allows to control the Fermi level in the doped layers with the corresponding advantages. However the exact mechanisms of molecular doping are still far from being fully understood.

We investigate the influence of doping in different material combinations of dopants and host materials. Seebeck measurements are used to study the energetic distance between Fermi energy and transport level of doped charge transport materials, e.g. fullerene C60 or N,N,N',N'-Tetrakis(4-methoxyphenyl)-benzidine (MeO-TPD). For n-doping of C60 a novel airstable dopant is presented.

For MeO-TPD and C60 a shift of the energetic distances from 180 meV down to 30 meV and from 120 meV down to 25 meV, respectively, is observed when increasing the doping concentration. Furthermore the influence of the temperature on conductivity and Seebeck measurements is shown. For MeO-TPD and C60 the activation energies of the conductivity are found to shift from 310 meV down to 210 meV and from 240 meV down to 60 meV, respectively, with increased doping concentration.

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HTL based SAM-system with improved carrier injection — ●MERVE ANDERSON, SYLVIA GANG, BENJAMIN FRIEBE, BJÖRN LÜSSEM, and KARL LEO — IAPP, TU Dresden

Organic electronics have received an increasing interest due to their mechanical flexibility, versatile chemical design and possibility of low-cost production. Various organic devices like light-emitting diodes (OLEDs), photovoltaics (OPVs), field-effect transistors (OFETs), and memory are already on the way to commercial applications.

The performance and lifetime of these devices are dependent on both the properties of the materials as well as the interfaces between the organic layers and between organic and inorganic layers (Ma et al., *Adv. Funct. Mater.*, 2010, 20, 1371-1388). In particular the control of the characteristic of the metal/organic injection contact is essential for reaching a high performance in these devices.

To optimize the injection contact, we synthesised a novel class of molecules that are based on a commercial hole transport material (HTL) and are able to assemble from solution onto metal electrodes. We characterized Au-electrodes modified with these self-assembled monolayers (SAMs) by UPS/XPS, and studied the performance of bottom electrode OFETs with pentacene as the active layer.

With this new SAM we achieve an enhanced OFET performance in terms of a low contact resistance, increased mobility and on/off ratio compared to conventional SAMs such as Perfluorodecanethiol (PFDT) (Boudinet et al., *Organic Electronics*, 2010, 11, 227-237) and Pentafluorobenzeneethiol (PFBT).

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Real time growth studies of organic-inorganic semiconductor hybrid structures — ●CHRISTOPHER WEBER, SEBASTIAN BOMMEL, and STEFAN KOWARIK — Institut für Physik der Humboldt Universität, 12489 Berlin, Deutschland

We combine time resolved optical and x-ray in situ methods to investigate the growth of organic semiconductor thin films on inorganic semiconductor substrates. We use organic molecular beam deposition (OMBD) to grow the organic semiconductor diindenoperylene (DIP) on three different ZnO surfaces. X-ray methods like X-Ray Reflectivity (XRR) and Grazing Incidence X-Ray Diffraction (GIXD) allow to determine the molecular alignment and roughness of the thin films. We also investigate the growth dynamics by simultaneous real time monitoring of anti-Bragg growth oscillations on different points in reciprocal space (q-space). Meanwhile optical methods like Differential Reflectance Spectroscopy (DRS) and Fluorescence Spectroscopy allow us to investigate the interdependency between structural and spectral changes during thin film growth. In this way we are able to study the correlation between molecular alignment and different surface termination of the substrates.

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Soft x-ray linear dichroism to explore molecular orientation in STXM — ●STEPHAN WENZEL¹, ANDREAS SPÄTH¹, BENJAMIN WATTS², and RAINER H. FINK¹ — ¹ICMM, Dept. Chemie & Pharmazie, Univ. Erlangen, Egerlandstraße 3, D-91058 Erlangen, Germany — ²Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen, Switzerland

Soft x-ray near-edge x-ray absorption fine structure (NEXAFS) is an ideal fingerprint tool for the study of organic substances. This also serves as an excellent contrast mechanism for scanning transmission x-ray microscopy (STXM). Linear dichroism which originates from the anisotropy of NEXAFS resonances further serves as a tool for the study of molecular orientation. We present some microspectroscopic studies of TCNQ and F₄-TCNQ, which are commonly used in organic electronic devices. Single crystals were prepared from saturated solutions on commercial ultrathin Si₃N₄ membranes and imaged in the PoLux STXM at the Swiss Light Source (SLS). We discuss analytical routines to derive the molecular crystal packing in individual nano- and microcrystals from hyperspectral images, e.g., from a series of images recorded at various photon energies (corresponding to a measurement of the NEXAFS spectrum in each pixel of the image series). Such studies can be extended to more complex materials like e.g. oriented polymers in organic solar cells, where the combination of structural and chemical analysis is inevitable. The PoLux STXM is supported by the BMBF (contract 05 KS7WE1).

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Photoionization cross section weighted DFT simulations as promising tool for the investigation of the electronic structure of open shell metal-phthalocyanines — ●MICHAEL VOGEL, FELIX SCHMITT, JENS SAUTHER, BENEDIKT BAUMANN, ANNA ALTENHOF, STEFAN LACH, and CHRISTIANE ZIEGLER — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern,

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The valence band structure of different metal-phthalocyanines (MePcs) was investigated by comparing ultraviolet photoelectron spectra (UPS) at different excitation energies with simulated spectra that take the different photoionization cross sections at these energies into account. The Kohn-Sham eigenvalue spectra, derived from density functional theory (DFT) calculations, using hybrid exchange-correlation functionals, were weighted with the photoionization coefficients in accordance with the used excitation energy. By applying these techniques the differences in the photoelectron spectra using He I and He II radiation can be reproduced and investigated. It will be shown that the 3d-orbitals of the used metal central atom of these molecules have a major influence. The changes at different excitation energies were studied for Fe, Co, and Cu central atoms to describe the chemical tailoring effects. Further the DFT calculations were used to get a detailed image of the electronic ground state.

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Characterization of the electronic and optical properties of 2-Aminopyrimidine-silver based crystals — ●ARTHUR RIEFER¹, EVA RAULS¹, WOLF GERO SCHMIDT¹, ION STOLL², JENS EBERHARD², and JOCHEN MATTAY² — ¹Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — ²Organische Chemie I, Universität Bielefeld, 33615 Bielefeld, Germany

The importance of organic semiconductors for many applications is due to their low fabrication effort and the possibility of tuning desired functions by chemical modification of their building blocks. In general, the properties of organic materials not only depend on their organic building blocks but also on the solid state assembly of the latter. Recently, the synthesis of a new family of organic semiconductors based on pentafluorophenyl 2-aminopyrimidine and silver salts (AgX with X=CO₂CF₃⁻, SO₃CF₃⁻, NO₃⁻) has been reported. Depending on the involved silver salt, X-Ray analysis show the compounds to be made

of 1-dimensional polymer strands with different geometries and crystal groups leading to differences in the electronic and optical properties. Therefore, we have studied pentafluorophenyl 2-aminopyrimidine and the compounds with Density Functional Theory (DFT). In detail, we calculated the band structures, the (joint) densities of states, and the dielectric functions in random phase approximation (RPA). For pentafluorophenyl 2-aminopyrimidine we obtained the energies of the HOMO and LUMO, as well as the Stokes shift by means of occupation constrained DFT. The influence of many-body effects is discussed.

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Vibrational analysis of ethyne-linked ZnTPP dimer — ●STEPHAN PETER KATE¹, SIMONA POP¹, NORBERT ESSER¹, KARSTEN HINRICHS¹, MATHIAS O SENGE², AOIFE RYAN², JÖRG RAPPICH³, and XIN ZHANG³ — ¹Leibniz Institut für Analytische Wissenschaften - ISAS - e.V., Albert-Einstein-Str.9, D-12489 Berlin, Germany — ²School of Chemistry, SFI Tetrapyrrole Laboratory, Trinity College Dublin, Dublin 2, Ireland — ³Helmholtz-Zentrum Berlin for Materials and Energy GmbH, Institute for Silicon Photovoltaics, Kekuléstrasse 5, Berlin, 12489, Germany

Recently, porphyrin oligomers have attracted much attention as pi-conjugated organic chromophores. Their possible advantages due to their extraordinary optical and electronic properties range from biosensors and organic solar cells to organic field-effect transistors. As a result of the pi-conjugation, the low-lying HOMO-LUMO electronic transitions allows the porphyrin oligomers to collect an extended low-energy part of the solar spectrum towards NIR spectral range. This study employs micro-Raman spectroscopy for the analysis of the vibrational modes of the ethyne-linked ZnTPP (tetraphenylporphyrin) dimer in comparison to its monomer. Their resonance Raman spectra were excited with the 633 nm (1.95 eV; HeNe laser) and 458 nm (2.71 eV; Y laser) emission lines which are located in the Q- and B-band regions of the optical absorption spectrum, respectively. The presence of the Raman-active ethyne stretching mode at 2150 wavenumbers is a fingerprint of the ethyne bridge used in the pi-conjugation of ZnTPP dimer.