

CPP 30: Poster: Organic Electronics and Photovoltaics

Time: Tuesday 18:15–21:00

Location: Poster B2

CPP 30.1 Tue 18:15 Poster B2

Microstructure of donor-acceptor conjugated polymer blends and annealing induced nano-aggregation observed by two-dimensional polarization fluorescence microscopy — ●DANIELA TÄUBER¹, YUXI TIAN¹, YUXIN XIA², OLLE INGANÄS², and IVAN SCHEBLYKIN¹ — ¹Chemical Physics, Lund University, Lund, Sweden — ²Biomolecular and Organic Electronics, Linköping University, Linköping, Sweden

Polymer-polymer bulk heterojunction solar cell devices combine solar energy harvesting with the fortune of polymer materials, which enable easy and inexpensive processing and flexibility of the material.

Their performance crucially depends on the organization of the conjugated polymer molecules. Studying blends of TQ1 and N2200 spin-cast from solution with two-dimensional polarization fluorescence microscopy we observe concentration dependent microstructures. Comparing polarization parameters from films as prepared with films annealed at 120°C, we find modifications pointing to enhanced nano-aggregation of the annealed polymer blend. These changes agree with modifications seen in fluorescence and absorption spectra and in fluorescence lifetime measurements.

D.T. acknowledges a personal research grant DFG-TA 1049/1-1.

CPP 30.2 Tue 18:15 Poster B2

Conformational preferences of conjugated benzothiadiazole-cored oligomers: the impact of through-space interactions — ●DEYAN RAYCHEV^{1,2}, OLGA GUSKOVA^{1,2}, and JENS-UWE SOMMER^{1,2,3} — ¹Dresden Center for Computational Materials Science, TU Dresden — ²IPF Dresden — ³Institute of Theoretical Physics, TU Dresden

Symmetrical benzothiadiazole-cored oligomers with thiophene or furan rings are widely used in experiments as structural blocks for organic electronics. Along with chemical composition, the molecular conformation plays a crucial role in crystal packing/self-assembly of these building moduli in thin films. In this work, we examine the conformational preferences analyzing possible through-space interactions (S...N, O...N, S...H, O...H), steric repulsion, electrostatics and donor/acceptor orbital interactions for a series of benzothiadiazole-based conjugated oligomers using DFT calculations (with different functionals and basis sets and taking into account the effects of the medium) and NCI procedure [1].

The financial support from ESF Young Investigators Group CoSiMa (TU Dresden) is highly appreciated.

[1] J. Contreras-García et al. *J. Chem. Theory Comput.* 7 (3), 625-632 (2011).

CPP 30.3 Tue 18:15 Poster B2

Influence of conformations in DPP-TH based molecular system on electronic structure and charge transport properties — MARIA V. MAKAROVA¹, SERGEY G. SEMENOV², and ●OLGA GUSKOVA^{1,3} — ¹IPF Dresden, Dresden, Germany — ²Petersburg Nuclear Physics Institute, National Research Centre "Kurchatov Institute", Gatchina, Russia — ³Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Such phenomenon as stereoisomerism can strongly influence on physical and chemical processes in molecular systems. In the present work, the role of conformational changes on charge transport process in diketopyrrolopyrrole-thiophene (DPP-TH) molecular system was theoretically investigated. Quantum chemical calculations of relative and reorganization energies, ionization potentials, electron affinities and intermolecular couplings were performed for two TH2-DPP-TH2 conformers. Calculations were carried out by M06-2X/cc-pVDZ method using GAUSSIAN09. Crystal structure predictions (Monte Carlo method) were performed using BIOVIA Materials Studio 8.0.

CPP 30.4 Tue 18:15 Poster B2

Manipulation and controlling the strength of the interfacial polarisation in OLED devices by doping — ●LARS JÄGER, TOBIAS D. SCHMIDT, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Most of the used electron transporting materials in organic light emitting diodes are known to be polar. This property modifies the internal electric field distribution of the device and therefore enables

an earlier flat band condition for the hole transporting side, leading to improved charge injection. Recently the interfacial polarisation has been investigated with regard to different materials and degradation effects, however, so far the influence of doping has never been looked at. Here we focus on the behavior in the case of doping of the polar electron transporting layer tris-(8-hydroxyquinolate) aluminum (Alq₃) with the hole transporting material 4,4'-bis[N-(1-naphthyl)-N-phenylamino]-biphenyl (NPB). By evaluating impedance spectroscopy data we can show that the limiting parameter is not the effective Alq₃ thickness. In fact the built up of the polarisation reaches a maximum for a 50% blend. Taking the permanent dipole moments of the molecules into account, an increasing contribution was found for a decreasing Alq₃ amount in the blend. This fact can be explained by a sterically mechanism in addition to the minimization of the dipole-dipole interaction.

CPP 30.5 Tue 18:15 Poster B2

Printing High Efficiency Solar Cells — ●DAN YANG and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Printing techniques hold a promising future for thin organic films. The realization of fast, low-cost and large areas manufacture lies within reach. In our work, we combine the printing technique with high power conversion efficiency (PCE) polymers to prepare organic solar cells. In the past few years, a new state-of-the-art low bandgap polymer with PCEs exceeding 7%, polythieno [3, 4-b]-thiophene-cobenzodithiophene (PTB7), has been developed as one of the most promising donor materials for organic solar cells. So far, research focused on PTB7 films prepared via spin coating to make such solar cells. In contrast, we prepare solar cells (PTB7 as donor) with printing the active layers. We measure the device function via I-V curves. In order to understand the influence of printing, we investigate the morphology of the active layers with GISAXS and the crystal orientation with GIWAXS.

CPP 30.6 Tue 18:15 Poster B2

Degradation processes in high-efficiency polymer solar cells — ●CHRISTOPH SENFTER, FRANZISKA LÖHRER, CHRISTOPH SCHAFER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

The application of polymers as active material in solar cells has several advantages over conventional silicon solar cells. Organic materials are typically cheap in production, flexible and lightweight, but their efficiencies and long term stabilities are far below the ones of their inorganic counterparts. In the last years, research has been focusing on the identification of new high-efficiency polymers like PTB7-Th with reported efficiencies surpassing 10 % in combination with PC71BM. However, little is known about the long-term stability of this polymer and its blends. Photo-oxidation and morphological changes of the active layer are two main aging processes, which lower the cell performance over time. To learn more about the degradation process, we investigate changes of the polymer under illumination using FT-IR spectroscopy. Additional investigation methods include optical characterization via UV/Vis and PL as well as morphological characterization using X-ray diffraction methods. The change in cell performance is probed by applying IV-measurements.

CPP 30.7 Tue 18:15 Poster B2

Hole mobility in bulk P3HT determined from first principles — ●ANDREAS LÜCKE¹, FRANK ORTMANN², SIMONE SANNA¹, EVA RAULS¹, UWE GERSTMANN¹, and WOLF GERO SCHMIDT¹ — ¹Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — ²Institute for Materials Science and Dresden Center for Computational Materials Science, Technische Universität Dresden, Germany

The temperature-dependent hole mobility for ideal Poly(3-hexylthiophene) (P3HT) crystals is calculated ab initio and compared with experimental data. Thereby the electronic structure as well as phonon frequencies and electron-phonon coupling constants are obtained from density functional theory. The P3HT transport properties are dominated by polarons due to the strong coupling between the charge carriers and the vibrating lattice. By providing a limit for ideal

P3HT crystals, our results allow for separating the polaron effects from disorder contributions onto the temperature dependent mobility. Furthermore a detailed analysis of important phonon modes is given that illustrates the polaron effects microscopically.

CPP 30.8 Tue 18:15 Poster B2

Investigation of the donor-acceptor coupling strength in DBP:C₇₀ solar cells — ●THOMAS ZEHEL, THERESA LINDERL, THOMAS LAMPE, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86159 Augsburg

The strength of the donor (D) acceptor (A) interaction can have an influence on the open circuit Voltage (V_{OC}) in organic solar cells as demonstrated by Vandewal *et al.* [1]. Here it is shown that the strength of the D-A interaction in Tetraphenyl-dibenzoperifluorene (DBP):Fullerene C₇₀ planar mixed hetero junction (PM-HJ) solar cells decreases with decreasing the amount of DBP in the mixed layer. However, no significant changes in V_{OC} for this D-A pairing can be observed. The coupling strength is obtained from electroluminescence (EL) and external quantum efficiency spectra of working devices. Temperature dependent EL measurements reveal two charge transfer peaks with different temperature dependence. At the same time the current voltage characteristics of the different devices show that only a small amount of DBP is necessary for efficient charge separation.

[1] Vandewal, K. *et al.*, Physical Review B, **2010**, *81*, 125204

CPP 30.9 Tue 18:15 Poster B2

Light-coupling and light trapping in periodically structured thin-film solar cells — THOMAS PFADLER and ●LUKAS SCHMIDT-MENDE — Universität Konstanz

Periodically structured TiO₂ electrodes are introduced to thin-film photovoltaics to tackle the typically partial light absorption. Arising consequences on light management in such thin-film solar cells are elucidated. Wavelength-scale patterns are transferred to the electron-selective TiO₂ bottom electrodes via direct laser interference patterning. In the main absorption region of the employed photoactive materials, the efficiency of the structure-induced light in-coupling is spectroscopically shown to be determined by the refractive index n (active material) with respect to $n(\text{TiO}_2)$. Beside the elucidation of light in-coupling in the main absorption region of the photoactive material, structure-induced light-trapping effects targeting at a resonant enhancement of the very weak tail-state absorption present in polymer:fullerene BHJ solar cells are additionally investigated. The presented approach paves the way to potentially close the gap between net optical and electric band gap of organic solar cells, which is stated as an intrinsic energy loss mechanism in donor-acceptor systems. Furthermore, fully vectorial electromagnetic simulations using the Discontinuous Galerkin Time Domain method were performed to obtain time-averaged Poynting vectors along with spatially resolved dependencies of the power loss densities. The simulations underline the experimental findings and further outline the tuneability of the absorption resonances towards arbitrary wavelength regions.

CPP 30.10 Tue 18:15 Poster B2

Disorder effects on Charge Transport in Rubrene Crystals — ●MICHEL PANHANS¹, DESANKA BOSKOVIC², PABLO ORDEJÓN^{2,3}, and FRANK ORTMANN¹ — ¹Institute for Material Science and Dresden Center for Computational Material Science, Technische Universität Dresden, 01062 Dresden, DE — ²ICN2 - Institut Catala de Nanociencia i Nanotecnologia, 08193 Bellaterra, ES — ³CSIC - Consejo Superior de Investigaciones Científicas, 08193 Bellaterra, ES

The understanding of charge transport in small-molecule organic semiconductors challenges both experimental and theoretical approaches since many years. This is mainly because transport phenomena in organic semiconductors are strongly influenced by vibrations and disorder effects (such as traps, dopants, structural disorder, etc.).

We present a charge transport approach based on ab initio calculations of all relevant parameters of the small molecules that tackles electron-phonon interactions both quantum-mechanically and semi-classically and includes disorder effects by suitable real space models.

The p-type charge transport in rubrene single-crystals FET's serves as a test case that provides a valuable reference for comparison with our charge transport simulations of rubrene crystals. Based on the present theory we studied band-like transport and phonon assisted hopping transport in the presence of two different sources of disorder and compared them quantitatively to existing experimental data. The analysis of both models illustrates important aspects of transport mechanisms occurring in organic small-molecule semiconductors.

CPP 30.11 Tue 18:15 Poster B2

Columnar axial orientation of discotic liquid crystals in nanoporous solids — ●KATHRIN SENTKER, KATRIN KNOPP, and PATRICK HUBER — Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg

The columnar axial orientation of discotic liquid crystals (DLC) in nanoporous silica or alumina membranes provides a high electrical conductivity along the pore axis, which is important for their applications in e.g. photovoltaic devices. The optical birefringence of the DLCs is a measure of their orientational order. In contrast to a radial orientation an axial orientation causes a negative birefringence. We successfully reproduced the experimental results of Calus *et al.* [1], showing that 11-hexakis(hexyloxy)triphenylene DLCs embedded in an untreated alumina membrane exhibit positive birefringence, hence a radial orientation. In order to achieve axial orientation we are going to chemically modify the membranes from hydrophilic to hydrophobic. Additionally, we are going to perform measurements with coronene-based DLCs as suggested by Duran *et al.* [2], supplemented by X-ray diffraction experiments to probe the translational order.

[1] Sylwia Calus, Andriy V. Kityk, Patrick Huber, Microporous and Mesoporous Materials 197 (2014)

[2] Hatice Duran *et al.*, ACS Nano 6, 11 (2012)

CPP 30.12 Tue 18:15 Poster B2

Energy losses in DIP/PDIR-CN₂ based solar cells. — ●EDUARD MEISTER¹, THERESA LINDERL¹, STEFAN SCHMIDT¹, THOMAS ZEHEL¹, PAUL BEYER², ANDREAS OPITZ², VALENTINA BELOVA³, ALEXANDER HINDERHOFER³, FRANK SCHREIBER³, and WOLFGANG BRÜTTING¹ — ¹Institut für Physik, Universität Augsburg, Germany — ²Institut für Physik, Humboldt-Universität zu Berlin, Germany — ³Institut für Angewandte Physik, Universität Tübingen, Germany

Perylene derivatives are widely used in organic electronics. Depending on the substitution at both ends of the molecular core, either donor- or acceptor-type behaviour is obtained. In this contribution we used diindenoperylene (DIP) as donor and N,N'-bis-(2-ethylhexyl)-1,7-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIR-CN₂) as acceptor and prepared donor/acceptor (D/A) solar cells with two different architectures: planar hetero junction (PHJ) and planar mixed hetero junction (PM-HJ). The *j*-*V* measurements displayed that the open circuit voltage V_{OC} of both architectures, PM-HJ and PHJ, is equal, where the short circuit current density j_{SC} as well as the efficiency for the PM-HJ cell is lower than for its PHJ pendant. In addition we determined from electroluminescence (EL) measurement two radiative CT states and from incident photon-to-current efficiency (IPCE) experiment at least four CT states. Taken as a whole, this D/A combination yields very low efficiency, most likely due to a strong interaction between DIP and PDIR-CN₂ accompanied by very high non-radiative energy losses detected with EL and IPCE measurements.

CPP 30.13 Tue 18:15 Poster B2

In situ polymerized insoluble semiconducting polymers for application in organic solar cells — ●JENNY LEBERT, ANNA SANINA, EVA KRATZER, and EVA M. HERZIG — Technische Universität München, Munich School of Engineering, Lichtenbergstr. 4, 85748 Garching

Organic semiconducting materials can be applied in optoelectronic devices such as organic light-emitting diodes and organic solar cells. The polymers employed usually exhibit a conjugated backbone of varying complexity which is equipped with insulating, alkyl side chains to make them processable from solution. While nowadays lab scale organic solar cells can easily perform at efficiencies above ten percent, they still suffer from fast degradation induced amongst others by external impacts such as water, oxygen and UV light. In situ polymerization offers the possibility to process polymers from solution without the need for solubilizing side chains. Thereby the amount of electrically insulating molecular parts in the film are reduced to a minimum. Moreover, the simplified chemical structure of the polymers leads to a higher stability. In this work, in situ polymerized polythiophene thin films are investigated in terms of their stability in organic solar cells. For this purpose, differently post-treated films are analyzed regarding their morphology, conductivity and optoelectronic properties.

CPP 30.14 Tue 18:15 Poster B2

Investigating the photoactive layer morphology of printed thin films for organic solar cells — ●OLIVER FILONIK^{1,2}, STEPHAN PRÖLLER¹, PETER MÜLLER-BUSCHBAUM³, and EVA M. HERZIG¹

— ¹Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — ²Technische Universität München, LS Erneuerbare und Nachhaltige Energiesysteme, 85748 Garching, Germany — ³TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany

Organic solar cells yield numerous advantages including flexibility, low material costs, and independence on rare resources. In particular, solution based processability enables fabrication techniques like printing, which is up-scalable to large area photovoltaics production in industrial processes. The photoactive layer morphology, consisting of a donor and acceptor material blend, is of utmost importance for the performance of the device due to its impact on the exciton generation, exciton separation and charge carrier transport in the device. Therefore, a deeper understanding of the parameters influencing the active layer's morphology is crucial.

Using a slot die coater, we print organic thin films used as the photoactive layer of an organic solar cell. We investigate the processing parameters as well as external influences on the film morphology in order to obtain insight into the crucial processing parameters for the photoactive layer. With this knowledge, we are able to optimize the production process of organic solar cells.

CPP 30.15 Tue 18:15 Poster B2

Diffusion of p-type Dopants in Organic Semiconductors — •DONGXIANG WANG^{1,2}, LARS MÜLLER^{2,3,4}, SEBASTIAN BECK^{2,4}, ROBERT LOVRINCIC^{2,3}, ULI LEMMER^{1,2}, and WOLFGANG KOWALSKY^{2,3} — ¹KSOP, Karlsruhe Institute of Technology, Germany — ²InnovationLab, Heidelberg, Germany — ³IHF, TU Braunschweig, Germany — ⁴KIP, Heidelberg University, Germany

Molecular doping of organic semiconductors is routinely applied in various devices such as organic light emitting diodes. Nevertheless, issues like the diffusion of dopants are still not solved for many material combinations. In this work, we investigate if this diffusion can be controlled to improve device performance. The starting device is a diode with two gold electrodes evaporated onto a substrate and the organic semiconductor material (P3HT) doped with certain p-type dopants such as F4TCNQ. Chlorobenzene is used as solvent for the solution-fabricating process. To get a general understanding of how dopant diffusion can be controlled, we start with an application of an electric field. Conductivity measurements as well as IR and UV-Vis spectroscopy are performed for the investigation. We show that the dopant distribution in the matrix material can indeed be controlled via an applied electric field. We will discuss how this effect can be utilized to improve the performance of an organic field effect transistor.

CPP 30.16 Tue 18:15 Poster B2

Influence of crosslinking on charge carrier mobility in PF2/6-derivatives — •FRANK-JULIAN KAHLE¹, IRENE BAUER², ANNA KÖHLER¹, and PETER STROHRIEGL² — ¹Department of Physics, University of Bayreuth, Germany — ²Department of Chemistry, University of Bayreuth, Germany

Cross-linking provides a good means to fabricate optoelectronic devices with multiple layers via solution processing. In the current work, a series of especially synthesized PF2/6 derivatives with different fractions of cross-linkable acrylate groups is investigated. Spectroscopic characterization and mobility measurements are carried out to assess the influence of introducing acrylate groups and crosslinking on material performance. For the regime of low to medium charge carrier density, relevant for OLEDs and OPVs, we used a novel technique based on the injection of charge carriers from the electrodes of an optoelectronic device: MIS-CELIV. This technique allows for the selective measurement of electron or hole mobility. By comparing crosslinked samples with pure PF2/6 as reference, we could show that the crosslinking process itself does not significantly influence hole mobility in the investigated system. An observed reduction of about one order of magnitude is attributed to structural differences caused by the introduction of acrylate groups. Furthermore, it turned out that the crosslinking process may be solely triggered by thermal activation and UV-illumination without the need of any photoinitiator, still achieving a densely linked network. This is of special interest as we have seen that a larger amount of photoinitiator may introduce traps for charge carrier transport.

CPP 30.17 Tue 18:15 Poster B2

Organic heterojunctions: Contact-induced molecular reorientation, interface states, and charge re-distribution — •PAUL BEYER¹, TINO MEISEL¹, ALEXANDER GENERALOV², ANA SOFIA ANSELMO³, and ANDREAS OPITZ¹ — ¹Institut für Physik, Humboldt-

Universität zu Berlin, Germany — ²Maxlab, Lund University, Sweden — ³Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Different relative molecular orientations at organic-organic heterointerfaces dictate the orbital overlap between neighboring molecules, as well as electronic and structural properties, which are crucial for organic electronic devices. In order to access these properties we utilize a multi-technique approach, consisting of I/V measurements, absorption and photoelectron spectroscopy.

As a donor/acceptor combination, we chose two perylene derivatives: diindenoperylene (DIP) and functionalized perylene alkyldiimide with cyano groups (PDIR-CN₂). The usage of different substrates allows us to tune the molecular orientation inside the grown thin films. We investigated different devices with relevant architectures – planar heterojunctions (PHJ) and planar mixed heterojunctions (PM-HJ).

From absorption measurements, we observed blend exclusive features, proving the creation of new charge transfer states, specifically charge transfer excitons. Depending on the molecular orientation and, thus, the interface geometries, we found clear changes in ionization energies compared to the pristine materials, stemming from differences in energy level alignment.

CPP 30.18 Tue 18:15 Poster B2

Ultrafast Dynamics of Charge Transfer in Polymer-Fullerene Systems — •STEFAN WEDLER¹, THOMAS UNGER¹, HEINZ BÄSSLER², and ANNA KÖHLER^{1,2} — ¹Experimental Physics II, University of Bayreuth, 95440 Bayreuth, Germany — ²Bayreuth Institute of Macromolecular Research (BIMF)

Exciton dissociation in organic semiconductors is a two-step process that consists first of an initial transfer of an electron from the photoexcited donor to the acceptor and second of the subsequent separation process of the resulting coulomb-bound interfacial electron-hole pair. Here, we have explored whether the initial electron transfer is thermally activated and can thus be described by a Marcus-type rate, or whether it is a temperature-independent tunneling-type process that is best modelled by a Miller-Abrahams rate. In order to investigate the influence of thermal activation on the transfer dynamics, we have performed temperature dependent ultrafast pump-probe spectroscopy on films of PCPDTBT-PCBM blends with a resolution of 200fs. The charge transfer is measured by monitoring the transient absorption of the polymer cation after excitation. We find no change in transfer dynamics upon cooling to 12K within our temporal resolution. This result suggests that initial charge transfer lacks thermal activation.

CPP 30.19 Tue 18:15 Poster B2

Preparation and Characterization of Ionic Transistors — •MARTIN GEBHARDT^{1,2}, LARS MÜLLER^{1,2}, ROBERT LOVRINCIC^{1,2}, and WOLFGANG KOWALSKY^{1,2} — ¹Institute for High-Frequency Technology, TU Braunschweig, Germany — ²InnovationLab GmbH, Heidelberg, Germany

In contrast to electron based transistors, most transmissions inside the human body depend on ions and molecules. To have an interface between electronics and the biological world, ion bipolar junction transistors (IBJT) were studied. The built IBJTs consist of two organic bipolar membranes and an electrolyte in between. When applying a voltage to the base of the IBJT, ions are injected into the junction and a current of opposite polarized ions flows from emitter to collector. In cut-off mode the junction is depleted of the base-ions and the current of the emitter-collector-ions stops. We present the fabrication of IBJTs and discuss the performance of them with respect to changes of the geometry.

CPP 30.20 Tue 18:15 Poster B2

Theoretical core level XPS and NEXAFS investigations of the C₆₀ derivative PCBM: the influence of oxygen adsorption — •IULIA EMILIA BRUMBOIU¹, LEIF ERICSSON², RICKARD HANSSON², ELLEN MOONS², OLLE ERIKSSON¹, and BARBARA BRENA¹ — ¹Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden — ²Department of Engineering and Physics, Karlstad University, SE-65188 Karlstad, Sweden

In recent years, organic photovoltaics (OPVs) have been developing as an alternative to silicon solar cells. Some of the advantages of OPVs are device flexibility, low production cost and low environmental impact. Device efficiencies have recently reached 10%, a limit that makes OPVs competitive on the market. One of the main issues that still needs to be resolved is the stability of the cells. Both the electron donor (or-

ganic polymer) and the electron acceptor (fullerene derivative) have been shown to undergo degradation during device functioning. We have addressed in this study one of the possible degradation mechanisms involving the electron acceptor PC₆₀BM. Specifically, we have studied by means of density functional theory (DFT) the possible final products of oxygen adsorption on the C₆₀ cage. Several configurations of PC₆₀BM with oxygen have been analysed from the point of view of the molecular structure, of the O 1s near edge x-ray absorption fine structure (NEXAFS) and of the x-ray photoelectron spectrum (XPS). We show that a joint O 1s XPS and NEXAFS study could provide insight into both the nature of the adsorbate (atomic or molecular oxygen) and the bonding configuration.

CPP 30.21 Tue 18:15 Poster B2

Chemical doping of semiconducting donor-acceptor polymers: a DFT study of the charge transfer — ●FLORIAN GÜNTHER^{1,2}, ANTON KIRIY³, SIBYLLE GEMMING^{1,4}, and GOTTHARD SEIFERT² — ¹Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — ²Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — ³Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — ⁴Institute of Physics, Technical University Chemnitz, Germany

Donor-acceptor (DA) polymers have recently been considered as promising candidates for novel organic electronics such as organic field effect transistors. Combining these systems with organic molecules having high electron affinity (low ionisation potential) leads to a charge transfer, and thus to doping of the organic semiconductor.

In this study, we theoretically evaluate the charge transfer between DA model compounds as Diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (DPP-TT) and p-dopant molecules as tetrafluorotetracyanoquinodimethane (F4-TCNQ) based on density functional theory (DFT) calculations. Furthermore, different structural formations are under consideration in order to obtain most stable configurations.

Interestingly, we observe in the lowest energy complex, the dopant molecule is located quite closely to the acceptor unit of the polymer (DPP) where the charge transfer process proceeds to the lowest extent.

CPP 30.22 Tue 18:15 Poster B2

Molecular doping of conjugated polymers with the strong Lewis acid tris(pentafluorophenyl)borane — ●MALAVIKA ARVIND¹, PATRICK PINGEL², and DIETER NEHER¹ — ¹University of Potsdam, Soft Matter Physics, Potsdam, Germany — ²Fraunhofer Institute for Applied Polymer Research, Potsdam, Germany

In the past years, conjugated polymers have acquired a great deal of interest as semiconductors in electronic devices due to their attractive properties such as mechanical flexibility and easy processability. Efficient charge transport through the semiconductor layers is a crucial requirement in electronic devices. Molecular doping provides an easy means of tuning and improving the transport properties of these materials. In this work, doping of the conjugated polymer poly(3-hexylthiophene) (P3HT) with the strong Lewis acid tris(pentafluorophenyl)borane (BCF) is studied using UV-Vis spectroscopy and conductivity measurements. By assigning the sub-band gap signals observed in the optical spectra of the doped solutions and layers to the known spectral signatures of the charged species in P3HT, the nature of charged species formed, the predominant mechanism of charge transfer between the dopant and polymer, and the doping efficiency is analyzed. While charge transfer is rather inefficient in solution, ca. 50 % of the employed dopant molecules undergo integer charge transfer with the polymer in solid state. Comparison with the well-known acceptor F4TCNQ reveals important differences with regard to the degree of ionization and the quality of the doped layer, which we assign to the better solubility and bulky structure of BCF.

CPP 30.23 Tue 18:15 Poster B2

Investigation and tuning of merocyanine dye thin films on ultra-flat substrates — ●THORSTEN LIMBÖCK, DIRK HERTEL, and KLAUS MEERHOLZ — Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln

Organic solar cells provide a low cost, yet, due to their thin film architecture, versatile alternative to the established silicon-based solar cells. One of the main challenges of organic photovoltaics is the relatively modest power conversion efficiency. To improve on the efficiency, the morphology of each individual layer has to be tuned in order to optimize the absorption, charge generation and charge transport. To investigate the morphology of dipolar molecules a merocyanine dye layer is grown in a controlled environment via vacuum deposition on ultra-flat

substrates graphite and mica in comparison to conventional organic photovoltaic electrode materials, such as ITO, MoO₃ or PEDOT. The morphologic behavior of its ordered growth and the changes therein for a variation of different parameters, such as layer thickness, evaporation rate and substrate temperature are investigated via atomic force microscopy and kelvin probe force microscopy. The achievable tuning range stretches from an amorphous form to large scale highly ordered layers with island sizes of several hundred μm². To investigate electric transport properties, organic field-effect transistors are built, which contain engineered layers of the merocyanine dye. The investigation is extended to other merocyanines having a lower polarity.

CPP 30.24 Tue 18:15 Poster B2

Charge transfer energies for organic donor acceptor pairs — ●JANNA ELISABETH RÜCKERT^{1,2}, SEBASTIAN SCHELLHAMMER^{1,2,3}, GIANAURELIO CUNIBERTI^{1,2,3}, and FRANK ORTMANN^{1,2} — ¹Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — ²Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — ³Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany
Organic solar cells depend heavily on the energetics close to the donor acceptor interface. We theoretically investigate the excitations of donor acceptor pairs based on C60 molecules and varying donor species. By means of time-dependent density functional theory simulations, we analyze the charge transfer energy and the absorption strength. We investigate the influence of the geometric configuration on the excitation energy and on the oscillator strength and find that the configuration of the molecular dimer has a strong impact on the absorption strength while the CT energy is weakly affected.

CPP 30.25 Tue 18:15 Poster B2

Effect of the donor orientation on the V_{OC} losses in small molecule organic bilayer solar cells. — ●STEFFEN ROLAND¹, NIVA RAN², THUC-QUYEN NGUYEN², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomie, Potsdam, Germany — ²University of California Santa Barbara, Center for Advanced Organic Photovoltaics, USA

Bilayer solar cells based on the donor molecule p-SIDT(FBTTh₂)₂ and the acceptor molecule C₆₀ show a significant difference in the V_{OC} of about 110 mV depending on whether the donor molecule exhibit an edge-on or face-on orientation. Here, we perform a detailed analysis of the losses determining the V_{OC} in these devices. By analyzing EQE and EL spectra related to the CT state, we find the effect of donor orientation on the CT energy not to be sufficient to explain the full V_{OC} difference. In accordance to this, we see almost no change of the HOMO energy in dependence of the orientation of the donor molecules. On the other hand, the absolute EL efficiency is significantly reduced in the bilayer cell with the edge-on oriented donor compared to the cell with face-on oriented donor molecules, pointing to increased non-radiative CT recombination. This shows that the molecular orientation can play a key role in determining non-radiative V_{OC} losses in organic photovoltaics.

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Spatial Orientation and Order of Structure-Defining Subunits in Thin Films of a High Electron Mobility n-Type Copolymer (P(NDI2OD-T2)) as Studied by Infrared Transition Moment Orientational Analysis (IR-TMOA) — ●ARTHUR MARKUS ANTON¹, ROBERT STEYRLLEUTHNER^{2,3}, WILHELM KOSSACK¹, FALK FRENZEL¹, DIETER NEHER², and FRIEDRICH KREMER¹ — ¹Universität Leipzig, Institut für Experimentelle Physik I, Leipzig, Germany — ²Universität Potsdam, Institut für Physik und astronomie, Potsdam, Germany — ³Freie Universität Berlin, Fachbereich Physik, Berlin, Germany

In order to investigate the molecular order in thin layers of P(NDI2OD-T2) the method of infrared transition moment orientational analysis (IR-TMOA), is employed. Structure-specific vibrational bands are analyzed in dependence on polarization and inclination of the sample film with respect to the optical axis. By means of IR specificity we deduce the molecular order parameter tensor for the respective moieties with regard to the sample coordinate system and determine independently the orientation and order of atomistic planes defined through the naphthalenediimide (NDI) and bithiophene (T2) units relative to the substrate, and hence, relative to each other. We observe that the polymer backbones in a 150 nm-thick film exhibit a pronounced in-plane anisotropy proving self-aggregated long range order, even though the

sample is spin-coated from solution. For μm -thick films the anisotropy vanishes while the inclination of the NDI unit remains basically unaffected. [Anton et al., *J. Am. Chem. Soc.* **137** (2015) 6034]

CPP 30.27 Tue 18:15 Poster B2

Charge Transport in Donor-Acceptor Polymeric Systems under Electric Fields — ●ANJA FÖRSTER^{1,2}, FLORIAN GÜNTHER^{1,2,3}, SIBYLLE GEMMING^{2,3}, and GOTTHARD SEIFERT^{1,2} — ¹Theoretical Chemistry, TU Dresden, Dresden, Germany — ²Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — ³Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Printable and foldable organic transistors are meant to revolutionize electronic applications. However, in comparison to their silicon counterparts their performance is currently still lacking. Thus, we investigate possible options of improving the charge transport in donor-acceptor polymers via DFT calculations.

The first focus point is the influence of gate-induced electric fields. Here, we concentrate on the preferable orientation of diketopyrrolopyrrole-dithienylthieno[3,2-b]thiophene (DPPT-TT) inside the transistor. We further analyze if source-drain induced electric fields have to be taken into consideration when describing the transport in DPPT-TT. We show that strong electric fields are required to yield significant changes in the transport properties.

A second option to improve the charge transport process is to functionalize DPPT-TT via fluoroalkyl chains. Here, the fluorine atoms introduce dipole fields and electron withdrawing sites. We concentrate on finding the composition of fluoroalkyl chains that yields the highest improvement in the charge transport process.

CPP 30.28 Tue 18:15 Poster B2

Nucleation of C70-aggregates on pentacene thin films for nanostructuring organic interfaces — ●JANINA ROEMER, SIMON NOEVER, STEFAN FISCHER, CLEMENS LIEWALD, and BERT NICKEL — Ludwig-Maximilians-Universität, Fakultät für Physik, München, Germany

Organic heterojunctions with well defined, nanostructured interfaces are desired for the investigation of interface effects. We use molecular beam deposition to create model-like, nanoscale interfaces by self-assembly of C70-aggregates on pentacene thin films. Size and distribution of these fullerene-islands can be tuned by the choice of evaporation rate and sample temperature.

An accompanying growth study utilizing x-ray Bragg scattering in reflection geometry, grazing incidence diffraction and atomic force microscopy on pentacene-C70 bilayer systems gives insight into the basic growth mechanism of the fullerene. In combination with in-situ measurements of thin film transistor characteristics during growth of the active layer, this allows us to correlate electronic effects, such as charging phenomena at the interface, with nanomorphology.

In future measurements we plan to apply photoresponse microscopy to study charge transfer at the pentacene-C70 heterojunction.

CPP 30.29 Tue 18:15 Poster B2

Rational design of thermally activated delayed fluorescence materials: The competition between internal conversion and non-radiative decay processes — ●PAUL KLEINE¹, RAMUNAS LYGAITIS^{1,2}, LUDWIG POPP¹, FLORIAN WÜST¹, OLAF ZEIKA¹, SIMONE LENK¹, REINHARD SCHOLZ¹, and SEBASTIAN REINEKE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — ²Department of Polymer Chemistry and Technology, Kaunas University of Technology, Lithuania

Under electroluminescence operation, about 75 % of the excitons formed in organic light-emitting diodes (OLEDs) come to life as triplet states. While phosphorescent OLEDs make use of rare metal complexes to increase triplet harvesting, the stability and substantial efficiency roll-off at higher current densities remain open issues. Although there has been an amazing progress in thermally activated delayed fluorescence (TADF) emitters, the overall understanding of the TADF unlocking molecular properties to upconvert triplet states is still in its infancy and the fundamental properties to tackle are still under debate. To increase the internal quantum efficiency of TADF materials, the competition between internal conversion, radiative, and non-radiative rates decides over good and bad emitter molecules. In this talk, we will present our recent efforts in the understanding of the basic concepts of TADF mechanism. Rational design and subsequent photophysical investigations of new types of TADF materials confirm the competition between multiple internal transfer rates which open the path to improved design structures for TADF in general.

CPP 30.30 Tue 18:15 Poster B2

First Solution-Processed White OLEDs Exhibiting TTA Delayed Fluorescence — ●MERVE WELNHOFER, CHRISTIAN TÖPEL, ANNE KÖHNEN, JÜRGEN SCHELTER, DIRK HERTEL, and KLAUS MEERHOLZ — Department of Chemistry, University of Cologne, Luxemburger Str. 116, 50939 Cologne, Germany

In past decades organic light emitting diodes (OLED) have drawn much attention due to their superior properties over the established lighting and display technologies. Although OLEDs have already found their way into commercial products, a major drawback is loss of three quarters of electrically generated excitons due to radiationless relaxation from triplet excitons. One approach to solve is to collect the triplet excitons by energy transfer between two triplet excitons to generate a singlet exciton relax radiatively by means of triplet-triplet annihilation (TTA). So far many organic molecules revealing TTA with different emission wavelengths are reported however none of them was suitable for solution processable OLEDs. We report on the first solution processed TTA type multilayer OLEDs containing oxetane functionalized (crosslinkable) anthracene derivatives that are emitting in the blue, green, yellow and red wavelength region. To our knowledge these devices are the first fully solution-processed OLEDs revealing TTA delayed fluorescence (DF). Additionally, we used these materials to fabricate the first solution-processed white DF-OLEDs.

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Thermally activated delayed fluorescence (TADF) in organic light emitting devices (OLEDs) utilizing carbazol-donor-benzofluoride-acceptor complexes — ●LUDWIG POPP¹, REINHARD SCHOLZ¹, PAUL KLEINE¹, RAMUNAS LYGAITIS^{1,2}, FLORIAN WÜST¹, ENI DOBBIBA¹, SIMONE LENK¹, and SEBASTIAN REINEKE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — ²Department of Organic Technology, Kaunas University of Technology, Lithuania

Thermally activated delayed fluorescence (TADF) takes place in fluorescent molecules where the energy splitting between the lowest excited singlet and triplet state (ST-splitting, Δ_{ST}) is about $k_B T$ at room temperature. Due to the small ST-splitting, the excited triplet states are easily converted into fluorescent singlet states via reverse intersystem crossing (RISC). This excitonic scheme is favorable for OLEDs, because it allows for making use of the large fraction of non-radiative triplets, which are formed under electroluminescence operation.

In this study, a new series of carbazol-donor-benzofluoride-acceptor complexes (" $x\text{F}y\text{Cz}$ ") is introduced where x denotes the number of fluorine atoms saturating the acceptor and y is the number of carbazol donor groups. Various investigations are shown such as absorbance and photoluminescence spectroscopy in solution and thin films, solvatochromism as well as the application and performance study of the emitters in actual OLEDs including e.g. j-V and luminance measurements, power efficiency and external quantum efficiency (EQE) up to 12 % for 1F4Cz.

CPP 30.32 Tue 18:15 Poster B2

The effect of the fullerene LUMO position on the CT properties in polymer:fullerene blends — ●TOBIAS THIEDE, JONA KURPIERS, and DIETER NEHER — Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany

In bulk heterojunction organic solar cells, one of the key parameters in solar cell efficiency, the open circuit voltage, has been shown to depend on the properties of the charge transfer (CT) state. These properties are again related to the energy gap between the highest occupied molecular orbital (HOMO) of the polymer and the lowest unoccupied molecular orbital (LUMO) of the fullerene acceptor. We present sensitive electroluminescence (EL) and external quantum efficiency (EQE) experiments on binary blends made of fluorinated copolymer 1F-PCPDTBT combined with the fullerene of different LUMO energy. By moving the LUMO of the fullerene we observe distinct changes in the absorption and emission properties. In particular, a significant increase of the EL efficiency accompanied by the appearance of emission from singlet excitons is seen when increasing the LUMO energy, as in blends with ICBA and ICTA. At the same time, the Voc loss due to non-radiative recombination is largely reduced. These findings help to understand the fundamental role of the energy landscape at the donor:acceptor interface and have important implications for designing future materials systems.

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Ion sensing with electrochemical gated organic field effect

transistors based on diketopyrrolopyrrole polymers — ●BENNO BUCHINGER, SVEN HÜTTNER, ANNA GRÄSER, and FABIAN HOFFMANN — Universität Bayreuth, Organic and Hybrid Electronics, MC I

Since conjugated polymers have the potential for biosensor applications we investigated the possibility of building electrochemical and bottom gated organic field effect transistors for sensing applications using different conjugated polymers based on DPP (Diketopyrrolopyrrole) derivatives as active material. DPP polymers are a promising type of polymers as they allow a high tenability between high electron and hole transport with high charge carrier mobilities as well as a high stability in ambient and aqueous environments. Ions can either interact with the surface of the polymer layer or diffuse into the bulk and interact with functional corresponding hydrophilic groups, inducing changes in the electronic properties. This work addresses the feasibility to use these polymers for sensing applications, i.e. detect different ions and ion concentrations in aqueous environments important for a row of bio-sensing applications.

CPP 30.34 Tue 18:15 Poster B2

Low temperature charge transport characterisation of low band-gap diketopyrrolopyrrole (DPP) based polymers — ●FABIAN HOFFMANN, BENNO BUCHINGER, and SVEN HÜTTNER — Universität Bayreuth, Organic and Hybrid Electronics, MC I

One of the most promising conjugated materials that emerged recently are conjugated polymers based on diketopyrrolopyrroles (DPP). Their semiconducting properties are directly related to their molecular ordering, molecular weight, purity and growth rate. In this context the material shows extraordinary high charge carrier mobilities in an OFET configuration due to the remarkable aggregating properties of the DPP moieties. Furthermore, they are stable at ambient conditions and can reach very low band gaps, which enables an absorption further in the red. At the same time they also show surprisingly low charge carrier mobilities in the bulk. We present temperature dependent OFET measurements to investigate the underlying charge transport processes. In particular, we address the influence of different processing conditions such as temperature and solvent vapour annealing.

CPP 30.35 Tue 18:15 Poster B2

Impact of PC[60]BM on the Photo-Degradation of PCPDTBT — ULF DETTINGER¹, HANS JOACHIM EGELHAUF², ●ANDREAS FRÜH¹, HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Eberhard-Karls-University, Institute for Physical and Theoretical Chemistry, Auf der Morgenstelle 18, D-72076 Tübingen, Germany — ²ZAE Bayern, Haberstrasse 2a, 91058 Erlangen, Germany

Organic photovoltaics (OPV) offers a promising solution for the energy demand in combination with challenging design requirements, although the stability of the device materials remains yet an important factor. UV-Vis and FTIR spectroscopy was used to study the photo-oxidation of the Low-Band-Gap Polymer PCPDTBT as pristine film and blended with PC[60]BM. The films were degraded under irradi-

ation of standard Air Mass 1.5 conditions under O₂ environment. It has been shown that the different monomer units of the polymer backbone are differently affected by the degradation. The unique kinetics of the accelerated degradation of PCPDTBT in the blend is studied in detail.[1] Reference: [1]*U. Dettinger et al. Chem. Mater. 2015, 27, S. 2299-2308

CPP 30.36 Tue 18:15 Poster B2

Modeling the Exciton Diffusion in Flat Heterojunction Organic Solar Cells — ●KARL-PHILIPP STRUNK^{1,2}, THOMAS PFADLER¹, and LUKAS SCHMIDT-MENDE¹ — ¹Universität Konstanz, Konstanz, Germany — ²Centre of Advanced Materials, Heidelberg, Germany

Organic solar cells have proven themselves to be a promising candidate towards a more energy efficient future. The performance of flat heterojunction solar cells is limited by the exciton diffusion length L_D of the active materials. For this reason exact knowledge of L_D is of significant importance when comparing different organic semiconductors. In this work, an organic system with state-of-the-art performance employing an exciton blocking layer of Tris[4-(5-phenylthiophen-2-yl)phenyl]amine (TPTPA) is studied. Based on experimental and simulated external quantum efficiency (EQE) spectra, it is shown that TPTPA contributes to the photocurrent, although exciton blockers are commonly believed to be non-photoactive. EQE spectra are simulated using a transfer matrix approach and a generalized diffusion equation for the exciton density, following previous publications. Furthermore, simulated EQE spectra are fitted to experimental data to obtain values of L_D for both donor and acceptor. L_D of the donor is measured experimentally using a time-resolved photoluminescence technique. The good agreement of experimentally and computationally obtained exciton diffusion lengths proves the selected algorithm to be a unique way to determine L_D from measurements of complete devices along with material characterization and simulations.

CPP 30.37 Tue 18:15 Poster B2

Studying the Effects of Degradation in Organic Solar Cell Materials — ●MICHAEL ADAMS¹, IAN HOWARD¹, BRYCE RICHARDS¹, ANDREAS WEU², and YANA VAYNZOF² — ¹Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany — ²Center for Advanced Materials, University Heidelberg, 69117 Heidelberg, Germany

Many factors have been reported to affect the stability of OPVs, among them are exposure to light, humidity, temperature and oxygen concentration. In order to develop strategies against these degrading effects we need to have a better understanding of the fundamental processes in the device's active layer. One of the most efficient OPV material combination to date is P3HT:PCBM. We perform transient absorption and streak camera measurements on P3HT:PCBM samples that have been prepared and degraded at the University of Heidelberg under various environmental conditions with the goal to identify differences in the photophysical processes occurring in these devices.