

CPP 37: Poster Session III

Topics: Controlling Phase Formation Dynamics in Solution Processed Semiconductors (37.1-37.4); Hybrid and Perovskite Photovoltaics (37.5-37.17); Molecular Electronics and Excited State Properties (37.18-37.23); Organic Electronics and Photovoltaics (37.24-37.55).

Time: Wednesday 11:00–13:00

Location: Poster B1

CPP 37.1 Wed 11:00 Poster B1

Key factors in the synthesis of template-oriented porous ordered titanium dioxide: solvents and catalysts — ●SHANSHAN YIN and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

As a crucial material for energy storage, TiO₂ has been widely studied during the past decades. Typically, when used as the active material of lithium-ion batteries or solar cells, TiO₂ thin films with specific structures always afford more advantages than classical bulk material. In this work, various intriguing structures have been synthesized with the template-oriented sol-gel method. Both, the hydrolysis and condensation reaction of TTIP, are confined into the PEO domain of the amphiphilic diblock copolymer during the sol-gel synthetic process. Since the polymer template can be fully removed with the calcination, the morphology control of the TiO₂ thin film is realized with controlling the phase separation behavior of the block polymer. In the present work, the influence of the solvent category and catalyst content on the morphology of TiO₂ thin film is discussed in detail. SEM and GISAXS measurements were carried out to study the pore structures of the TiO₂ films.

CPP 37.2 Wed 11:00 Poster B1

Ordering and crystallization in thin films of diketopyrrolopyrrol-based semiconducting copolymers — ●SHAYAN VAZIRIEH LENJANI, MARIO ZERSON, QIAN WANG, MICHAEL SOMMER, and ROBERT MAGERLE — Fakultät für Naturwissenschaften, TU Chemnitz, Chemnitz, Germany

Semiconducting polymers based on diketopyrrolopyrrol (DPP) combine a number of favorable properties, such as straightforward chemical synthesis and photostability with an outstanding charge carrier mobility in organic electronic devices. Despite this success, the structure formation processes in thin films are poorly understood. With atomic force microscopy (AFM), we study thin films of DPP copolymers prepared from different solvents, polymer concentrations, and temperatures. During drying, a complex sequence of structural rearrangement processes occurs. In solution, the polymers partly form aggregates. At higher polymer concentrations, different types of lyotropic liquid crystalline phases form as indicated by terrace formation and the observed surface textures. During the final drying, the polymer chains partly crystallize and form crystalline lamellae that are typical for semicrystalline polymers. From arrays of pointwise measured amplitude-phase-distance curves, we reconstruct three-dimensional depth profiles of the specimen's top 10 nm surface layer. These high-resolution volume images reveal different types of surface structures with unprecedented resolution.

CPP 37.3 Wed 11:00 Poster B1

What is the role of planarity and torsional freedom for aggregation in organic semiconductor materials? — ●STEFAN WEDLER¹, AXEL BOURDICK², STEPHAN GEKLE², FABIAN PANZER¹, CAITLIN MCDOWELL³, GUILLERMO C. BAZAN³, THUC-QUYEN NGUYEN³, and ANNA KÖHLER^{1,4} — ¹Soft Matter Optoelectronics, University of Bayreuth — ²Biofluid Simulation and Modeling, University of Bayreuth — ³Center for Polymers and Organic Solids, UC Santa Barbara — ⁴BIMF, University of Bayreuth

Planarity and rotational freedom play an important role for the aggregation process in organic semiconductors. Stiff and planar molecules seem to aggregate more easily. However, it is not clear whether these factors are a prerequisite or just a side effect of aggregation. We investigate the importance of planarity for aggregation using two small conjugated molecules, which consist of typical building blocks and differ only by the rigidity of their central unit. Their aggregation properties are compared by absorption and luminescence spectroscopy, both temperature dependent in solution as well as in-situ upon spincoating during film formation. MD simulations and DFT calculations reveal intermolecular arrangements. Our results suggest that planarity and torsional rigidity are indeed needed to promote aggregation, though too much rigidity can obstruct the pathway to ordered structures.

CPP 37.4 Wed 11:00 Poster B1

Investigating the Role of Planarity and Torsional Freedom for Aggregation in Organic Semiconductor Materials with the Help of MD and DFT Simulations — STEFAN WEDLER¹, ●AXEL BOURDICK², STEPHAN GEKLE², FABIAN PANZER¹, and ANNA KÖHLER¹ — ¹Experimental Physics II, University of Bayreuth — ²theoretical Physics VI, Biofluid Simulation and Modeling, University of Bayreuth

Organic photovoltaics has become a rapidly developing field, in which a lot of interesting systems are investigated for potential industrial applications. An ongoing challenge hereby is to relate the aggregation to the macroscopic properties of the solar cells. Planarity and rotational freedom play an important role during the aggregation process but the details of the mechanism is poorly understood. We use MD and DFT simulations to gain insights at molecular length scales which is difficult to access by experiments alone. We investigate two small conjugated molecules with a tandem like design structure, which differ in the planarity of the central donor units. The aggregation properties are investigated by optical experiments (presented on the accompanying poster by S. Wedler et al [1]), which we support with simulations. Free energy calculations and an investigation of the properties of the aggregates lead to a better understanding of the importance of planarity and rotational freedom.

[1]: Poster, What is the role of planarity and torsional freedom for aggregation in organic semiconductor materials?, S. Wedler et. al.

CPP 37.5 Wed 11:00 Poster B1

Water-processed active layers for hybrid photovoltaics using spray deposition techniques — ●LAUTARO DÍAZ PIOLA, VOLKER KÖRSTGENS, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Hybrid solar cells aim to combine the advantages of both, inorganic and organic materials in the active layer. The stability and high carrier mobility of the inorganic component, together with the potential low-cost production and feasibility of producing flexible devices from the organic component make the hybrid approach promising. In particular, the possibility for wet chemical device preparation in the organic material allows the use of scalable thin film coating techniques. Most of the research in this direction use organic solvents for the solar cell preparation, which does not lead to a full environmentally friendly approach. Therefore, the use of water soluble components for the organic material is of interest. In the present investigation we study the morphology of active layers for hybrid solar cells that are fully water processed using industrially scalable techniques such as spray coating. The investigation of the mesoscale structure and of the crystal structure is carried out via the scattering techniques GISAXS and GIWAXS, respectively, while UV/vis measurements are performed to study the absorption properties.

CPP 37.6 Wed 11:00 Poster B1

Impact of microstructure of hybrid perovskite powders on the mechanical properties of completely dry processed perovskite layers via pressing — ●MAXIMILIAN SCHULTZ¹, NICO LEUPOLD², KONSTANTIN SCHÖTZ¹, RALF MOOS², and FABIAN PANZER¹ — ¹Soft Matter Optoelectronics — ²Department of Functional Materials, all University of Bayreuth, Bayreuth, 95440, Germany

Optoelectronic devices based on hybrid perovskites have undergone a remarkable development within the last few years. However, state of the art processing approaches such as solution processing or evaporation suffer from an intrinsically high complexity, as the actual perovskite crystallization and its film processing happen simultaneously and are inextricably interconnected.

Here we present an alternative, entirely dry processing approach, which decouples perovskite crystallization and film formation, by using readily prepared perovskite powders and produce films by appropriate mechanical pressure treatment. We show how the used pressure and the powder microstructure, i.e. particle size and stoichiometry af-

fect the mechanical stability, compactness and surface roughness of the pressed layers. We further address how specific temperature treatment during the pressing step can be used to improve the properties of the pressed layer.

CPP 37.7 Wed 11:00 Poster B1

The 2-Step deposition method of mixed perovskites as a route to highly tunable optoelectronic properties — ●LENNART REB and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching, Germany

Mixed-cation lead mixed-halide perovskite solar cells with their impressive increase in efficiency over the last years, exceeding 22 per cent recently, are promising to play a role for future and sustainable power generation. Typically, the well-established 1-step spin-coating deposition technique is used for the perovskite layer to achieve these high efficiencies. In contrast, the 2-step deposition technique takes full advantage of the chemical tuneability of the perovskite semiconductors. Probing such perovskite thin films of different chemical compositions and concentrations with grazing incidence small- and especially wide-angle X-ray scattering allows assessing their morphological and crystalline structure. Spectroscopic measurements, e.g. ellipsometry, external quantum efficiency measurements, impedance spectroscopy, complement the structural investigations and thereby help us to increase our knowledge of some still poorly understood physical mechanisms in perovskite solar cells. More importantly, this is a necessary step to be able to tune the fascinating optoelectronic properties of perovskite to access the full range of other promising applications, such as photo-detectors and light emitting diodes.

CPP 37.8 Wed 11:00 Poster B1

Characterization and Encapsulation of Perovskite Solar Cells — ●BENJAMIN PREDESCHLY, LENNART REB, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching, Germany

Perovskite Solar Cells (PSCs) with their upscalable low-cost production from solution and their flexibility, suited for new application fields, are promising for future energy generation. Impressive power conversion efficiency (PCE) of more than 20 percent was reached recently as a result of optimized preparation techniques and material compositions. However, PSCs exposed to ambient conditions, especially humidity, show a decreasing PCE with time, making long-term stability a bottleneck towards commercialization. We process PSCs with the champion architecture and investigate them by various methods like external quantum efficiency measurements, scanning electron microscopy and grazing incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS) to relate the morphological changes to the degradation of the device performance. To improve the long-term stability, we develop a simple but effective method for mechanical encapsulation, protecting the PSC with a flexible foil from humidity. We track the PCE of the encapsulated PSCs over time, with a substantial improvement of the long-term stabilization in ambient condition, which is supported by GIWAXS measurements. Reaching long-term stability for PSCs is an important step towards their success.

CPP 37.9 Wed 11:00 Poster B1

Mesoporous Titania Backfilled with Heavy Element Containing Small Molecules and High-Efficiency Polymer PTB7-Th for Hybrid Photovoltaics — ●RAPHAEL MÄRKEL¹, NURI HOHN¹, EMANUEL HUPF², GAETANO MANGIAPIA³, MATTHIAS POMM³, ERIC RIVARD², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — ²University of Alberta, Department of Chemistry, Edmonton, Canada — ³Helmholtz-Zentrum Geesthacht at Heinz Maier-Leibnitz Zentrum, Garching

Hybrid photovoltaic devices have recently attracted significant research attention due to improvements in efficiency by tailoring the organic-inorganic interface. Mesoporous titania films are synthesized utilizing polystyrene-*b*-polyethyleneoxide diblock copolymer templating in a sol-gel approach. A hybrid photovoltaic active layer is then achieved by infiltrating the organic component into the resulting mesoporous titania scaffold. We investigate the backfilling of organic polymer PTB7-Th and novel tellurophene Phen-Te-BPinPh small molecule into the mesoporous titania films by ToF-GISANS. While the backfilling efficiency of PTB7-Th proves to be sensitive to the polymer concentration, Phen-Te-BPinPh is backfilled easily into the titania matrix due to its small size. Complementary X-ray scattering techniques are used in

obtaining the SLD profile required for ToF-GISANS analysis and the crystal structure of respective thin films. Conclusions derived from real space investigation via SEM are found in agreement with these results.

CPP 37.10 Wed 11:00 Poster B1

Comparative study of interface modification and passivation approaches on low-temperature SnO₂ and their effect on perovskite solar cell performance — ●MAX GRISCHEK, PHILIPP TÖCKHORN, GANNA CHISTIANKOVA, LUKAS KEGELMANN, and STEVE ALBRECHT — Helmholtz-Zentrum Berlin, Berlin, 12489, Germany.

SnO₂ is a widely used electron transporting material (ETM) in planar n-i-p-type perovskite solar cells (PSC). It allows high Voc above 1.15 V and efficiencies close to 21%. In addition, low process temperatures make SnO₂ a suitable ETM for flexible foils or monolithic silicon-perovskite tandem solar cells. However, high device efficiencies require thorough optimization of the SnO₂ surface. This study investigates modification and passivation approaches on SnO₂ and compares their effect on chemical composition, energetics, charge carrier extraction, interface recombination and performance in PSCs. Firstly, a dipole interlayer between SnO₂ and the absorber is utilized to reduce the SnO₂ workfunction and its conduction band offset to the absorber, as implied by UPS. This is shown to reduce interface recombination losses and increase the device Voc, as revealed by absolute PL and J-V measurements. Similar effects are observed when introducing very thin interlayers of PCBM/PMMA mixtures. The best PSC performance is achieved by an O₂-plasma treatment of the SnO₂ surface. Using J-V, TRPL and absolute PL measurements, less non-radiative recombination and faster charge carrier extraction are observed. This plasma treatment leads to reduced hysteresis and an enhancement in device efficiency to 18.1%.

CPP 37.11 Wed 11:00 Poster B1

Preparation of Mg_xZn_{1-x}O nanoparticles through a wet chemical route for applications in optoelectronic devices — ●ANDREAS RINGLEB and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Zinc oxide (ZnO) is an n-type semiconductor and a promising candidate for applications in various types of optoelectronic devices due to its wide direct bandgap of about 3.3 eV and high exciton binding energy of approximately 60 meV. The targeted substitution of Zn with magnesium enables a tunable band gap of Mg_xZn_{1-x}O between 3.3 and 7.8 eV through control of the Mg-content. Mg_xZn_{1-x}O nanoparticles have been prepared from acetate precursors through a wet chemical route. Thin films have been deposited on quartz and FTO coated glass substrates from pastes by doctor-blading and subsequent drying and/or annealing. XRD and SEM have been used to study the morphology and crystal structure of these films. The modulation of the band gap has been confirmed by UV-Vis spectroscopy. Elemental composition has been studied by XPS and EDX. Nanoparticle size has been measured by means of dynamic light scattering (DLS). A focus has been put on the homogeneity and porosity of the resulting films since they are especially suited for future applications in hybrid photovoltaics, such as dye-sensitized solar cells (DSCs), quantum-dot solar cells (QDSCs) or perovskite solar cells (PSCs).

CPP 37.12 Wed 11:00 Poster B1

Time-Resolved Microwave Conductivity on Lead Halide Perovskite Films — ●PATRICK DÖRFLINGER¹, ANDREAS BAUMANN², ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Perovskite solar cells are one of the most promising new photovoltaic technologies with steadily rising efficiencies. To further improve their potential performance and stability, it is essential to understand their optoelectrical properties as well as to develop novel, not yet established, perovskite materials. These must be extensively characterized prior to solar cell fabrication. With Time-Resolved Microwave Conductivity (TRMC) the mobility and lifetime of photogenerated charge carriers in a perovskite layer can be determined in a non-contact way. The TRMC measurement technique is based on the interaction of an applied electro-magnetic field with the charge carriers in the semiconductor material, which leads to a time-dependent change in conductance. We use TRMC to probe the charge carrier dynamics in various perovskite materials, such as methylammonium lead iodide and mixed cation and halide perovskite.

CPP 37.13 Wed 11:00 Poster B1

Influence of Ammoniumvaleric Acid on the Current-Voltage Hysteresis of $MAPbI_3$ Thin Films on Microstructured Electrode Arrays — •JONAS GLASER, JONAS HORN, RAFFAEL RUESS, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

As organic-inorganic lead halide perovskite solar cells have emerged as promising technology for low-cost and highly efficient photovoltaics, issues such as long term stability and hysteresis in the current-voltage characteristics are put into focus of interest. Microstructured metal electrode arrays can be used to investigate electrical and interface properties of such semiconducting layers. In this work, thin films of methylammonium lead iodide ($MAPbI_3$) were prepared on microstructured platinum arrays in order to study the I - V -characteristics under different applied voltages. Partial substitution of methylammonium by ammoniumvaleric acid was found to reduce the observed hysteresis and, also, decreased the measured current densities by about one order of magnitude. It was found that the appearance of the hysteresis strongly depends on the chosen measurement conditions, e. g., scan rate and voltage range. Therefore, we assume that the application of an external electric field leads to alignment of dipoles and migration of ions and vacancies in the perovskite thin films, which then shows two kinds of I - V -hysteresis, one for smaller voltages that is not influenced by the scan rate and another one for larger applied electric fields whose extent depends on the scan rate.

CPP 37.14 Wed 11:00 Poster B1

Electrical Characterization of the Double Perovskite $Cs_2AgBiBr_6$ — •FABIAN SCHMITZ, JONAS HORN, and DERCK SCHLETTWEIN — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik

Hybrid organic-inorganic lead halide perovskites have been investigated intensively during the last decade. Issues of chemical stability, interfacial contact formation and the toxicity of lead represent the main present challenges for perovskite solar cells. Fully inorganic absorbers, such as the double perovskite $Cs_2AgBiBr_6$ provide a possible solution to some of these problems. Despite rather fast nongeminate recombination, this material is not only a promising approach to overcome the stability issues but also facilitates ambient processing with less problematic solvents and reduces the toxicity problems of prospective cells.[1] We prepared such inorganic layers to evaluate their suitability as absorber or buffer layers in solar cells by measuring their I - V -characteristics in the dark and under illumination, incident photon conversion efficiency and open circuit voltage decay. Further, we measured the electronic properties of $Cs_2AgBiBr_6$ layers using symmetric metal contacts in order to investigate I - V -hysteresis, which is a good indicator of contact characteristics in perovskite solar cells.

[1] R. Kentsch, M. Scholz, J. Horn, D. Schlettwein, K. Oum, T. Lenzer, *J. Phys. Chem. C*, **122**, 25940 (2018).

CPP 37.15 Wed 11:00 Poster B1

Charge Carrier Dynamics of the Double Perovskite $Cs_2AgBiBr_6$ — •ROBIN KENTSCH¹, MIRKO SCHOLZ¹, JONAS HORN², DERCK SCHLETTWEIN², KAWON OUM¹, and THOMAS LENZER¹ — ¹Physikalische Chemie, Universität Siegen, Adolf-Reichwein-Str. 2, 57076 Siegen, Germany — ²Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Hybrid lead perovskites have reached power conversion efficiencies above 23% in photovoltaic applications. Yet, major drawbacks remain. These include the toxicity of lead as well as the insufficient long-term stability. The ongoing search for environmentally friendly alternatives has identified so-called "double perovskites" with the general formula $A_2MM'X_6$ as potential replacements. Here, we report results for the charge carrier dynamics of the lead-free silver-bismuth double perovskite $Cs_2AgBiBr_6$ by employing time-resolved optical spectroscopy and electrical measurements.[1] Upon photoexcitation, we identify fast charge carrier cooling processes and pronounced coherent oscillations in the picosecond range. This is consistent with strong electron-phonon coupling. Furthermore, excitonic contributions are found. Electron-hole recombination occurs in the time range from several hundred picoseconds to microseconds. Implications of this charge carrier dynamics for the energy conversion efficiency of this lead-free perovskite in the real device will be discussed.

[1] R. Kentsch, M. Scholz, J. Horn, D. Schlettwein, K. Oum, T. Lenzer, *J. Phys. Chem. C*, **122**, 25940 (2018).

CPP 37.16 Wed 11:00 Poster B1

Unravelling the origin of double peak emission of hybrid perovskites — •KONSTANTIN SCHÖTZ¹, ABDELRAHAM ASKAR², WEI PENG³, DOMINIK SEEBERGER¹, TANAJI P. GUJJAR¹, MUKUNDAN THELAKKAT¹, SVEN HÜTTNER¹, OSMAN BAKR³, KARTHIK SHANKAR², ANNA KÖHLER¹, and FABIAN PANZER¹ — ¹University of Bayreuth, 95440 Bayreuth, Germany — ²University of Alberta, Edmonton, AB T6G 1H9, Canada — ³King Abdullah University of Science and Technology (KAUST), Thuwal23955-6900, Kingdom of Saudi Arabia

The optical properties of hybrid perovskites are known to be sensitively interconnected with their structure, which is soft and thus prone for changes. Double photoluminescence (PL) peaks have been reported at low temperatures, and recently also at room temperature, though there is still no consensus about the origin of this double PL peak structure. Here we show that the occurrence of the additional PL peak is not limited to one specific material composition and that it occurs in single crystals as well as in thin films, rendering it a general phenomenon. We systematically investigate the origin of this additional PL feature by measuring and analyzing temperature-dependent one- and two-photon-induced PL. Together with fluence dependent measurements, optical modelling and systematic surface treatments, we can differentiate the impact of various possible physical and optical effects such as e.g. self-absorption, excited state diffusion or surface states, in order to gain a detailed and elaborated understanding on the occurrence of multiple PL peak phenomena in hybrid perovskites.

CPP 37.17 Wed 11:00 Poster B1

Using polymeric hole-injection layers for solution-processed Perovskite-based light-emitting diodes — •TASSILO NAUJOKS¹, THOMAS MORGENSTERN¹, MANUEL ENGELMAYER¹, MATTHEW JUROW², YI LIU², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, United States of America

Replacing common organic emitters with Lead-Halide Perovskites, like $CsPbBr_3$, is a promising approach towards low cost, efficient and narrow emission-band LEDs. While showing high photoluminescent quantum-yields in thin films [1], achieving similarly high performance in elec devices proves to be challenging. Protection of the hole injection layer either by shielding films or orthogonal solvents has a huge effect on the optoelectronic properties. A hole-injection layer for a solution-processed emitter should not be impaired by the respective solvent. Such films can be formed by crosslinked polymers.

In this study we investigate the synergy of poly-TPD as hole-injection polymer and $CsPbBr_3$ quantum dots as emitter in an otherwise common organic LED stack. Furthermore the use of different polymers or combinations show significantly increased efficiency. The efficiency proves to be correlated to the respective solvent susceptibility of the layers. The findings are of huge importance for future applications of lead-halide perovskites in optoelectronic lighting applications.

[1] BECKER, MICHAEL, *et. al.* Nature **553**, 189 (2018)

CPP 37.18 Wed 11:00 Poster B1

p-type doping of organic semiconductors with polycyclic acceptors — •ADRIANA RÖTTGER¹, BERTHOLD WEGNER¹, ANDREAS OPITZ¹, and NORBERT KOCH^{1,2} — ¹Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Predictions about ion pair formation (IPA) of organic donor/acceptor blends can be made based on redox-potentials measured by cyclic voltammetry in solution or based on ionisation energies (IE) / electron affinities (EA) measured on thin films by direct / inverse photoelectron spectroscopy. Here, we investigate the accuracy of these predictions for two different organic semiconductor systems in solutions and thin films. At first optical absorption spectroscopy is employed to determine IPA yield in mixtures of two pyrene derivatives as donors and three polycyclic acceptors, which exhibit similar chemical structures. Since the predictions from redox potential and IE/EA do not differ significantly, both prove accurate. The second system consists of the polymer P3HT doped with the same set of acceptors. Again, optical absorption spectroscopy was used to determine the presence of ionic molecular species as well as formed polarons in P3HT. These predictions also prove accurate. In addition, scanning force microscopy and current-voltage measurements were performed to examine the impact of doping on surface morphology and electrical conductivity of P3HT films, respectively.

CPP 37.19 Wed 11:00 Poster B1

Ultrafast photophysics of TIPS-tetracenophane — ●CLEMENS ZEISER¹, ANDREAS GÖTTLER², LUCA MORETTI³, MARGHERITA MAIURI³, GIULIO CERULLO³, TETSUHIKO NAGAHARA^{3,4}, HOLGER F. BETTINGER², and KATHARINA BROCH¹ — ¹Institut für Angewandte Physik, Universität Tübingen, Germany — ²Institut für Organische Chemie, Universität Tübingen, Germany — ³Dipartimento di Fisica, Politecnico di Milano, Italy — ⁴Department of Chemistry and Materials Technology, Kyoto Institute of Technology, Japan

Singlet exciton fission is a process which could help to improve the power-efficiencies of silicon solar cells by providing a solution to overcome the Shockley-Queisser-Limit. Tetracene is one of the most promising compounds for application as a singlet fission layer [1] and its photophysical properties thus need to be well understood. Chemically linked tetracene dimers [2] provide an opportunity to alter the relative orientation of two tetracene monomers and, thus, to study its influence on the singlet fission time constant. Here we report on the photophysics of the linked TIPS-tetracene dimer TIPS-tetracenophane (TIPS-TCP) [3], where the two tetracene monomers are doubly linked and facing each other directly. Using transient absorption spectroscopy on thin films of TIPS-TCP, we find a singlet lifetime significantly longer than that of tetracene and interpret this finding as an ultrafast creation of a triplet pair state, but a hindered separation of the two triplets.

[1] R. W. MacQueen et. al., *Mater. Horiz.* **5** (2018) [2] N. V. Korovina et. al., *J. Am. Chem. Soc.* **140** (2018) [3] H. F. Bettinger et. al., *Org. Chem. Front.* **4** (2017)

CPP 37.20 Wed 11:00 Poster B1

Ab initio many-body study of the electronic structure of the Lewis acid Tris(pentafluorophenyl)borane (BCF) — ●RICHARD SCHIER, ANA M. VALENCIA, and CATERINA COCCHI — Physics Dept., Humboldt-Universität zu Berlin und IRIS Adlershof

Doping in organic semiconductors is an attractive area of research for molecular electronics. The Lewis-acid tris(pentafluorophenyl)borane (BCF)[1] is a strong electron acceptor already successfully employed as a p-dopant in organic semiconductors[2]. However, a clear understanding of its electronic structure is still missing. We fill this gap in a first-principles study based on density-functional theory with hybrid functionals and many-body perturbation theory, including the GW approximation, as implemented in the MOLGW code[3]. For comparison, we relate BCF to its building block hexafluorobenzene (C6F6).

For BCF, we find that both the LUMO and the HOMO are non-degenerate. The LUMO is mainly localized around the boron atom, consistent with the electron-withdrawing character of this molecule. On the other hand, the HOMO is distributed only on the phenyl-rings without any participation of the boron. From GW, the HOMO energy of BCF and C6F6 differs by about 250 meV, suggesting that these two molecules have approximately the same ionization potential.

[1] Körte et al., *Angew. Chem.* **56**, 8578 (2017) [2] Pingel et al., *Adv. Electron. Mater.* **2**, 1600204 (2016) [3] Bruneval et al., *Comput. Phys. Commun.* **208**, 149 (2016)

CPP 37.21 Wed 11:00 Poster B1

The statistics of photoluminescence quantum yield measurements — ●FELIX FRIES, HEIDI THOMAS, MAX GMELCH, TIM ACHENBACH, and SEBASTIAN REINEKE — IAPP, Technische Universität Dresden, 01187 Dresden, Germany

Measuring the photoluminescence quantum yield (PLQY) is both a well-known and often used method within many different fields of luminescent materials. Knowing a material's PLQY not only allows estimating its use for applications but also gives further insights into the physics within. Calculating the radiative rate of a fluorescent decay is only one of many examples. The common setup comprises a light-source for excitation, an integrating sphere, and a spectrometer or photodiode for signal detection. However, to assure accurate results the measurement relies on a very stable light source.

Here we show that even with low cost devices as LEDs, reliable values with a low statistical error can be obtained. Therefore, we investigate the importance of a right statistical treatment of the measured data. Furthermore, sources of systematic errors in the setup can easily be detected that way.

Evaluating the results of PLQY measurements on solid-state samples of organic molecules showing both fluorescent and phosphorescent emission at room temperature (biluminescence), we are able to deduce information about the singlet's and triplet's PLQY separately and also about intermolecular interaction processes like singlet-triplet annihilation.

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CPP 37.22 Wed 11:00 Poster B1

Molecular design of λ^6 -phosphorus compounds for OLED applications — ●JULIANA NAIR, JONAS KÖHLING, GERD-VOLKER RÖSCHENTHALER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic light emitting diodes (OLEDs) are one of the leading technologies used as active optoelectronic device in displays. Currently, in OLED displays the most challenging quest is to synthesize and design efficient and stable blue emitters. To achieve this goal it is of great interest to evaluate possible molecules prior to synthesis and to optimize their molecular design.

In this study a large amount, i.e. 151 derivatives, of λ^6 -phosphorus fluorescent compounds were evaluated regarding their light emitting properties. As basic structure the central phosphorous atom is bound to one derivative of 8-Quinololinol as well as 4 Fluorine atoms. 8-Quinololinol was systematically varied by introduction of substituents from strong electron withdrawing groups (EWG) towards strong electron donating groups (EDG). Besides the mesomeric and inductive electron withdrawing and donating effects also the position of the substituent has a crucial influence on the calculated emitting wavelength of these fluorophores. To determine the emitting wavelength of an isolated molecule time-dependent density functional theory (B3LYP/6-31+G(d,p)) was employed. EWGs tend to increase the bandgap if placed on the benzene ring of the ligand, where EDGs show the same effect when substituted on the pyridine ring of the ligand. This allows to tune the calculated bandgap between 3.2 - 4.1 eV.

CPP 37.23 Wed 11:00 Poster B1

Micro-Refractometry and Local-Field Mapping with Single Molecules — ANDREI V. NAUMOV^{1,2}, ALEXEY A. GORSHELEV¹, MAXIM G. GLADUSH^{1,2}, TATIANA A. ANIKUSHINA^{1,2}, ALINA V. GOLOVANOVA^{1,2}, JÜRGEN KÖHLER^{3,4,5}, and ●LOTHAR KADOR³ — ¹Institute for Spectroscopy, Russian Academy of Sciences, Moscow 108840, Russia — ²Moscow State Pedagogical University, Moscow 119435, Russia — ³University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — ⁴University of Bayreuth, Spectroscopy of Soft Matter, 95440 Bayreuth, Germany — ⁵Bavarian Polymer Institute, 95440 Bayreuth, Germany

Single-molecule spectroscopy at cryogenic temperatures was used to measure and map the local index of refraction in a solid with nanometer resolution. The natural zero-phonon linewidth of 1950 single terrylene molecules in a matrix of polycrystalline *n*-hexadecane was measured at $T = 1.5$ K where thermal broadening effects are absent. The linewidth is then determined by the excited-state lifetime which depends on the local density of states of the electromagnetic field, i.e., the local refractive index. The spatial resolution is on the order of a few nanometers; it is given by the accuracy with which fluorescing single molecules can be localized. Unexpectedly large fluctuations of the local refractive index between 1.1 and 1.9 were found. Three different distance ranges could be roughly identified, in which the fluctuations have different magnitudes.

CPP 37.24 Wed 11:00 Poster B1

Voltage-dependent shift of the emission spectra of exciplex OLEDs — ●THOMAS SCHRÖTHER, THOMAS ZECHEL, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Exciplexes are excited states between two different molecules in an organic light emitting diode (OLED). After electrical excitation, the hole is located in the highest occupied molecular orbital (HOMO) of the donor material and an electron occupies the lowest unoccupied molecular orbital (LUMO) on the acceptor. These states are recently used to improve the external quantum efficiencies in OLEDs.

In this work we investigated the electroluminescence spectra of the material combination m-MTDATA:BPhen forming exciplex states in OLED devices using two layouts, where the molecules were either mixed or in separate planar layers. After varying the applied voltage, it was possible to discern between two different kinds of spectral shifts that depend on the layout by fitting the data with multiple Gaussian functions. In the mixed OLED the positions of the individual peaks are constant but their contribution to the emission changes. Whereas every single Gaussian shifts with constant height in the planar device resulting in a shift of the whole curve. Based on the theoretical description by Monkman and Al Attar [1] as well as Linderl [2], we present two models to explain this observed difference.

[1] H. A. AL ATTAR, A. P. MONKMAN, *Adv. Mat.* 28 (36), 8014–8020 (2016), DOI: 10.1002/adma.201600965

[2] T. LINDERL, PhD thesis, University of Augsburg (2017).

CPP 37.25 Wed 11:00 Poster B1

Monitoring Singlet/Triplet Interconversion in OLEDs — ●ULLI VON GOSCINSKI, DIRK HERTEL, and KLAUS MEERHOLZ — University of Cologne, Institute of Physical Chemistry, Luxemburger Str. 116, 50939 Cologne, Germany

In order to reach highest efficiencies in organic light-emitting diodes (OLEDs), excitons from both, singlet as well as triplet states, have to be harvested. Initially, they are distributed in a ratio of 1:3 according to spin statistics. Usually, a conversion between these states by intersystem crossing or reverse intersystem crossing is required to realize highly efficient OLEDs e.g. devices based on thermally activated delayed fluorescence (TADF) [1]–[2]. The rate of interconversion can be directly manipulated by small magnetic fields (< 150 mT). We utilize these magnetic field effects, namely magneto conductivity (MC), magneto electroluminescence (MEL) and magneto photoluminescence (MPL) to monitor singlet/triplet conversion events. The correlation of MEL and MPL is essential to clarify the underlying mechanism because of the different initial population of the singlet and triplet levels upon electro- or photoexcitation. Temperature dependent luminescence and conductivity measurements allow further insights in the nature of spin state conversion in organic emitter molecules.

[1] Zhang, Q. et al., *Nat. Photonics* 8, 326–332 (2014).

[2] Kaji, H. et al., *Nat. Commun.* 6, 8476 (2015).

CPP 37.26 Wed 11:00 Poster B1

Kinetic Monte Carlo simulations of energy transfer processes in an organic light emitting diode — ●LEANNE PATERSON and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic light emitting diodes (OLEDs), utilise small organic molecules, in order to achieve an emissive electroluminescent layer. Ultra-thin, lightweight and flexible characteristics offer a highly enticing substitute, in comparison to their inorganic counterpart. It is therefore understandable why there has been a large amount of research, focused on enhancing the efficiency and stability of OLEDs. However, achieving a blue OLED, which is both efficient and stable, has proven to be problematic. The challenge originating with the limitations of the individual blue emitters, be that phosphorescent or fluorescent. Commercially, stability is prioritised, in order to achieve a long-lived consumer product, but with battery life on portable devices being the cost of any inefficiency, it is vital that blue OLEDs become more efficient. By developing a Kinetic Monte Carlo (KMC) code, for the study of excited molecule energy transfer, the individual emitters can be studied. Making direct comparisons to experimentally achieved results, it is possible to investigate processes, such as Förster resonance energy transfer (FRET) and Dexter energy transfer. Using the KMC code a unicoloured phosphor-sensitised fluorescence (UPSF) OLED and the corresponding energy transfer processes are explored. The fundamental efficiency and lifetime limits are identified, providing a clear insight, and expanding on experimentally achieved results.

CPP 37.27 Wed 11:00 Poster B1

Derivates of Imidazo[1,5-a]pyridine as Blue Light-Emitters for OLED — ●GEORG ALBRECHT¹, CARINA RÖSSIGER², JASMIN MARTHA HERR², HARALD LOCKE², HISAO YANAGI³, RICHARD GÖTTLICH², and DERCK SCHLETTWEIN¹ — ¹Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — ²Justus-Liebig-Universität Gießen, Institut für Organische Chemie — ³Nara Institute of Science and Technology

1,3-disubstituted imidazo[1,5-a]pyridines are discussed for applications in material science as new and oxidation-stable blue emitters, e.g. for organic light emitting diodes (OLED). We investigated the stepwise change of physical properties in solution and solids when introducing nitrogen atoms and/or increasing sizes of aromatic rings as substitutional moieties. As an extension, a larger homologue, i. e., imidazo[1,5-a]quinoline was also studied. Absorption and emission spectra as well as quantum yields were measured and interpreted based on DFT calculations. Single crystals were grown from solution or by entrainer sublimation and thin films were prepared by physical vapor deposition. Fluorescence microscopy was used to investigate on crystal emission. Comparing the results obtained at thin films and in solution, the molecular coupling in the different phases is assessed and their applicability in OLED devices is discussed.

CPP 37.28 Wed 11:00 Poster B1

Excimer formation in carbazole-based host materials for OLEDs — ●EIMANTAS DUDA¹, ALEXANDER RUDNICK¹, SERGEY BAGNICH¹, DANIEL WAGNER², PETER STROHRIEGL^{2,3}, and ANNA KÖHLER^{1,3} — ¹Soft Matter Optoelectronics, Department of Physics, University of Bayreuth, Germany — ²Macromolecular Chemistry I, Department of Chemistry, University of Bayreuth, Germany — ³ayreuth Institute of Macromolecular Research, University of Bayreuth, Germany

We present a detailed spectroscopic study on bipolar OLED host materials in solution and in neat film from 10K to room temperature. The hole-transporting part is based on the carbazole moiety, while the electron-transporting part is based on triazine moiety. We find that the tendency to excimer formation depends sensitively on the planarity of the molecule, counterintuitively with more excimer formation for the planar ones. Quantum chemical calculations indicate that this results from excited state localization onto the outer carbazole moiety for the non-planar compounds.

CPP 37.29 Wed 11:00 Poster B1

Density of States at the Interface of Organic Permeable-Base Transistors — ●HENNING ISEKE, FELIX DOLLINGER, HANS KLEEMANN, and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Dresden, Germany

Organic permeable-base transistors (OPBT) are among the best performing organic transistors reaching on/off ratios of $>10^8$ and transition frequencies of >40 MHz. These vertical transistors resemble solid-state triodes where the current is controlled by the potential of a permeable electrode denoted as base. As for other organic transistors, the knowledge of the interfacial density of states is a key in order to develop an in-depth understanding of the device operation as well as degradation processes. However, for OPBTs, this interfacial density of states has not been revealed so far.

D. V. Lang et. al proposed a method to determine the density of states in organic field effect transistors by means of temperature dependent transfer characteristics. Here, we validate this method and discuss under which conditions it is applicable to OPBTs. Furthermore, we carry out systematic device investigations under various stress conditions, and discuss how this stress affects the interfacial density of states. This study helps to develop a deeper understanding of the underlying mechanisms of degradation in OPBTs. Moreover, it enables more systematic approaches for device optimization due to the knowledge of the interfacial density of states.

CPP 37.30 Wed 11:00 Poster B1

Influence of Humidity on Work Function of PEDOT:PSS Thin Films — ●AMAN ANAND^{1,2}, RICO MEITZNER^{1,2}, SHAHIDUL ALAM^{1,2}, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany

Poly (3,4-ethylenedioxythiophene): poly (styrene sulfonate) (PEDOT: PSS) is the most common and successful commercial conductive polymer used in the field of optoelectronics. Its properties are high transparency in the visible range, high electrical conductivity, excellent chemical and physical stability, high ductility, good film-forming properties, and high work function among the other polymers. PEDOT: PSS is highly hygroscopic in nature, which limits its applications. In the present work, the influence of moisture content due to hygroscopicity of the PEDOT: PSS thin film is in regard to the change of work function. Different modifications on the PEDOT: PSS which wants to lead to better compatibility in forming contacts with organic semiconductors.

CPP 37.31 Wed 11:00 Poster B1

IR spectroscopic investigation of precursor aromatization of poly(p-phenylene) — ●RAINER BÄUERLE^{1,2}, ALI ABDULKARIM³, KARL-PHILIPP STRUNK^{1,4}, JAN FREUDENBERG^{2,3}, DANIEL JÄNSCH^{2,3}, SEBASTIAN BECK^{1,2}, and ANNEMARIE PUCCI^{1,2} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²InnovationLab, Heidelberg — ³Organisch-chemisches Institut, Universität Heidelberg — ⁴Centre for Advanced Materials, Universität Heidelberg

Two challenges of the long-desired prototype of a conjugated polymer semiconductor poly(para-phenylene) (PPP) are its difficult synthesis and its insolubility. Both problems have been recently overcome by

a new precursor route. [1] We investigate and compare the thermal aromatization of a kinked and a linear precursor polymer using IR spectroscopy and UV-vis ellipsometry on thin films.

For a kinked precursor polymer we find that the aromatization speed increases with increasing temperature and decreases with decreasing layer thickness yielding unordered PPP induced by the unordered precursor.

In contrast to this, the aromatization kinematics of a linear precursor is independent from layer thickness and already the thin film of the precursor exhibits near-range order which is passed through to the converted PPP. The low conversion temperature (<250 °C) makes our PPP feasible for fabrication of plastic devices. It was further proven that PPP is long-time stable and shows no degradation.

[1] A. Abdulkarim et al., *J. Am. Chem. Soc.*, 2016, 138 (50), pp 16208-16211

CPP 37.32 Wed 11:00 Poster B1

Polarisation anisotropy in organic guest-host systems — ●FELIX HÖHNLE, THOMAS MORGENSTERN, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Exciting dye molecules with linearly polarised light leads to an anisotropic excited state population of the emitters' transition dipole moments (TDMs). Depending on different depolarisation effects before light emission –such as rotational diffusion (mostly in solutions), intra- and intermolecular exciton migration or conformational changes of molecules– the emitted light can also be partly polarised. The extent of the latter is quantified by the anisotropy value r . It relates the intensities emitted with polarisation parallel and perpendicular with respect to the polarisation of the exciting light.

In this work we probed thin solid films of commonly used organic emitters doped into a matrix. It could be shown that polarisation anisotropy can be increased by decreasing the dye concentration in the guest-host system, which must be due to reduced intermolecular exciton transfer since no other processes should be present in a solid film. Depending on the exact material, values close to the theoretical maximum of $r = 0.4$ were reached. Additionally, we see that excess energy of excitons affects the migration process and thus the anisotropy.

The above effect can also influence TDM orientation measurements which aim to improve device efficiencies. At low dye concentrations, the hindered equilibration of excitons to all orientations upon light emission can lead to erroneous (pseudo-horizontal) orientation values.

CPP 37.33 Wed 11:00 Poster B1

Comparison of a solution-based doping process and doping via coevaporation for thin layers of organic semiconductors — ●MARIUS GEBHARDT, THERESA LINDERL, EDUARD MEISTER, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, Germany

For the use of organic layers in thermoelectric devices a high electrical conductivity and Seebeck coefficient combined with low thermal conductivity is essential. In this work we focus on increasing the electrical conductivity by different doping approaches.

Thin evaporated layers of the electron donor molecules DIP, 6T and DBTTF, on top of which the strong electron acceptor F4-TCNQ dissolved in solution was spincoated, are compared to coevaporated layers with F6-TCNNQ as the electron acceptor. To study the degree of doping as well as to discern between ion pair (IPA) and charge transfer complex (CTX) formation the transmission spectra of the samples were measured. The impact of the doping processes on the surface and bulk morphology was examined via atomic force microscopy and X-ray diffraction. Strong indications for the formation of charge transfer crystals are observed in some of the discussed material combinations. First conductivity measurements, however, indicate that the electrical transport is affected in different ways.

CPP 37.34 Wed 11:00 Poster B1

From spin-coating to slot-die printing in organic solar cells: Where do we lose the efficiency? — ●DANIEL KROH¹, JEGADESAN SUBBIAH², DOOJIN VAK³, DAVID JONES², and ANNA KÖHLER¹ — ¹Soft Matter Optoelectronics, University of Bayreuth — ²School of Chemistry, Bio21 Institute, University of Melbourne, Australia — ³CSIRO Manufacturing, Melbourne, VIC 3168, Australia

The field of solution-processed organic solar cells (OSCs) has been dominated by polymeric semiconductors, though molecular materials with high power conversion efficiencies (PCEs) in OSCs have been reported and are attractive due to their reduced batch-to-batch vari-

ation. For example, devices based on the donor molecule BQR are thermally stable and show a low thickness dependence of the active layer with PCEs reaching 10.7%. These properties suggest BQR as an excellent choice for roll-to-roll processing, which is relevant for industrial fabrication. However, within the transition from spin coated to slot-die printed devices a drop in efficiency appears. Although this drop is commonly observed, its reason is not clear. We use time resolved and temperature dependent UV-Vis absorption and photoluminescence spectroscopy to investigate the formation of spin-cast and slot-die coated films and the resulting morphology in-situ during the deposition process of BQR:PC70BM blends. Comparing the two deposition methods allows us to get a better understanding of the correlation between film morphology and device performance. With this insight, we can optimize the conditions of the slot-die printing process to reduce the drop in PCE, which is an important step towards industrial fabrication.

CPP 37.35 Wed 11:00 Poster B1

Understanding the mechanism behind the novel doping of organic semiconductors via Lewis Acids — ●SIMON BIBERGER¹, VIKTOR BRUS², DAVID CAO², BRETT YURASH², DIRK LEIFERT³, THUC-QUYEN NGUYEN², and ANNA KÖHLER¹ — ¹Experimental Physics II, University of Bayreuth, Bayreuth, Germany — ²Center for Polymers and Organic Solids, UCSB, Santa Barbara, USA — ³Organisch-Chemisches Institut, Westfälische Westfälische Wilhelms-Universität, Münster, Germany

To p-dope organic semiconductors F4TCNQ is commonly used. This doping mechanism relies on the electron transfer from the HOMO of the semiconductor to the LUMO of the dopant. This occurs by a match of those energy levels. For a solution-processed semiconductor this approach suffers from the differential solubility of the dopant, the charge-transfer complex and of the polymer what ultimately limits the processability of the doped semiconductor. In this study we use electrophilic Lewis acids to p-dope conjugated polymers. Work by Zalar et al. (*Adv. Mat.* 2014, 26, 727-727) showed an increased mobility after addition of Lewis acid. Yet the mechanism behind this doping approach is still elusive. To understand this approach we systematically investigate the effect of structural and electronic factors by varying, e.g., the donor and acceptor strength of the polymer. Optical and electrical characterization, using, e.g., optical spectroscopy and EPR, were performed to understand the influence of the adduct formation on the properties of the polymer.

CPP 37.36 Wed 11:00 Poster B1

Consequences of Ionic Adsorption on the Photovoltage in Dye-sensitized Solar Cells — ●RAFFAEL RUESS¹, SABINA SCARABINO², ANDREAS RINGLEB¹, KAZUTERU NONOMURA³, NIKOLAOS VLACHOPOULOS³, ANDERS HAGFELDT³, GUNTHER WITTSTOCK², and DERCK SCHLETTWEIN¹ — ¹Justus-Liebig-Universität Gießen, Institut für Angewandte Physik — ²Universität Oldenburg, Institute of Chemistry — ³Ecole Polytechnique Federale de Lausanne, Institute of Chemical Sciences and Engineering

Reversible redox couples that allow faster charge transfer than the classical I^-/I_3^- can improve the performance of dye-sensitized solar cells (DSSCs). In our work we study a cationic Co-based redox couple that promises high open-circuit photovoltages V_{oc} by reducing the energy-loss during the dye regeneration process. However, we found that such cations lead to different surface reactions with oxide semiconductors compared to the anionic I^-/I_3^- . By using photoelectrochemical and optical techniques we noticed that the semiconductor surface charge plays a major role in determining V_{oc} by stabilizing or destabilizing the electronic states in the semiconductor. Further, light-harvesting of the dye is influenced by electric fields arising from adsorbed ions at the semiconductor surface inducing a Stark effect on the molecular orbitals. We conclude that the ionic character of electrolyte components such as the redox couple or electrolyte additives significantly influence the energetics in the cell and, thus, V_{oc} . Our work shows that the control of semiconductor surface charge is key in improving the DSSC performance.

CPP 37.37 Wed 11:00 Poster B1

Comparison of sequential and solution-mixed doping of poly(3-hexylthiophene) in thin films using the Lewis acid BCF — ●DOMINIQUE LUNGWITZ¹, AHMED E. MANSOUR¹, ANDREAS OPITZ¹, and NORBERT KOCH^{1,2} — ¹Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Molecular doping of organic semiconductors is a commonly used technique to increase the conductivity and tune the electronic structure. Sequential doping method allows for an improved film morphology with controlled dopant load by avoiding agglomeration of polymer and dopant before deposition as observed partially for solution-mixed doping [1]. Herein, we investigate the changes in the electronic structure by photoemission spectroscopy and dopant distribution for sequentially and solution-mixed doping of poly(3-hexylthiophene) (P3HT) in regiorandom (RRa) and regioregular (RRe) forms. The Lewis acid dopant tris(pentafluorophenyl)borane (BCF) is applied for p-doping. We find that the solution-mixed process results in homogeneous bulk doping with an increase in the ionization energy for both P3HT regularities. However, for sequential doping by vapour exposure of thin RRa-P3HT films, a saturation for the BCF load is found at the surface and Fermi-level pinning is observed due to interfacial doping of the top polymer surface. Furthermore our results demonstrate that dopant molecules tend to diffuse more in RRe-P3HT than in RRa-P3HT films once they are sequentially doped and result in intermixed doped P3HT similar to solution mixed doping.

CPP 37.38 Wed 11:00 Poster B1

Thiophene based Semiconductors and Graphene Oxide for Organic Solar Cells — ●ROY SCHAFFRINNA^{1,2}, MARTINA SCHWAGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Hochschule München, Fakultät für Angewandte Naturwissenschaften und Mechatronik, 80335 München

The polymers poly(3-hexylthiophene), poly(3-thiopheneacetic acid), poly(3-thiopheneethanol) and the related copolymers are prepared starting from the respective monomer units by chemical oxidative polymerization. Graphene has also been oxidized to graphene oxide, which due to its functional groups is much more soluble in organic solvents and forms far more homogeneous layers than pure graphene and is also liquid processable. The synthesized molecules are used either as electron donor or electron acceptor in the organic solar cell and are characterized via infrared, absorption and fluorescence spectroscopy. The organic materials are electrically conductive due to their extended conjugated π -electron system and therefore require neither heavy metals / heavy metal complexes nor dopants for charge transport and can be easily deposited via spin-coating from a solution.

CPP 37.39 Wed 11:00 Poster B1

Molecular orientation of diketopyrrolopyrrole (DPP)-based donor-acceptor copolymers in thin films — ANDREAS FRÜH¹, ●SVEN BÖLKE¹, FLORIAN TRILLING², ULLRICH SCHERF², THOMAS CHASSÉ¹, and HEIKO PEISERT¹ — ¹Institute of Physical and Theoretical Chemistry, University of Tuebingen, Auf der Morgenstelle 18, 72076 Tuebingen, Germany — ²Makromolekulare Chemie und Institut für Polymertechnologie, Bergische Universität Wuppertal, Gausstrasse 20, 42119 Wuppertal, Germany

Novel low band gap (LBG) polymers are interesting materials for organic-based devices because of their high absorption in the solar spectrum and favourable electronic properties. For applications, the self-organization in thin films is an important issue in which the chemical structure determines largely the arrangement of the polymer chains.

Promising materials in this context are diketopyrrolopyrrole (DPP)-based donor-acceptor copolymers, where the DPP unit is inscribed into a double-stranded ladder framework leading to partially ladderized step-ladder polymers with high charge transfer mobilities, attributed to the highly aggregated, π -stacked conformation of DPP.

In the present study, we use polarization dependent IR spectroscopy in transmission to investigate the preferred orientation of DPP-based donor-acceptor copolymers in about 300 nm thin films. Analyzing vibrations with differently oriented transition dipole moments, we discuss the preferred molecular orientation of the polymers in context with the chemical structure. Transition dipole moments were calculated using DFT.

CPP 37.40 Wed 11:00 Poster B1

Following the morphology formation of printed non-fullerene active layer for solar cells — ●XINYU JIANG¹, SEBASTIAN GROTT¹, TOMMASO RICCIPELLI¹, VOLKER KÖRSTGENS¹, KERSTIN WIENHOLD¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH³, WEI CAO¹, SHANSHAN YIN¹, LIN SONG¹, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²DESY, Notkestr. 85, 22607 Hamburg — ³KTH, Department of Fibre and Polymer Technology, SE-100 44

Stockholm, Sweden

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements via novel organic synthesis methods and optimized fabrication routes, especially with respect to their potential roll-to-roll processing for large-area device manufacturing. Printing techniques allow for up-scaling to industrial-oriented scale which is not the case for laboratory deposition techniques like spin coating. In the present work, we fabricated an active layer which contains a low band gap donor polymer (pffBT4T-2DT) with a non-fullerene acceptor (EH-IDTBR) for solar cells by using a slot-die printing technique. To observe the structure formation of polymer domains at a larger length scale, grazing incidence small-angle X-ray scattering (GISAXS) was used in-situ during the printing process. BHJ solar cells based on printed active layer film were fabricated, which showcases the suitability of the printing technique.

CPP 37.41 Wed 11:00 Poster B1

Investigation on the influence of morphological modifications on the power-conversion efficiency of fullerene-free organic solar cells — ●GORAN IVKOVIC IVANDEKIC, SEBASTIAN GROTT, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Highly efficient organic solar cells have received significant attention in recent years. The properties, such as light weight, flexibility and the possibility to be processed at low cost, allow a wide range of application in the field of electronic devices. Although great progress has been made with fullerene-based cells, weak light absorption in the visible spectrum along with high production costs of fullerene derivatives is motivating the increased effort in developing a promising alternative. This study attempts to further improve fullerene-free organics solar cells by modifying the morphology of the photo-active layer. To substitute the fullerene, ITIC is chosen, and a low-bandgap PBDB-T is used. Different PBDB-T:ITIC bulk-heterojunction blends are processed by varying the solvents. The prepared solar cells are characterized using several experimental techniques. To get insight into the inner morphology of the applied bulk-heterojunction grazing-incidence small-angle X-ray scattering (GISAXS) and grazing-incidence wide-angle X-ray scattering (GIWAXS) are used. These information are related to photo-electronic characteristics obtained from UV-vis and PL measurements and current density-voltage curves, in order to get a full understanding of the applied donor-acceptor system.

CPP 37.42 Wed 11:00 Poster B1

Photophysical properties of ternary non-fullerene organic solar cells — ●ALI SAHIN, DIRK HERTEL, and KLAUS MEERHOLZ — University of Cologne, Luxemburgerstr.116, Cologne, Germany

Organic solar cells (OSC) are considered an attractive alternative to conventional inorganic solar cells. The benefits OSC offer, result from their favorable low-cost fabrication and their application in thin-film form. The active layer of an OSC is typically composed of two components in a bulk-hetero junction (BHJ) mixture, an electron donor (p-type semiconductor) and an electron acceptor (n-type semiconductor). Upon light excitation the formed exciton has to diffuse by typically 10-30nm to reach to D-A interface, where it dissociates into free charge carriers. Fullerene derivatives have dominated as acceptors for many years, but recently non-fullerene acceptors - mostly of ADA motif - have entered the scene [2]. Ternary BHJ cells with three components in the active layer represent one way to finetune the interface. Therefore, a series of new n-type ADA-acceptors were investigated with regard to their photophysical properties and in combination with various p-type conjugated polymers. Conductivity measurements of the neat materials and mixtures were carried out in field-effect transistors and compared with the photo-CELIV and TPV measurements in corresponding BHJ films. The charge carrier lifetime and the recombination rates were determined in order to correlate the molecular properties and BHJ properties in the thin-film with the photovoltaic parameters in binary and ternary OSC.

[2] Y. Lin et al., J. Am. Chem. Soc., 2016, 138(9), 2973-2976.

CPP 37.43 Wed 11:00 Poster B1

N-type C₆₀ thin films for thermoelectric applications — ●KONSTANTIN BARKO¹, ALEXANDER STEEGER¹, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Efficient waste heat recovery by thermoelectric generators requires p-

and n-type semiconductors with high figures of merit $zT = \sigma S^2 T / \kappa$. Therefore, it is a key challenge to find materials with a high ratio of electrical conductivity σ to thermal conductivity κ . In this regard, organic semiconductors appear an appropriate class of compounds as they offer low thermal conductivities and can be doped to increase their electric conductivities. However, the search for stable n-dopants turns out to be challenging. As a promising host, fullerene C₆₀ thin films has shown κ -values as low as 0.16 W/(mK)[1] and have been successfully n-doped with acridine orange base [2]. Using this material combination as a starting point, we analyze the thermoelectric characteristics of n-doped C₆₀ thin films as function of dopant concentration in the relevant temperature range from 300 K to 400 K. The transport properties are discussed in relation to the underlying thin film morphology estimated by AFM and X-ray diffraction. Furthermore, we pursue the concept of tuning the relative positions of transport-level and Fermi-energy which determines the macroscopic Seebeck coefficient S . These results are discussed in view of implementing n-doped fullerene layers in thin film thermoelectric generators. [1] M. Sumino et al. Appl. Phys. Lett. 99(2011)093308 [2] F. Li et al. J. Appl. Phys. 100(2006)023716

CPP 37.44 Wed 11:00 Poster B1

Investigating Triplet Exciton Losses in PBDB-T:ITIC Bulk Heterojunction Solar Cells — ●JOHANNES JUNKER¹, MARIA KOTOVA¹, ALBERTO PRIVITERA², ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV¹ — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Department of Physics, Oxford University, Oxford, United Kingdom

Organic bulk heterojunction solar cells based on small molecule non-fullerene acceptors (NFA) received a lot of attention in the past few years as their power conversion efficiency rapidly exceeded the 13% mark. So far, little is known about the photophysics of Polymer:NFA blends. By using spin-sensitive techniques, i.e. photoluminescence and electrically detected magnetic resonance (PLDMR, EDMR), we investigated triplet exciton generation in films of neat Poly[(2,6-(4,8-bis(5-(2-ethylhexyl)thiophen-2-yl)-benzo[1,2-b:4,5-b']dithiophene))-alt-(5,5-(1',3'-di-2-thienyl-5',7'-bis(2-ethylhexyl)benzo[1',2'-c:4',5'-c']dithiophene-4,8-dione))] (PBDB-T), 3,9-bis(2-methylene-(3-(1,1-dicyanomethylene)-indanone))-5,5,11,11-tetrakis(4-hexylphenyl)-dithieno[2,3-d:2',3'-d']-s-indaceno[1,2-b:5,6-b']dithiophene (ITIC), their blends and solar cells. In all films we found triplet excitons and CT states at low temperatures. However, in devices operated at ambient conditions, the triplets disappear. We discuss these results in a picture of strongly suppressed triplet exciton generation compared to fullerene-based solar cells.

CPP 37.45 Wed 11:00 Poster B1

Investigating the influence of morphology on the charge-carrier mobility in organic field-effect transistors — ●TOBIAS MEIER¹, HEINZ BÄSSLER^{1,2}, and ANNA KÖHLER^{1,2} — ¹Soft matter optoelectronics, University of Bayreuth, 95440 Bayreuth, Germany — ²Bayreuth Institute of Macromolecular Research, University of Bayreuth, 95440 Bayreuth, Germany

For organic semiconductors it is well known that the charge-carrier mobility depends sensitively on the morphology of the organic semiconductor film. The charge-carrier mobility is one of the most important properties for the application of organic semiconductors as it determines the performance of devices such as organic solar cells and field-effect transistors (OFETs). However, computational models to investigate this morphology-mobility relationship are still rare. Here, we have developed a kinetic Monte Carlo model approach to simulate charge transport in OFETs that greatly reduces the computational costs at higher charge-carrier concentrations through an effective energy landscape. This is necessary in order to simulate larger device sizes enabling the introduction of morphological aspects. Our model enables us to study the influence of conjugation length and their alignment in the film in the charge transport process.

CPP 37.46 Wed 11:00 Poster B1

Dipolar doping of organic semiconductors to enhance carrier injection — ●ALEXANDER HOFMANN¹, VIVIEN WESSELS¹, SIMON ZÜFLE², STÉPHANE ALTAZIN², KOHEI SHIMIZU³, BEAT RUHSTALLER², HISAO ISHII³, and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Institute of Computational Physics, ZHAW, 8401 Winterthur, Switzerland — ³Center for Frontier Science, Chiba University, Chiba, 263-8522 Japan

We have investigated the prototypical polar organic system *N,N'*-Di(1-

naphthyl)-*N,N'*-diphenyl-(1,1'-biphenyl)-4,4'-diamine (NPB) doped with tris-(8-hydroxyquinolate) aluminum (Alq₃) in different ratios by various electrical and optical techniques. Throughout all devices and measurements, a maximum of injected charge carriers and current for low to moderate doping ratios is observed. The strong dipole moment of polar organic materials like Alq₃, if not oriented perfectly isotropic, will lead to the buildup of a giant surface potential (GSP). It has been shown previously, that depending on polarity and carrier species, injection can be improved or hindered¹. By combining electrical² and optical measurements as well as simulations, we find a complex relation of positive and negative effects on overall device performance that, besides the influence of the GSP on injection and doping on transport, also reveal a change in NPB energy levels provoked by the dipolar surrounding.

[1] Organic Electronics **39**, 244-249 (2016) [2] Journal of Applied Physics **122**, 115502 (2017)

CPP 37.47 Wed 11:00 Poster B1

Charge transfer effects in donor and acceptor mixed systems of DNTT and PDIF-CN₂ — ●NADINE RUSSEGGER, LENA MERTEN, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

One very important and fundamental process for organic semiconductors (OSCs) is the charge transfer effect between electron donor and electron acceptor molecules.

In this work, the charge transfer effect of weakly interacting organic semiconductor thin film mixtures is comprehensively investigated. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) as donor and *N,N'*-1H,1H-perfluorobutyl-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIF-CN₂) as acceptor.

The structural, optical and electronic properties of the intermolecular interactions were characterized using a range of experimental methods. The structure of the mixed phase polymorph was evaluated by surface X-ray scattering. The charge transfer in the equimolar mixed film of DNTT and PDIF-CN₂ was characterized by absorption, photoluminescence as well as in-situ differential reflectance spectroscopy.

The results allow us to determine correlations between structural properties and charge transfer effects within the mixed systems of DNTT and PDIF-CN₂.

CPP 37.48 Wed 11:00 Poster B1

Mixing behaviour of small molecule organic semiconductors 6T and PDIF-CN₂ — ●LENA MERTEN, NADINE RUSSEGGER, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

Mixtures of small molecule organic semiconductors are a promising research field due to their various applications in organic electronics. For most applications a specific degree of order and mixing is desired, thus the mixing behaviour of dissimilar organic molecules is to be investigated.

We prepared thin films from mixtures of α -sexithiophene (6T) and *N,N'*-1H,1H-perfluorobutyl-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIF-CN₂), as donor and acceptor type molecules, respectively.

The mixed films exhibit strong long-range phase separation. Film properties were characterized structurally and optically during and after growth. The structural characterizations were done post-growth by AFM and X-ray scattering, the optical investigation by absorption spectroscopy, photoluminescence and ellipsometry, complemented by in-situ differential reflectance spectroscopy to monitor the evolution of optical properties during growth.

CPP 37.49 Wed 11:00 Poster B1

Morphology Formation and Stability of Organic Supramolecular Structures — ●ASENA CERHAN¹, CHRISTOPHER GREVE¹, MICHAEL BUCHHORN¹, BERND WITTMANN², FELIX WENZEL³, HANS-WERNER SCHMIDT³, RICHARD HILDNER^{2,4}, and EVA M. HERZIG¹ — ¹Dynamik und Strukturbildung-Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ²Lehrstuhl für Spektroskopie weicher Materie, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ³Makromolekulare Chemie I, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth — ⁴Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4 9747 AG Groningen, Netherlands

Organic, supramolecular systems can exhibit extreme transport properties. To understand such fascinating material properties, we study the morphology of such systems under various external conditions.

As the aromatic interactions have great effects on the temperature-dependent dynamic behaviour of supramolecular assemblies, the temperature studies were combined with scattering experiments. Using chemically different material systems and studying their structure in various solvents in solution, but also in thin films, we systematically investigate the importance of chemical composition versus processing conditions on the final self-assembled (super-)structure. The temperature studies with simultaneous scattering and photoluminescence measurements, furthermore, lend us insights into the stability and formation of such organic, supramolecular structures.

CPP 37.50 Wed 11:00 Poster B1
influence of UV-light on charge injection across hybrid metal oxide/organic interfaces — ●MEYSAM RAOUFI, ULRICH HÖRMANN, and DIETER NEHER — Institute of Physics and Astronomy, University of Potsdam, Potsdam

Selective charge injection into organic semiconductors is crucial for the performance of organic opto-electronic devices. Surface modification of metal oxides with self-assembled monolayers (SAMs) allows engineering of the work function (WF) to align with the charge transport levels of organic semiconductors. [1] At the same time, it has also been shown that irradiation with UV-light (light-soaking) has a pronounced effect on the electronic properties of metal oxides [2]. Here, we study the combined effect of light-soaking and surface modification on the WF and hole injection properties of ZnO. By Kelvin probe measurements in a UV-free environment we determine the WF of SAM modified ZnO prior to and after intentional light-soaking. We carefully modulate the level of photo-doping of the metal oxide layer and track the WF changes. This allows us to correlate the hole injection current from ZnO into P3HT in unipolar devices with the change in injection barrier height. Our results illustrate a severe dependence of the ZnO/organic contact on the history of light exposure. Valid conclusions about the contact energetics are only possible, if the sample history is precisely known. Importantly, despite being considered as a typical n-type material, properly treated ZnO forms an ohmic contact for hole injection. [1] I. Lange et al., *Appl. Phys. Lett.* 106, (2015). [2] G. Lakhwani et al., *J. Phys Chem C*. 114, (2010).

CPP 37.51 Wed 11:00 Poster B1
Long-term durability measurement of LHC-based DSSC under constant illumination — ●AIKE WEISSMANN¹, FABIAN SCHMID-MICHELS¹, NINA LÄMMERMANN², LUTZ WOBBE², ANDREAS HÜTTEN¹, and OLAF KRUSE² — ¹Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — ²Faculty of Biology, Algae Biotechnology & Bioenergy, Bielefeld University, Germany

With the recent surge in interest in light harvesting complexes (LHC) as a substitution for more traditional choices of dye in dye-sensitized solar cells (DSSC), the question of stability of the biological compounds becomes more pressing. LHC are required to withstand effects of photobleaching, heat and possibly hostile electrolytic environments to ensure the longevity of the created devices. This is necessary for LHC to be able to become a low-cost, low-toxicity alternative to the more commonplace dyes. To this end, LHC-based DSSC have been kept under constant illumination for an extended (> 48h) period of time, while their power output, short-circuit current and open-circuit voltage had been measured at least once per hour.

CPP 37.52 Wed 11:00 Poster B1
Investigation of Sub-Molecular Parts in Mixtures for Organic Photovoltaics — ●ARTHUR MARKUS ANTON¹, RICO MEITZNER², SHAHIDUL ALAM², HARALD HOPPE², and FRIEDRICH KREMER¹ — ¹Peter Debye Institute for Soft Matter Physics, Leipzig University — ²Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena

Nowadays, renewable sources of energy together with low-cost device manufacturing are highly demanded. For this purpose, the application of organic photovoltaics (OPV) appears to be suitable for reducing environmental impact as well as direct technology cost by "green" and low-cost synthesis combined with great-scale casting methods. Despite the advantages of fullerenes in OPV, such as high electron mobility or a low LUMO energy level, their commercial application is restricted through high synthesis costs and chemical instabilities. In order to overcome these detriments, non-fullerene acceptors have obtained considerable attention. Blends of PBDB-T:ITIC achieved efficiencies up to 11% in bulk heterojunction solar cells [1]; blends of AnE-PVstat:ITIC, instead, fall short, although photoluminescence in-

dicates efficient quenching of donor emission [2]. It is believed that orientation and order of molecular units play an essential role for the performance of organic semiconductors [3]. Thus, a novel approach by means of FTIR spectroscopy is employed in order to analyze sub-molecular parts in polymer:acceptor blends. [1] W. Zhao et al., *Adv. Mater.* 28 (2016), 4734; [2] S. Alam et al., *Chem. Pap.* 72 (2018), 1769; [3] A. M. Anton et al., *J. Am. Chem. Soc.* 137 (2015)

CPP 37.53 Wed 11:00 Poster B1
Determination of morphological evolution in bulk heterojunction polymer solar cells — ●HONGWON KIM, TOMMASO RICITELLI, XINYU JIANG, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Organic solar cells have been progressed via novel organic materials indicating improved efficiencies as well as high stability. Bulk heterojunction (BHJ) polymer solar cells offer the advantage of a high power/mass ratio combined with a mechanical flexibility. However, the achieved best efficiency values still stay behind that of other solar cell technologies, which demonstrates the needs for more fundamental understanding. In the present study, BHJ solar cells are investigated which consist of a low-bandgap donor (PffBT4T-2OD) and a non-fullerene acceptor (EH-IDTBR). The active layers are investigated with X-ray scattering techniques to track morphological evolution during the ageing processes via different external conditions. In addition, with spectroscopic measurements under identical conditions we get insights into changes on a molecular level.

CPP 37.54 Wed 11:00 Poster B1
Coupled organic-inorganic nanostructures with mixed linker molecules — ●FLORIAN GRASSL¹, EDUARD MEISTER¹, ANDRE MAIER², MARCUS SCHEELE², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Institute for Physical and Theoretical Chemistry, University of Tübingen, 72076 Tübingen, Germany

Coupled organic-inorganic nanostructures (COINs) utilize organic semiconductors as crosslinking ligands to facilitate charge conduction between semiconductor nanocrystals. They offer the perspective to combine efficient carrier transport with a high degree of structural order [1], as it has been successfully demonstrated in field-effect transistors [2]. A well-known and working organic ligand is 1,2-Ethanedithiol (EDT), especially with PbSe nanocrystal [3]. Here we focus on the introduction of a mixture of two organic ligands. Using the dip-coating technique of fabricating COIN layers from PbS nanocrystal with a mixture of Zinc β -Tetraaminophthalocyanine (Zn4APc) and EDT as organic linker molecules, we elucidate the carrier transport and device performance. We compare this mixture of linker molecules with single Zn4APc- and EDT-ligands in transistors, diodes and solar cells.

[1] M.Scheele *et al.*, *Physical Chemistry Chemical Physics* (2015), doi:10.1039/c4cp03094j
 [2] A.André *et al.*, *Chemistry of Materials* (2015), doi:10.1021/acs.chemmater.5b03821
 [3] J.Luther *et al.*, *Nano Letters* (2008), doi:10.1021/nl802476m

CPP 37.55 Wed 11:00 Poster B1
Investigation of the templating effect of graphene on organic molecular layers — ●MAX REIMER, SELINA OLTJOF, and KLAUS MEERHOLZ — University of Cologne, Luxemburger Str. 116, Germany

Electrical and optical properties of many organic semiconducting molecules are highly anisotropic. Therefore these properties will depend on the packing and ordering motif when deposited as thin films. However, most of the time when such molecules are used in organic electronic devices the growth mode is rather amorphous. Being able to grow layers with an engineered order could dramatically improve their properties such as absorption, emission, and most importantly mobility [1]. In the past years, monolayer graphene has proven to be a useful templating material [2] for subsequent material growth. Using this approach and optimizing the preparation conditions we are able to achieve an ordered and oriented growth mode for merocyanine dyes; this versatile material class is highly interesting for the use in organic photovoltaics. Two in-situ methods, low energy electron diffraction (LEED) and ultraviolet photoelectron spectroscopy (UPS), allow us to observe the packing motif and the width of the energetic levels in the region of the highest occupied molecular orbital (HOMO) which is connected to the degree of order of the molecular layer. We further exploit atomic force microscopy (AFM) which provides information about the grain size of the formed crystalline regions. The optimized

film growth allows us to improve the IV characteristic of basic organic devices containing these molecules. [1] Guillaume Schweicher et al.,

IJC 2014, 54, 595-620 [2] Ti Wang et al., Sci. Rep. 2016, 6, 28895