

CPP 46: Poster Session IV

Topics: Fundamental Physics of Perovskites (46.1-46.7), Hybrid and Perovskite Photovoltaics (46.8-46.21), Organic Electronics and Photovoltaics (46.22-46.47), Molecular Electronics and Photonics (46.48-46.51), Excitons, Plasmons and Polaritons in Molecular Systems (46.52-46.53), Electrical, Dielectrical and Optical Properties of Thin Films (46.54-46.58).

Time: Wednesday 11:00–13:00

Location: Poster A

CPP 46.1 Wed 11:00 Poster A

Control of Charge-Carrier Concentration in Lead-Free Perovskite Thin Films Consisting of Formamidinium Tin Iodide

— •PASCAL SCHWEITZER, JONAS HORN, RAFFAEL RUESS, and DERCK SCHLETTWEIN — IAP, JLU Giessen, Germany

As a promising substitute material for toxic lead perovskites we investigated formamidinium tin iodide. Thin films were prepared by spin-coating in a one-step approach. The crystal structure was confirmed by XRD, the microstructure of the films was studied by SEM and the optical absorption characteristics (Burstein-Moss-shift) were investigated by UV-vis spectroscopy. To discuss optoelectronic applications of such films, understanding of the electronic characteristics is essential. Different measurement geometries and contact materials were tested in order to provide reliable electrical studies. Inert contact materials and symmetrical electrodes were used to concentrate on perovskite materials properties rather than the influence of additional hole- and electron transport layers in typical device structure. To avoid severely high charge carrier concentrations caused by self-doping, this was limited by intentional mixing with tin fluoride to compensate tin vacancies. Current-voltage-characteristics served to discuss hysteresis in the materials which led to insight into polarization effects that are crucial, e.g. for perovskite solar cells under working conditions. We applied impedance spectroscopy to Schottky-type contacts to follow the space charge capacity under potential variation. Thereby we determined the charge carrier concentration in dependence of permittivity via Mott-Schottky analysis.

CPP 46.2 Wed 11:00 Poster A

Charge Injection from $CH_3NH_3PbI_{3-x}Cl_x$ to Organic Semiconductors Detected With sub-ps Transient Absorption Spectroscopy— •JONAS HORN¹, IULIA MINDA², HEINRICH SCHWOERER², and DERCK SCHLETTWEIN¹ — ¹Institute of Applied Physics, JLU Giessen, Germany — ²Laser Research Institute, Stellenbosch University, South Africa

Presently, inverted perovskite solar cells are heavily studied. The charge transfer processes between the perovskite layer and the charge extraction layers is one of the key factors in solar cell performance. In most of these architectures, a combination of PEDOT:PSS as transparent hole conductor and PCBM as n-type semiconductor is used. In this study, pump-probe absorption spectroscopy with femtosecond resolution is used to determine the injection time of photo-generated charge carriers from the perovskite to the PEDOT:PSS and PCBM layers. A characteristic signal was identified to be caused by holes injected into the PEDOT:PSS layer by comparing the transient signals of photo-excited perovskite films with and without PEDOT:PSS interface. This signal appears within the resolution of the measurement setup (<200 fs) proving ultrafast charge carrier injection. Changes in the transient signals characteristic for the perovskite layer as reflected in the time constants obtained by global analysis confirmed this observation. We could also show ultrafast as well as slow injection of electrons into PCBM based on the decay of signals characteristic for the excited state of the perovskite as well as the appearance of characteristic PCBM signals.

CPP 46.3 Wed 11:00 Poster A

In-situ monitoring of sequential conversion of $MAPb(IxBr1-x)3$

— •CAROLIN REHERMANN, KATRIN HIRSELANDT, ABOMA MERDASA, and EVA UNGER — Helmholtz-Zentrum Berlin, Young Investigator Group Hybrid Materials Formation and Scaling, Berlin, 12489, Germany

Metal halide perovskites are an interesting material for tandem solar cells due to their band gap tunability, band gaps up to 3 eV can be prepared by exchanging halides.1 Burschka et al.2 introduced the 2-step method. Three competing processes might occur: direct conversion/intercalation, dissolution-reformation and ion exchange.3

In this work, the second step is monitored by in-situ UV-vis mea-

surements. The second step is the conversion from a lead iodide film into a mixed halide perovskite film $MAPb(IxBr1-x)3$. Using MABr we can track the different conversion kinetics between a direct conversion and a dissolution-reformation process. The influence of different reaction parameters is investigated.

In-situ UV-vis measurements show an initial evolution of a spectral signature characteristic for the absorption onset of the direct conversion product, $MAPbBrI2$. Upon progression, this signature disappears in favor of the pure dissolution-reformation product $MAPbBr3$. Changes in spectral signature during a post-conversion annealing step prove that ionic equilibration occurs.

1. Unger et al. Journal of Materials Chemistry A 2017, 5 (23), 11401-11409. 2. Burschka et al. Nature 2013, 499 (7458), 316-319. 3. Ko et al. Chemistry of Materials 2017, 29 (3), 1165-1174.

CPP 46.4 Wed 11:00 Poster A

Combinatorial Investigation of Co-Evaporated $CsPbI_3$ Thin Films

— •PASCAL BECKER, JUSTUS JUST, and THOMAS UNOLD — Helmholtz-Zentrum Berlin, Germany

Lead halide Perovskite materials have recently emerged as very promising new material for thin film solar cell absorbers yielding power conversion efficiencies of above 22%. Highest power conversion efficiencies are found for Pb-based inorganic-organic halides, which tend to chemically decompose at elevated temperatures. Inorganic lead halide perovskites such as $CsPbI_3$ are significantly more stable and well suited candidates for high efficient tandem solar cells due to their high bandgap of 1.8 eV. However, much less is known about the crystal structure and optoelectronic properties of these compounds.

We synthesized combinatorial samples of $CsPbI_3$ thin films with a spatial gradient in composition by co-evaporation of CsI and PbI_2 . Applying X-ray diffraction mapping, X-ray fluorescence mapping and UV-vis mapping on these samples we are able to investigate the phase diagram of this compound as well as the optoelectronic properties of the different phases. Depending on the composition and growth temperature we find a transition from the yellow phase to the brown phase in $CsPbI_3$ as well as segregation of excess CsI and PbI_2 .

CPP 46.5 Wed 11:00 Poster A

In-Situ Investigation of Ion Migration and Aggregation in Organolead Halide Perovskite Films— •YU ZHONG¹, CARLOS ANDRES MELO LUNA², RICHARD HILDNER², CHENG LI¹, and SVEN HUETTNER¹ — ¹Macromolecular Chemistry I, University of Bayreuth, Bayreuth, Germany — ²Experimental Physics IV, University of Bayreuth, Bayreuth, Germany

During current-voltage(J-V) measurements, perovskite solar cells(PSCs) exhibit a certain photo-induced instability and hysteresis phenomenon. Firstly, we study the light-induced behavior in $CH_3NH_3PbI_3-xCl_x$ film in-situ, by employing wide-field photoluminescence(PL) microscopy to obtain both the spatially- and temporally-resolved PL image. Along with the increase of the PL intensity under continuous illumination, some areas render PL inactive. A faster and more obvious PL decay process was observed with a higher excitation energy. By characterizing this excitation energy dependent PL decay, we suggest that the PL quenching can be ascribed to an aggregation of iodide ions. Secondly, by introducing phenyl-C61-butyric acid methyl ester(PCBM) in PSCs, hysteresis phenomenon is suppressed. The results of wide-field PL image and temperature dependent J-V curve measurement confirm that PCBM molecules decrease the mobility and increase the activation energy of iodide ions. This real-time investigation of the light soaking of perovskite films provides more details to improve the performance of PSCs. The suppression of the iodide ions movement, e.g. involving PCBM, is a concern for better performance and stability of PSCs.

CPP 46.6 Wed 11:00 Poster A

Influence of hole selective contacts in inverted perovskite solar cells— •KATRIN HIRSELANDT¹, ANIELA CZUDEK¹, CELLINE

AWINGO², STEFFEN BRAUNGER¹, CAROLIN REHERMANN¹, THOMAS DITTRICH², and EVA UNGER¹ — ¹Helmholtz-Zentrum Berlin, Young Investigator Group Hybrid Materials Formation and Scaling, Berlin, 12489, Germany — ²Helmholtz-Zentrum Berlin, Institute Silicon Photovoltaics, Berlin, 12489 Berlin, Germany

Planar solution processed perovskite solar cells have reached efficiencies above 20 % and their stability have improved during the past years [1,2]. In device preparation, reproducibility is a major obstacle due to perovskite absorber inhomogeneity and interfacial properties [3].

In this study we investigated four different types of planar inverted perovskite solar cells, comparing the cesium-containing triple cation perovskite with the archeotypical methylammonium lead iodide (MAPI) as absorber materials as well as two different hole transporting materials (HTMs): Poly[bis(4-phenyl)(2,4,6-trimethylphenyl)amine] (PTAA) and Poly(3,4-ethylenedioxythiophene) polystyrene (PEDOT:PSS) as selective contact layer.

The best and most reproducible performance of 16 % on average was achieved for MAFACs on PTAA. These devices also exhibited the least photocurrent hysteresis and are hence the most robust and reproducible architecture tested.

[1] K. A. Bush et al., *Nature Energy* (2017), 2, 17009 [2] M. A. Green et al., *Prog. Photovoltaics* (2017), 25, 3-13 [3] C. Bi et al., *Nature Communications* (2015), 6, 7747

CPP 46.7 Wed 11:00 Poster A

Measurement development for hysteresis characterization of perovskite solar cells — ● ANIELA CZUDEK¹, LUKAS KEGELMANN¹, AMRAN AL-ASHOURI¹, STEVE ALBRECHT¹, and EVA UNGER^{1,2} — ¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — ²Lund University, Department of Chemical Physics, Lund, Sweden

Evaluating the performance of perovskite solar cells can be intricate due to transient current-voltage phenomena on different time scales. Current-voltage measurements in different scan directions may exhibit varying degrees of discrepancy - often referred to as hysteresis - which makes defining the 'right' measurement conditions difficult. We here present a procedure to assess the steady-state solar cell performance of perovskite devices using an iterative - perturb and observe - maximum power point tracking algorithm. This methodology is directly used to also investigate the transient response of devices upon voltage perturbation around maximum power point. The time constants of transient current response allows for a quantitative comparison of different device architecture types and determine the minimum delay time (voltage settling time) required to perform current-voltage measurements at quasi-steady-state condition of the device. We will show and discuss how this methodology was utilized to quantitatively compare perovskite solar cells of different architecture types, contact layers and perovskite absorber composition.

CPP 46.8 Wed 11:00 Poster A

Investigation of inorganic nanoparticles and low band-gap polymers for printed hybrid solar cells — ● GAETANO MANGIAPIA and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Printed solar cells represent a potential alternative to the use of conventional cells. Because of their low-cost, low-weight, production simplicity, and possibility to be used on curved or flexible substrates, they have progressively captured the attention of applied research. Printed hybrid solar cells combine the above mentioned advantages with the use of hybrid photovoltaics, where two different semiconductors (organic and inorganic) compose the active layer. Although PCE values need to be boosted up for industrial applications, the possibility to chemically modulate the properties of the organic part (e.g. by adding or changing a functional group) allowed foreseeing the capability to tune both the optical and electronic properties, an essential requirement for finding new and highly efficient materials. We study bulk heterojunction hybrid solar cells composed of the low band-gap polymer PTB7 and its derivatives and inorganic ZnO nanoparticles. We correlate optical and morphological properties of the active layer. Characterization involves X-ray and neutron scattering techniques in combination with photophysical measurements.

CPP 46.9 Wed 11:00 Poster A

Hybrid solar cells based on metal oxides and water-soluble polythiophenes — ● JIABIN GU¹, VOLKER KÖRSTGENS¹, KLARA STALLHOFFER², HRISTO IGLEV², REINHARD KIENBERGER², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS

Funktionelle Materialien, 85748 Garching — ²TU München, Physik-Department, LS Laser und Röntgenphysik, 85748 Garching

Environmentally friendly processing of hybrid solar cells with the solvent water is feasible with an active layer consisting of laser-ablated metal oxides and a water-soluble polythiophene [1]. Zinc oxide and titanium dioxide particles are processed with laser ablation in water. The obtained nanoparticles are investigated regarding the size distribution and crystallinity. Spray-deposition as a cost-effective preparation method has been utilized as technique to produce films of the laser-ablated nanoparticles, the active layers including polythiophenes and the corresponding hybrid solar cells. Films have been characterized with optical and spectroscopic methods as well as with x-ray characterization techniques. The influence of differences of bandgap, crystallinity and mesoscale morphology on the photovoltaic performance of the obtained devices is discussed. [1] Körstgens et al., *Nanoscale* 7, 2900 (2015).

CPP 46.10 Wed 11:00 Poster A

Use of Triphenylamine Dyes With Metal Complex Electrolytes in ZnO-Based Dye-Sensitized Solar Cells . — ● ANDREAS RINGLEB, RAFFAEL RUES, and DERCK SCHLETTWEIN — IAP, JLU Giessen, Germany

Dye-sensitized solar cells (DSSCs) may serve as an alternative to silicon-based solar cells because of low energy-payback-times and expected low costs, in particular, if the porous ZnO is prepared by electrodeposition. The triphenylamine-based organic dye D35CPDT (also known as LEG4) has been frequently used as a sensitizer with good efficiency on TiO₂ in combination with modern Co- and Cu-based electrolytes which have a high redox potential and allow fast and effective regeneration without high overpotentials. In the present work we study the combination of these different successful approaches. Porous ZnO has been electrodeposited on AZO-coated glass. Adsorption of LEG4 to the ZnO surface has been studied by varying pre-treatment of the films and optimized samples have been used to prepare DSSCs. These have been studied by means of current-voltage characteristics and detailed photoelectrochemical methods such as impedance spectroscopy, dynamic illumination and time-resolved experiments. A focus has been put on the analysis of recombination of injected electrons from the ZnO/dye interface to the redox electrolyte as one of the main loss channels in DSSCs and on mass transport of the electrolyte through the porous sensitized photo anode as an additional limiting factor.

CPP 46.11 Wed 11:00 Poster A

Control of surface electronic parameters of ITO using dipolar monomolecular layers. — ● MEYSAM RAOUFI¹, ULRICH HÖRMANN¹, EMIL LIST KRATOCHVIL², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomy, Potsdam-Golm, Germany — ²Humboldt University, Institute for Physics, Berlin, Germany

In organic electronic devices, the injection of holes and electrons from the electrodes into the organic semiconductors is a key issue for their efficient operation. Different chemical and physical treatments have been proposed to improve hole injection and minimize the injection barrier height as a result of increasing the work function of ITO. A particularly interesting approach is the deposition of dipole layers by molecular self-assembly[1,2].

Here, by applying self assembled monolayers of different phosphonic acids, we study how the efficiency of hole injection across a hybrid surface correlates with the change in barrier height. Fine tuning of the injection barrier is achieved by mixing molecules with different electrostatic dipoles. Finally, by incorporating photo-switchable molecules into the SAM, we gain control over the energetics at the organic/inorganic interface and its injection properties.

1. A. Sharma, A. Haldi, P. J. Hotchkiss, S. R. Marder, and B. Kippelen, *J. Appl. Phys.* 105, (2009). 2. I. Lange, S. Reiter, M. Pätz, A. Zykov, A. Nefedov, J. Hildebrandt, S. Hecht, S. Kowarik, C. Wöll, G. Heimel, and D. Neher, *Adv. Funct. Mater.* 24, 7014 (2014).

CPP 46.12 Wed 11:00 Poster A

Work-Function Modification of Transparent Conductive Electrodes and Investigation of Organic Electron-Transport-Layers for Use in Perovskite Solar Cells — ● BERTHOLD WEGNER^{1,2}, FEDERICO PULVIRENTI³, JAY PATEL⁴, NAKITA NOEL⁴, HENRY SNAITH⁴, SETH MARDER³, and NORBERT KOCH^{1,2} — ¹Helmholtz-Zentrum Berlin, Germany — ²Humboldt-Universität zu Berlin, Germany — ³Georgia Institute of Technology, Atlanta, USA

— ⁴University of Oxford, UK

Minimizing electron-collection losses at the electron-selective contact in organic-inorganic halide perovskite solar cells is crucial to achieve better device performance and long-term stability. Here, we report on the modification of fluorinated tin oxide (FTO) used as transparent electrode in perovskite devices, and the comparison of two classes of organic semiconductors with similar electron affinities for their use as efficient electron-transport-layers (ETL) in perovskite solar cells. Ultraviolet photoelectron spectroscopy (UPS) reveals that deposition of a moderately air-stable organometallic dimer on the FTO surface leads to a decrease in work-function (WF) by more than 1 eV. Furthermore, UPS and x-ray photoelectron spectroscopy (XPS) are used to study the energy level alignment between the dimer-modified FTO and the ETL layers, and whether the dimer reacts with or diffuses into the ETL layer. Perovskite solar cells employing such modified electron-selective contacts were fabricated showing increased power conversion efficiencies.

CPP 46.13 Wed 11:00 Poster A

Suppressed Ionic Migration in 2D-Ruddlesden-Popper Perovskite — ●CHENG LI¹, ANTONIO GUERRERO², HUAN LONG¹, YU ZHONG¹, JUAN BISQUERT², JIANPU WANG³, and SVEN HUETTNER¹ — ¹Organic and Hybrid Electronics, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth, Germany — ²Institute of Advanced Materials (INAM), Universitat Jaume I, 12006 Castelló, Spain — ³Institute of Advanced Materials (IAM), Nanjing Tech University (NanjingTech), 30 South Puzhu Road, Nanjing 211816, China

Organometal trihalide perovskite solar cells (PSCs) are still suffering from the problem of hysteresis and stability. Recently, another class of perovskite - two dimensional (2D) Ruddlesden-Popper (RP) halide layered perovskites have attracted attention. In this work, first, we fabricate 2D RP perovskites using 1-naphthylmethylamine iodide (NMAI) as the precursor. Then we characterize the built-in potential in the device using electroabsorption spectroscopy. Further, we utilize time-resolved photoluminescence (PL) image microscopy and impedance spectroscopy (IS) on perovskite films to investigate both the spatial and temporal evolution of ion migration under external electric fields. Our approach enables us to quantitatively characterize the kinetic processes and determine the mobility of these ions, which is around one order of magnitude lower compared with the one in 3D perovskite. Following that, temperature dependent J-V curve enables us to obtain the activation energy of ions inside. Hence, decrease of J-V curve hysteresis and the improvement on stability are ascribed to the suppressed ion migration.

CPP 46.14 Wed 11:00 Poster A

Radiative efficiency in planar metal-organic-perovskite solar cells — ●SIMON BERGER¹, PHILIPP RIEDER¹, DAVID KIEMASCH¹, KRISTOFER TVINGSTEDT¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

In order to achieve an ideal solar cell with any material system, it is necessary to strive for the radiative efficiency limit. Here we evaluated the capability of planar perovskite solar cells in (p-i-n)-layout to emit light by EL-spectroscopy. In this technique charge carriers are injected into the solar cell to recombine and the emitted photons are being detected. We fabricated and evaluate devices with different hole transport layers namely PTAA, PEDOT-PSS and p-TPD. The MAPbI₃ and (MAPbBr₃)_x(FAPbI₃)_(1-x) perovskites were prepared by both the one-step and two-step method. We show the impact of these different charge selective layers and the applied voltage on the electro-luminescence characteristics and compute $V_{OC,Rad}$ in the radiative limit for each material.

CPP 46.15 Wed 11:00 Poster A

Charge Carrier Dynamics in Methylammonium Lead Iodide probed by TRMC and TRPL — ●NATHANIA HENNING¹, MANUEL ULLRICH¹, LIUDMILA KUDRIASHOVA¹, ANDREAS BAUMANN², ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Organo lead halide perovskites, such as methylammonium lead iodide (MAPI), have attracted great attention to the field of thin film photovoltaics due to their outstanding electrical and optical properties.

The mobility and the lifetime of photogenerated charge carriers are among the fundamental quantities which define the performance of solar cell devices. In this work, we perform combined analysis of transients, provided by two electrodeless characterisation techniques: time-resolved microwave conductivity (TRMC) and time-resolved photoluminescence (TRPL). Complementary TRMC and TRPL characterisation of perovskite thin films aims to improve numerical fits and provide characteristic lifetimes as global fit parameters.

CPP 46.16 Wed 11:00 Poster A

Time-Resolved Microwave Conductivity on Perovskite Materials for Solar Cells — ●MANUEL ULLRICH¹, NATHANIA HENNING¹, LIUDMILA KUDRIASHOVA¹, ANDREAS BAUMANN², ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Perovskite solar cells have attracted much attention in recent years, since their power conversion efficiencies increased steadily and exceeded 20 %. To further improve their performance and relate this to the preparation route, optoelectronic properties need to be investigated. We use time-resolved microwave conductivity (TRMC) to elucidate and quantify charge carrier mobilities and lifetimes. This electrodeless technique is based on the interaction of photoexcited charge carriers with the applied electro-magnetic field (GHz), leading to a time-dependent change in conductance. We focus on methylammonium lead iodide (CH₃NH₃PbI₃) as an active layer and examine different processing conditions, which affect the perovskite crystallinity and finally the charge carrier dynamics. Furthermore the impact of different transport layers on the charge carrier lifetime is investigated.

CPP 46.17 Wed 11:00 Poster A

Characterization of mm sized CH₃NH₃PbI₃ crystals grown by Inverse Temperature Crystallization — ●STEFAN KIESMÜLLER¹, STEFAN VÄTH¹, SEBASTIAN HAMMER¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Organo lead halide perovskites are an important subject of research due to their promising properties concerning photovoltaics. Up to now, mostly thin films with poly-crystalline nature are formed from solution or vacuum deposition techniques. The role of crystallinity and crystal domain size on the functionality of the perovskite solar cell is in the focus of present research. In order to probe the fundamental properties like the charge carrier transport of the hybrid perovskite semiconductors and its limitations very often large crystals have been studied. Here, we used the technique of Inverse Temperature Crystallisation to grow methylammonium lead iodide (MAPI) crystals of different size and crystal quality. This growth technique for crystals is based on the effect of reverse solubility of some materials in special solvents in remarkably short growth times. The so grown MAPI crystals are characterized by means of X-ray diffraction and scanning electron microscopy. The optical properties are studied by photoluminescence. Finally, Time-of-Flight measurements were performed to investigate the fundamental charge carrier transport.

CPP 46.18 Wed 11:00 Poster A

Cs₂AgBiBr_xI_{1-x}: A Novel Lead-Free Material for Perovskite Solar Cells — ●MELINA ARMER¹, MATHIAS FISCHER¹, LIUDMILA KUDRIASHOVA¹, ANDREAS BAUMANN², and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

As conventional perovskite solar cells contain lead and therefore suffer toxicity issues, finding alternative lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, we present a novel lead-free material for solar cells, Cs₂AgBiBr_xI_{1-x}, permitting straightforward spin-coating from solution. The films have been characterized using steady state and time-resolved optical spectroscopy. The morphology and quality of the as prepared films has been evaluated using a scanning electron microscope and X-ray Diffraction. It has been found that solution processed Cs₂AgBiBr_xI_{1-x} forms polycrystalline thin films with crystalline domains in the micrometer range. Further, we observed photoluminescence in the visible region (around 658 nm) with long lifetimes up to 1,6 μs in the visible region by steady state and time resolved photolu-

minescence measurements. Due to the encouraging optical properties, the straightforward solution processing and its uniform polycrystalline morphology we propose $\text{Cs}_2\text{AgBiBr}_x\text{I}_{1-x}$ to be a promising candidate for the application in lead-free perovskite solar cells.

CPP 46.19 Wed 11:00 Poster A

Rotational dynamics of methyl ammonium ions in the hybrid organic-inorganic perovskite $\text{CH}_3\text{NH}_3\text{PbI}_{2.94}\text{Cl}_{0.06}$ by means of QENS investigations — ●GÖTZ SCHUCK¹, FREDERIKE LEHMANN^{1,2}, and SUSAN SCHORR^{1,3} — ¹Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — ²Universität Potsdam, Institut für Chemie, Potsdam OT Golm, Germany — ³Institute of Geological Sciences, Freie Universität Berlin, Berlin, Germany

Perovskites with ABX_3 - structure show a huge possibility on element substitutions on A-, B- and X-site which leads to a broad variety of physical properties. Our main field of interest is chloride substituted methyl ammonium lead triiodide in which A is the organic unit $[\text{CH}_3\text{NH}_3]^+ = \text{MA}$, $\text{B} = \text{Pb}_2^+$ and $\text{X} = \text{I}_{3-x}\text{Cl}_x$. The aim is to get an inside into the interrelationship of static and dynamic structure of $\text{MAPbI}_{3-x}\text{Cl}_x$ and MAPbCl_3 by studying the temperature dependent methyl ammonium dynamics by means of QENS investigations in order to understand the influence of chloride on the rotational dynamics of the methyl ammonium cation.

In recent QENS investigations on MAPbI_3 [1] two quasielastic components were identified in the tetragonal ($165 \text{ K} < T < 327 \text{ K}$) and cubic ($T > 327 \text{ K}$) phase. From the QENS results, it was interpreted that in the cubic and tetragonal phases the MA ion exhibit four-fold rotational symmetry perpendicular to the C-N axis (C_4) along with three-fold rotation parallel to the C-N axis (C_3), while in the orthorhombic $Pnma$ phase ($T < 165 \text{ K}$) only C_3 rotation is present.

[1] Li et al., Nature Communications 2017, 8, 16086

CPP 46.20 Wed 11:00 Poster A

Charge carrier recombination in planar n-i-p and p-i-n perovskite solar cells - the role of interfaces — ●D. KIEMASCH¹, K. TVINGSTEDT¹, L. GIL-ESCIRG², C. MOMBLONA², M. SESSOLO², A. BAUMANN³, H. BOLINK², and V. DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — ²Instituto de Ciencia Molecular, Universidad de Valencia, 46980 Paterna, Valencia, Spain — ³Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany

Charge carrier recombination processes in organo-metal halide perovskite solar cells are one of the most studied research topics in this new class of photovoltaic materials. Usually, time resolved photoluminescence (tr-PL) is used to study recombination in perovskite layers. Here, crystals or films with or without charge selective layers are being probed. In contrast, only a few experimental approaches have been presented on complete perovskite solar cells using charge selective layers and contacts.

We report on charge carrier recombination dynamics in planar n-i-p and p-i-n perovskite solar cells with different organic charge selective layers. The perovskite layers have been prepared by vacuum deposition leading to efficiencies in the range of 20% for the n-i-p and 17% for the p-i-n layout. To explain this difference between both type of devices we studied charge carrier recombination dynamics with steady state and transient electrical measurements demonstrating the importance of interface recombination in perovskite solar cells.

CPP 46.21 Wed 11:00 Poster A

Red-shifting the band gap of Perovskite photovoltaics using Sn/Pb metal mixtures — ●ANTONIO GÜNZLER and MICHAEL SALIBA — Adolphe Merkle Institute, Fribourg, Switzerland

Perovskite solar cells using only Pb at the metal position currently achieve record performances. Partial replacement of Pb by Sn has the advantage of using less toxic Pb.

In addition, Pb-Sn mixtures have an earlier absorption onset towards the near IR broadening the absorption spectrum. This is especially useful for thin-film perovskite-perovskite tandem cells already achieving up to 19% efficiency to date with the potential to reach values beyond 40%.

Furthermore, other optoelectronic applications require tunability of the band gap.

We aim to improve the fundamental understanding of the correlation between the perovskite structure and its optoelectronic properties under variation of the Sn content.

CPP 46.22 Wed 11:00 Poster A

Interfacial charge transfer and temperature dependent charge carrier transport in organic heterostructure field-effect transistors — ●EDUARD MEISTER, STEFAN SCHMIDT, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, Germany

In this work we studied interfacial charge transfer (CT) happening in hetero-structure field-affect transistors (FETs) based on vapour deposited small molecules. We used diindenoperylene (DIP) as donor (D) and N,N'-bis-(2-ethylhexyl)-1,7-dicyanoperylene-3,4:9,10-bis(dicarboxyimide) (PDIR-CN₂) as acceptor (A) and fabricated D/A as well as A/D heterostructure FETs and used additionally two different contact materials, tetrathiafulvalene tetracyanoquinodimethane (TTF-TCNQ) and aluminum, for preferred hole and electron injection into DIP, respectively. DIP deposited on thermally treated and smoothed tetratetracontane [1] exhibits a electron as well as a hole field-effect mobility μ in the range of $0.1 \text{ cm}^2/\text{Vs}$, whereas PDIR-CN₂ shows only *e*-transport with μ in the same range. As reported previously [2] partial ground state CT between DIP and PDIR-CN₂ molecules takes place resulting in significant changes in the transistor characteristics. In total, we have identified five different working regimes of heterostructure FETs. Temperature dependent measurements of the mobility in the donor and the acceptor indicate among others a significant difference between hole and electron transport in DIP.

[1] L. Pithan et al., *J. Chem. Phys.* **143** (2015) 164707.

[2] V. Belova et al. *J. Am. Chem. Soc.* **139** (2017) 8474.

CPP 46.23 Wed 11:00 Poster A

Conjugated polymers with alternating benzothiadiazole-diketopyrrolopyrrole units for OTFTs: Synthesis and DFT/MD simulations — ●RENÉ DANIEL MÉNDEZ LÓPEZ^{1,2}, DEYAN RAYCHEV^{1,2}, ANTON KIRIY¹, OLGA GUSKOVA^{1,2}, and JENS-UWE SOMMER^{1,2,3} — ¹Leibniz IPF — ²DCMS, TU Dresden — ³Institute for Theoretical Physics, TU Dresden

Organic semiconducting polymers are adequate for large area and low cost electronic device applications, such as organic thin film transistors (OTFTs). The joint theoretical/experimental studies are crucial for understanding the charge transport in ambipolar OTFTs, in which both electrons and holes are mobile. Here we report on the synthesis, characterization and simulations of a polymer consisting of diketopyrrolopyrrole (DPP) and benzothiadiazole (B) units. DPP is a versatile building block for OTFTs and its synthesis is straightforward and inexpensive. The π - π intermolecular interactions, the solid-state packing, and optical properties are dependent on the nature of the conjugated blocks adjacent to DPP core. Here, furan (F) is proposed as such an adjacent unit, linking DPP and B blocks in the conjugated backbone. The synthesis of the PDPP-FBF copolymer was performed following Ref.1. From the experiments, the π - π distance, the HOMO-LUMO energy levels and the charge carrier mobilities are characterized. These values are compared with the results of simulations in order to get a deeper understanding of the parameters governing the mobility. This work is funded by ERDF and Free State of Saxony via ESF project CoSiMa 100231947.[1] P. Sonar et al. Chem. Commun., 2012, 48, 8383.

CPP 46.24 Wed 11:00 Poster A

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} — ¹Experimental Physics II, 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, however, 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). Yet, there is no comprehensive theoretical description available for this complex morphology-mobility relationship. Here, we use a kinetic Monte Carlo model to simulate charge transport in OFETs in order to investigate the interplay between the morphology of the semiconductor and the charge-carrier mobility. We focus on the role of conjugation length in the charge transport process and on the importance of ordered domains. Parameters considered include the temperature dependence, charge-carrier concentration and film thickness.

CPP 46.25 Wed 11:00 Poster A

Flexible all-carbon solution-gated FETs for pH sensing — •DANIEL HÜGER¹, DAVID KAISER¹, CHRISTOF NEUMANN¹, UGO SASSI², MATTEO BRUNA², MARIA KÜLLMER¹, and ANDREY TURCHANIN¹ — ¹Institute for Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — ²Nokia Bell Labs, Cambridge CB3 0FA, UK

Flexible electronics have shown extensive applications in the areas of biology, chemistry, and medicine. We employ single-layer graphene (SLG) grown by methane Chemical Vapor Deposition on Cu foils transferred on PEN substrates and amino-terminated 1 nm thick carbon nanomembranes (CNMs) generated by electron-beam induced crosslinking of aromatic self-assembled monolayers to engineer hybrid NH₂-CNM/SLG field effect transistors. Passivation of the electrodes for the operation of the devices in liquid is realized by self-assembly of hexadecanethiol on the Au contacts. We present the results achieved with these van der Waals heterostructure devices in solution-gated field effect transistors for pH-sensing and compare their performance to that of devices realized on standard SiO₂/Si substrates.

CPP 46.26 Wed 11:00 Poster A

Imidazo[1,5-a]pyridine und -quinoline as a New Class of Materials for Light Emitting Devices — •JASMIN MARTHA HERR^{1,3}, GEORG ALBRECHT^{2,3}, HISAO YANAGI³, DERCK SCHLETTWEIN², and RICHARD GÖTTLICH¹ — ¹Institute of Organic Chemistry, JLU Giessen, Germany — ²Institute of Applied Physics, JLU Giessen, Germany — ³Nara Institute of Science and Technology, Japan

1,3-disubstituted imidazo[1,5-a]pyridines are receiving increased interest for applications as organic semiconductor thin films, mainly regarding organic light emitting diodes (OLED). Characteristic for these molecules is a blue luminescence with a large Stokes shift and high quantum yields (QY).[1,2] The goal of this work is to explore the potential of this class of materials by introducing specific electron-withdrawing or electron-donating substituents to the chromophore system. A microwave-assisted one-pot synthesis was developed for this purpose which provides a simple and affordable approach towards this new and interesting class of materials. Thin films were prepared by physical vapor deposition (PVD) onto quartz glass. These films and solutions of the molecules were investigated by UV-Vis and fluorescence spectroscopy, as well as lifetime measurements of the excited state to then compare the measurements in solution to those in the solid phase. [1] G. Volpi, G. Magnano, I. Benesperi, D. Saccone, E. Priola, V. Gianotti, M. Milanese, E. Conterposito, C. Barolo and G. Viscardi, *DyesPigm.* **2017**, 137, 152-164. [2] F. Shibahara, R. Sugiyama, E. Yamaguchi, A. Kitagawa and T. Murai, *J.Org.Chem.*, **2009**, 74, 3566-3568.

CPP 46.27 Wed 11:00 Poster A

Optimization and Characterization of Blue OLEDs based on Molecular TADF Emitters — •FELIX KLINGERT¹, NIKOLAI BUNZMANN¹, SEBASTIAN WEISSENSEEL¹, ANDREAS SPERLICH¹, NIKITA DRIGO², MOHAMMAD KHAJA NAZEERUDDIN², and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Group for Molecular Engineering of Functional Materials, EPFL, CH-1951 Sion, Switzerland — ³Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Realizing efficient and stable blue organic light emitting diodes (OLEDs) that meet display requirements has proven to be a challenging endeavor. Most organic molecules with a bandgap big enough to emit blue light suffer from either poor efficiency or a short lifespan. A modern approach of increasing efficiency is a process called thermally activated delayed fluorescence (TADF). Here, we fabricate blue OLEDs through thermal evaporation based on a molecular TADF emitter and characterize them by means of their current-electroluminescence-voltage characteristics, emission spectra and external quantum efficiency. From these measurements we draw conclusions about the electro-optical properties of the emitter molecules and their suitability as a material for blue OLEDs.

CPP 46.28 Wed 11:00 Poster A

Solution-processed Dual Wavelength Organic Near-Infrared Photodetectors — •YAZHONG WANG, ZHENG TANG, BERNHARD SIEGUMUND, ZAIFEI MA, JOHANNES BENDUHN, DONATO SPOLTRE, and KOEN VANDEWAL — Technische Universität Dresden, Nöthnitzer Str. 61, 01187 Dresden, Germany

Optical sensors that are capable of detecting photons at two or multiple specific wavelengths are highly interesting because they can identify target objects or materials much more precisely by detecting the reflected, transmitted or emitted photons at two or multiple characteristic wavelengths. In this work, optical simulations using Transfer Matrix Method (TMM) were performed on organic devices to achieve dual wavelength narrowband detection in the near-infrared spectral range of 700 ~ 1100 nm. The devices exploit charge-transfer (CT) states, formed at the interface of blended organic donating and accepting materials. Combined with a Fabry-Pérot resonant cavity, the CT absorption can be dramatically enhanced at certain wavelengths. Our results show that two detection wavelengths can be tuned independently from 650 to 1100 nm. The spectral resolution (full width at half maximum - FWHM) of the detection bands varies between 10 and 30 nm, and we achieved peak EQEs above 10%. A possible application of such photodetectors is moisture detection, where two of the characteristic absorption peaks of water are located at around 750 and 960 nm. By optimizing the thickness of the two photo-absorbing layers in a tandem device structure, the detection bands can be tuned to match with those two wavelengths for simultaneous and precise detection.

CPP 46.29 Wed 11:00 Poster A

Printed fullerene free organic thin films for photovoltaic applications — •RODRIGO DELGADO, SEBASTIAN GROTT, and PETER MÜLLERBUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

During the past decade, organic photovoltaics (OPVs) have attracted considerable attention owing to their outstanding characteristics, such as potential low-cost fabrication, high throughput, light weight, flexibility and easy processability. Fabrication techniques for these OPVs devices vary depending on the materials used, and include vacuum evaporation, spin-coating, inkjet printing, doctor-blading, spray casting, screen printing and roll-to-roll printing. Among these, the scalability of the printing processes makes them attractive for industrial application. In this study, the influence of different ratios of donor:acceptor PBDB-T:ITIC for thin film bulk heterojunction (BHJ) OPVs deposited by printing methods are explored. In order to characterize these solar cells their current-voltage characteristics as well as their absorbance spectra are measured. Additionally, the inner morphology of the active layers is probed with advanced scattering techniques, to correlate structure information with the obtained photoelectrical properties of the devices.

CPP 46.30 Wed 11:00 Poster A

A comparative study of thin organic layers for photovoltaic applications using spin and spray coating — •DEBAMITRA CHAKRABORTY, SEBASTIAN GROTT, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Bulk-heterojunction organic solar cells have emerged as a promising alternative for conventional silicon based solar cells because of their potential to be light weight, flexible and semi-transparent, which makes them versatile for many applications. Though the most popular scientific method of processing solar cell is spin coating, they can also be processed with solution based methods which enables the possibility to use low cost manufacturing processes like roll-to-roll printing or spray casting. In this study we investigate thin films of different mixtures of conjugated polymers and small acceptor molecules forming organic bulk hetero junctions, which were processed by spin coating or spray casting. Thereby we want to investigate the influence of the different processing techniques on the film morphology and photophysical properties. The structure is analyzed with scattering techniques and correlated with the obtained photophysical properties.

CPP 46.31 Wed 11:00 Poster A

Investigation of low band-gap polymers for highly efficient organic solar cells — •CHRISTOPH BILKO, FRANZISKA C. LÖHRER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

In contrast to silicon-based solar cells, organic photovoltaics offer a wide range of advantages. Due to their flexibility and tunable optical properties, sun harvesting in areas not accessible to conventional solar cells could be greatly increased using organic solar cells, e.g. on curved or flexible surfaces. Other advantages are the lighter weight and potentially lower production costs. In the last years, the formerly poor efficiencies of organic photovoltaics have been greatly increased. However, further improvements in the device architecture and stability are

needed to reach industrially relevant efficiencies. To enhance the performance of solar cells, recent research efforts focus on identifying new highly efficient materials. One way to achieve this is the development of low band-gap polymers, which absorb light of lower energies and can, therefore, increase the overall absorption. Prominent representatives for these kinds of polymers are PTB7 and its derivatives, which can achieve efficiencies of over 10 %. Our work focuses on the comparison of different low band-gap polymers regarding their optical and structural properties. Applied characterization techniques include optical absorption and microscopy measurements as well as X-ray scattering methods. Exploratory solar cells link the power conversion efficiency to parameters such as the active layer composition and morphology.

CPP 46.32 Wed 11:00 Poster A

Investigation of novel material systems for increasing the efficiency of organic solar cells — ●CHRISTIAN WEINDL, FRANZISKA C. LÖHRER, and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

In the last decade, interest in organic photovoltaics has increased strongly with enhanced performance values. Even though organic solar cells cannot compete with conventional solar cells in terms of efficiency and long-term stability yet, they have reached the point of industrial application due to a range of unrivaled advantages. Apart from their light weight and their highly tunable optical and mechanical properties, organic solar cells can be produced in an easy and cheap, solution-based way which offers the possibility of mass production via roll-to-roll processing. Their advantages play a particular role in areas not accessible for conventional solar cells, such as curved, flexible or transparent surfaces as well as mobile devices. In our work, we investigate novel material systems used to increase the performance of organic solar cells in terms of efficiency as well as long-term stability. Here, we present insights into the correlation of optical and morphological properties of polymer-based organic photovoltaics by combining real-space imaging and X-ray scattering techniques with optical spectroscopy.

CPP 46.33 Wed 11:00 Poster A

Spontaneous generation of interlayers in OPVs with silver cathodes using additives in a P3HT:PCBM layer — BASEL SHAMIEH¹, GITTI FREY¹, and ●UWE VOGEL² — ¹Israel Institut of Technology, Haifa 32000, Israel — ²Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

We report a new efficient methodology for processing interlayers by the spontaneous segregation of an additive to a silver cathode. The driving force for this special migration is the chemical interaction between the thiol end group of the additive HEG-DT and the silver. In addition, we report modification of the silver work function at the interface and effectively increase the device Voc which enhances the device efficiency by 76%.

CPP 46.34 Wed 11:00 Poster A

Morphological Investigations on fullerene-free bulk heterojunction blends for photovoltaic applications — ●SEBASTIAN GROTT¹, LORENZ BIESSMANN¹, NITIN SAXENA¹, WEI CAO¹, SIGRID BERNSTORFF², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Elektra-Sincrotrone Trieste, 34149 Basovizza, Italy

Organic solar cells have been in the focus of research for decades due to their advantages in versatility, flexibility, low-cost manufacturing processes, like roll-to-roll-printing, and the tuneable characteristics. These properties open up a wide field of applications and represent an alternative for conventional photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional, values over 11% have been reported. In particular, fullerene-free bulk heterojunction (BHJ) blends receive an increasing attention. We investigate the inner morphology of such BHJ systems. Different compositions of PBDB-T and ITIC BHJ films are studied with advanced x-ray scattering techniques. The obtained structure information is correlated with current density-voltage characteristics and the absorbance of the active layers.

CPP 46.35 Wed 11:00 Poster A

Improvement of Organic Solar Cell Morphology and Device Operation due to Controlled Polymer Aggregation in Solution — ●SHAHIDUL ALAM^{1,2}, RICO MEITZNER^{1,2}, CHRISTIAN KÄSTNER³, CHRISTOPH ULBRICHT⁴, DANIEL A. M. EGBE⁴, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

— ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — ³Institute of Thermodynamics and Fluid Mechanics, Technische Universität Ilmenau, Am Helmholtzring 1, 98693 Ilmenau, Germany — ⁴Institute of Polymeric Materials and Testing, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Aggregation of organic semiconductors (OS) generally positively impacts the device performance of polymer solar cells. Aggregation and specifically intermolecular electronic coupling leads to extended absorption spectra by formation of new absorption bands. In addition, more ordered domains of OS improve the free charge carrier generation yield and also reduce recombination rates of free charges located in the ordered phases due to energy relaxation within. Thus, aggregation enhances charge carrier mobility and lifetime, resulting in an improved charge extraction under operating conditions. Here we report progress in controlling polymer aggregation in solution by introduction of anti-solvent additives. The impact of polymer aggregation on photovoltaic performance was investigated by various spectroscopic methods.

CPP 46.36 Wed 11:00 Poster A

Investigation of light harvesting complex LHCBM6 for dye-sensitized solar cells — ●FABIAN SCHMID-MICHEL¹, NINA LÄMMERMANN², OLAF KRUSE², and ANDREAS HÜTTEN¹ — ¹Center for Spinelectronic Materials and Devices, Physics Department, Bielefeld University, Germany — ²Faculty of Biology, Algae Biotechnology & Bioenergy, Bielefeld University, Germany

Light harvesting complexes (LHC) or antenna complexes participate in photosynthesis by harvesting sunlight and transferring the excitation energy to the reaction centre. By channelling this energy elsewhere it is possible to use LHC either as a dye for dye-sensitized solar cells or as energy harvesters for artificial photosynthesis (AP). Solving this challenge could lead to a more efficient regenerative fuel production. To investigate LHCBM6, dye sensitized solar cells were prepared on ITO glass with the LCHs bound to TiO₂ nanoparticles. Different binding types were evaluated by electrical measurements and microscopy. Long-term electrical measurements provide insight into the long-term stability.

CPP 46.37 Wed 11:00 Poster A

Composition control and photovoltaic properties of binary polymer:fullerene blends — ●LORENA PERDIGÓN-TORO¹, YUEQI YANG¹, ELISA COLLADO-FREGOSO¹, HARALD ADE², and DIETER NEHER¹ — ¹University of Potsdam, Institute of Physics and Astronomy, Germany — ²Department of Physics and ORaCEL, North Carolina State University, Raleigh, North Carolina 27695, USA

Organic solar cells consist of blends of two or more semiconductors with distinct electronic structures, namely electron donors and acceptors. The morphology of the blend can vary greatly depending on numerous conditions, such as the nature of the materials or the processing. When employing an amorphous polymer and small molecules such as fullerenes, the morphology comprises at least two phases: one phase nearly pure in fullerenes and a second where the macromolecules and fullerenes are intimately intermixed. The initial polymer:fullerene ratio and the annealing temperature play deciding roles on the composition of these two phases. Recent work suggested an unique dependence of the fill factor of solar cells made from binary blends with composition contrast.

In this work, we use PCDTBT:PC71BM as reference to obtain a system ranging from a well-separated blend to a one phase blend. Devices annealed above the critical temperature exhibit much lower fill factor, pointing to increased geminate and/or non-geminate recombination. Various techniques such as bias assisted charge extraction (BACE) and time delayed collection field (TDCF) are used to disentangle these processes and analyse field-assisted charge generation and extraction.

CPP 46.38 Wed 11:00 Poster A

Influence of PMMA protection layers on Ozone degradation of P3HT and MDMO-PPV — ●ANDREAS FRUEH¹, HANS-JOACHIM EGELHAAF², HEIKO PEISERT¹, and THOMAS CHASSÉ¹ — ¹Universität Tübingen, IPTC, Auf der Morgenstelle 18 D-72076 Tübingen, Germany — ²ZAE Bayern, Auf AEG, Bau 16, 1. OG, Fürther Str. 250, D-90429 Nürnberg

The fast degradation of organic polymer materials remains a major problem in organic electronics and optoelectronic devices. We study the influence of PMMA cover layers on the photo oxidation and the degradation by ozone of two prototype poly-

mers: poly(3-hexylthiophene) (P3HT) and Poly[2-methoxy-5-(3*,7*-dimethyloctyloxy)-1,4-phenylenevinylene] (MDMO-PPV) using optical spectroscopies. PMMA films with layer thicknesses of for example 65 nm slow the ozone-degradation down by a factor of 2600. PMMA films do not provide protection against photo oxidation at AM 1.5 in dry or humidified synthetic air.

CPP 46.39 Wed 11:00 Poster A

Printed films of conjugated polymers and small acceptor molecules — ●KERSTIN WIENHOLD and PETER MÜLLER-BUSCHBAUM — TU München, Physik Department, LS Funktionelle Materialien, 85748 Garching

Organic photovoltaics are a promising alternative to conventional silicon solar cells as they offer several potential advantages e.g. low weight, high mechanical flexibility and low-cost production. Recent research focuses on identifying new high-efficiency polymers and acceptor molecules to reach high power conversion efficiencies (PCEs). To date, a PCE of 13% could be obtained with a PBDB-T-SF: IT-4F based organic solar cell devices. The fluorinated conjugated polymer PBDB-T-SF acts as a donor whereas the fluorinated small molecule IT-4F acts as an electron acceptor. Both molecules are promising for photovoltaic applications as they show higher absorption coefficients, higher efficiency in exciton separation and charge transport as well as enhanced chemical stability as compared with their non-fluorinated counterparts. However, before commercialization, the solar cell performance must be optimized and an up-scale of the thin layer deposition is necessary. Printing of the individual layers of the solar cells can overcome the up-scale challenge. We print thin PBDB-T-SF: IT-4F films. Characterization techniques such as UV/Vis spectroscopy, photoluminescence and scattering methods such as GISAXS and GIWAXS are applied to get a deeper insight into the composition and morphology of the active layer of the printed films with the aim to further improve the solar cell efficiencies.

CPP 46.40 Wed 11:00 Poster A

Charge transport in layered organic semiconductors — ●ANIRBAN MONDAL and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Mainz, Germany

Modern organic electronic devices comprise of many semiconducting layers. The performance of these heterostructures is predominantly determined by the relative alignment of ionization potentials and electron affinities in each layer with respect to each other. Despite the continued scientific interest, predicting energy-level alignment at organic heterointerfaces is still a challenge in computational materials science. Using the adapted to charge systems Ewald summation technique and exploring the long-range nature of the charge-multipole interactions, we demonstrate that the density of states is a function of layer thickness and the environment in which this layer is embedded. These results contribute to the understanding of functional heterointerfaces for organic light emitting devices.

CPP 46.41 Wed 11:00 Poster A

Charge Localisation and Quantitative Chemical p-Doping in Single-Wall Carbon Nanotubes — ●BERND STURDZA¹, MICHAEL AUTH¹, KLAUS H. ECKSTEIN², FLORIAN OBERNDORFER², ANDREAS SPERLICH¹, TOBIAS HERTEL², and VLADIMIR DYAKONOV^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — ³Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Single-Wall Carbon Nanotubes (SWNTs) meet the requirements for various applications due to their particular electronic properties. As in other semiconductors the influence of defects and doping is highly important for future technologies. Recent studies indicated charge carrier localisation in AuCl₃ doped (6,5) SWNTs implied by changing exciton dynamics using indirect all-optical measurements [1]. Here we show direct quantitative studies of p-doping in SWNTs employing electron paramagnetic resonance (EPR). By comparison to a spin count reference sample quantitative EPR yields direct access to doping concentrations. We were able to quantify the p-doping concentrations on the SWNTs for various doping ratios, further receiving new insight into charge carrier confinement.

[1] Eckstein et al., Localized Charges Control Exciton Energetics and Energy Dissipation in Doped Carbon Nanotubes, ACS Nano 2017, DOI:10.1021/acsnano.7b05543

CPP 46.42 Wed 11:00 Poster A

Modeling morphologies with liquid crystalline order in copolymers with conjugated blocks — ●JIANRUI ZHANG, KURT KREMER, and KOSTAS DAOULAS — Max Planck Institute for Polymer Research, Mainz, Germany

Block copolymers (BCP) with conjugated blocks are interesting for organic electronics. Because of the π - π stacking interactions between aromatic rings in the backbone and short side chains, conjugated blocks can form liquid crystals (LC) with collective planar order or crystalline phases. Therefore, the phase behavior of BCP with conjugated blocks is significantly more complex comparing to classical BCP and their properties are less understood. Here we investigate the effects of collective planar order on conformational and structural properties of these materials. For this purpose, we employ a generic model, where conjugated blocks can create collective planar order characterized by biaxial nematic symmetry. We consider diblock copolymers consisting of one flexible and one conjugated block, and restrict our study to the simplest case – lamellar phase. First Monte Carlo (MC) simulations in the canonical ensemble are used to locate approximately the region of the parameter space where lamellae are formed. Then variable box-shape MC simulations are performed to find optimized lamellae with uniform stress. The optimized lamellae comprise alternating amorphous and biaxial layers, formed by flexible and conjugated blocks respectively. Interestingly, we find that different biaxial layers have the same preferred chain alignment direction but different π -stacking directions. This observation indicates decorrelation between biaxial layers.

CPP 46.43 Wed 11:00 Poster A

Influence of Morphology on Mobility in Perylene Bisimide Polymer Systems — ●HAZEM BAKR¹, JULIAN KAHLE¹, MUKUNDAN THELAKKAT², and ANNA KÖHLER^{1,3} — ¹Experimental Physics II, Uni Bayreuth — ²Macromolecular Chemistry I, Uni Bayreuth — ³BIMF, Uni Bayreuth

We investigate how morphological and conformational order affects the charge transport in two different perylene bisimide (PBI) based polymers. The two PBIs used differ in their sidechains, thus leading to different morphologies. Time resolved photoluminescence measurements in solution and film have shown the presence of two emitting species, present at different amounts. A long lived one with a lifetime of 20 ns which is attributed to excimer emission and a short lived one with a lifetime of 4 ns assigned to the PBI monomer emission. Using electron only devices, we determine the electron mobility using space charge limited current (SCLC) measurements. The differences in charge mobilities and their relation to the film morphology are discussed.

CPP 46.44 Wed 11:00 Poster A

Efficient doping of poly(3-hexylthiophene) using the strong Lewis acid tris(pentafluorophenyl)borane — ●MALAVIKA ARVIND¹, PATRICK PINGEL², CHRISTIAN RÖTHEL³, SILVIA JANIEZ², INGO SALZMANN⁴, and DIETER NEHER¹ — ¹University of Potsdam, Germany — ²Fraunhofer Institute for Applied Polymers, Germany — ³Karl-Franzens Universität Graz, Austria — ⁴Humboldt Universität zu Berlin, Germany

Molecular doping provides a convenient way of improving the conductivity and transport properties of organic materials. In this study, we use tris(pentafluorophenyl)borane (BCF)- a well soluble, strong Lewis acid that is known to serve as a p-dopant[1], to dope the semiconducting polymer poly(3-hexylthiophene) (P3HT). Analysis of the sub-band gap signals in the UV-Vis-NIR spectra of BCF doped P3HT solutions and thin films indicates a doping process similar to that in F4TCNQ-P3HT, despite the obvious structural dissimilarity between the two dopants.[2] However, grazing incidence x-ray diffraction (GIXRD) experiments reveal important differences between the two systems. While co-crystal formation is observed in F4TCNQ-P3HT films[3], such features are absent in the BCF-P3HT system. By employing different techniques for film preparation and doping, we succeeded in fabricating doped films with high structural homogeneity and outstanding electrical conductivities.

[1] Welch et al., J. Am. Chem. Soc., 133 (2011) 4632

[2] Pingel, Arvind et al., Adv. Electron. Mater., (2016) 2: 1600204

[3] Mendez, Salzmänn et al. Nat. Comm., (2015), 6, 8560

CPP 46.45 Wed 11:00 Poster A

Drift, Diffusion, and Immobilization of Organic Dopant Molecules - Challenges and Prospects — ●SEBASTIAN BECK^{1,2}, PATRICK REISER^{2,3}, HEIKO MAGER^{1,2}, VIPILAN SIVANESAN^{1,2},

JAKOB BERNHARDT^{1,2}, FRANK SIMON BENNECKENDORF^{2,4}, LARS MÜLLER^{1,2,5}, and ANNEMARIE PUCCI^{1,2} — ¹Kirchhoff-Institut für Physik, Universität Heidelberg — ²InnovationLab, Heidelberg — ³Surface Science Division, TU Darmstadt — ⁴Organisch-Chemisches Institut, Universität Heidelberg — ⁵Institut für Hochfrequenztechnik, TU Braunschweig

A precise adjustment of dopant distribution is crucial for the functionality of organic electronic devices. Therefore, a lot of effort is made to control the molecular composition in devices throughout fabrication. However, diffusion processes as well as drift of organic dopant molecules can alter the carefully planned device architecture resulting in device fatigue. Therefore, detailed studies of diffusion and drift properties as well as a method to immobilize organic dopant molecules are needed to further improve device performance. In this study, the drift of dopant molecules, such as F4TCNQ and Mo(tfdCO₂Me)₃, in external electric fields was investigated. IR micro-spectroscopy of doped P3HT layers in combination with electrical measurements was used to clarify the underlying processes. Additionally, the diffusion properties of Mo(tfdCO₂Me)₃ in sequentially doped P3HT layers with varying regioregularity were studied by in-situ IR and Photoelectron spectroscopy. We further present an UV triggered immobilizing procedure and introduce it to derivatives of the n-type dopant N-DMBI.

CPP 46.46 Wed 11:00 Poster A

Exploring the design of a complex and versatile Kinetic Monte Carlo code, for organic electronics applications — ●LEANNE PATERSON and DENIS ANDRIENKO — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

There is a vast and continuously growing interest in the field of organic electronics. Although in its infancy with respect to inorganic competitors, it is clear that the use of organic materials in electronic devices can offer a cheaper, flexible and highly variable alternative. In order for the field to advance and maximise the capabilities of such devices, it is vital to understand the molecular processes involved. Kinetic Monte Carlo (KMC) simulations offer a method to investigate the movement of charge carriers through the organic material, with the possibility to incorporate effects such as recombination of carriers and coulomb interaction. Charge carrier movement in organic semiconductors can be described via a "hopping" mechanism. Each carrier hop or event, takes the system from state "a" to "b", there is a corresponding rate for this transition and a probability for it to occur, which can be represented by the master equation. KMC is one method of solving this master equation, giving a randomly generated trajectory of carrier movement within the organic material. The KMC code presented, uses a two-level variable step size method (VSSM) algorithm, to increase computational efficiency. The algorithm proceeds with pre-computed rates, calculated using Marcus theory, which are grouped corresponding to carrier type and position.

CPP 46.47 Wed 11:00 Poster A

Structural models of the n-type nickel-tetrathiooxalate polymers: A combined DFT/MD approach — ROMAN TKACHOV^{1,2}, LUKAS STEPIEN², ROBERT GRAFE², ●OLGA GUSKOVA³, ANTON KIRYI³, HEIKO REITH⁴, and CHRISTOPH LEYENS^{1,2} — ¹TUD, Helmholtzstr. 7, 01062, Dresden — ²Fraunhofer IWS, Winterbergstr. 28, 01277, Dresden — ³IPF Dresden, Hohe Str. 6, 01069, Dresden — ⁴IFW Dresden, Helmholtzstr. 20, 01069, Dresden

In this work, the 3D models of the n-type nickel-tetrathiooxalate polymers poly(Ni-tto) and poly[Kx(Ni-ett)] have been studied for the first time using DFT, the crystal packing prediction, all-atom MD simulations and experiments [1,2]. As a result, possible unit cells for both polymers are suggested, having densities and the XRD patterns close to the experimental ones [2]. The predicted 3D packings consist of two structural elements: the π -stacked columns and the herringbone arrangements with counterions intercalating in-between stacks. From the all-atom MD simulations, the close contacts S...Ni, S...S, the distributions of counterions and the thermal disorder are characterized. This distinguishes our approach from the previously reported ones either on a linear idealistic chain [3] or on 3D models without counterions [4]. We are currently focusing on the calculations of the Seebeck coefficient for 3D models of polymers as promising elements for thermoelectric applications. This work is supported by SAB (Proj.100245366) and AiF (IGF-Proj.18165BR). [1] R. Tkachov et al Tetrahedron, 2017, 73, 2250. [2] R. Tkachov et al Polym. Chem., 2017 (submitted). [3] D. Tiana et al PCCP, 2014, 16, 14463. [4] T. Vogt et al JACS 1988, 110, 1833.

CPP 46.48 Wed 11:00 Poster A

LT-UHV-STM investigations on single benzylnaphthoic diimides adsorbed on metal(111)-surfaces — ●BERTRAM SCHULZE LAMMERS¹, RENÉ EBELING¹, ELENA DIRKSEN², THOMAS J. J. MÜLLER², and SILVIA KARTHÄUSER¹ — ¹Peter Grünberg Institut (PGI-7) and JARA-FIT, Forschungszentrum Jülich GmbH, Germany — ²Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität Düsseldorf, Germany

LT-UHV-STM investigations allow the detailed characterization of the adsorption behavior and the geometry of 2-dimensional molecules physisorbed on atomically flat surfaces up to their orbital structure. As functionalized naphthalene diimides (NDIs) received current interest due to their possible use as small molecular acceptors for various applications in molecular electronics, we deduced the adsorption behavior and the electronic behavior of these molecular compounds by STM. Here the 2,7-dibenzyl 1,4,5,8-naphthalenetetracarboxylic diimide (BNTCDI), which consist of a large π -conjugated NDI backbone and two benzyl-groups connected to the central part, have been studied as prototypical 3-dimensional NDI compounds. Recent results [1] for BNTCDI on the Pt(111)-surface verified the 3-dimensional structure of the adsorbed molecule with the phenyl groups standing vertically with their phenyl plane on the substrate. In addition to these results the electronic and topographic structure of BNTCDI adsorbed on different (111)-surfaces was investigated in detail and compared to DFT based calculations on BNTCDI in the gas phase and its orbital symmetry of the HOMO and the LUMO. [1] DOI: 10.1021/acs.jpcc.7b09911

CPP 46.49 Wed 11:00 Poster A

Spin crossover iron(II) coordination polymer with fluorescent properties: correlation between emission properties and spin state — CHARLES LOCHENIE¹, ●KONSTANTIN SCHÖTZ², FABIAN PANZER², HANNAH KURZ¹, BERNADETTE MAIER¹, FLORIAN PUCHTLER⁴, SEEMA AGARWAL⁵, ANNA KÖHLER^{2,3}, and BIRGIT WEBER¹ — ¹Inorganic Chemistry II, Universität Bayreuth — ²Experimental Physics II, Universität Bayreuth — ³Bayreuth Institute of Macromolecular Research, Universität Bayreuth — ⁴Inorganic Chemistry I, Universität Bayreuth — ⁵Macromolecular Chemistry II, Universität Bayreuth

Spin crossover complexes show great potential as molecular switches or data storage devices. For a good performance as such, the switching between the high spin (HS) and the low spin (LS) state should be abrupt and show a stable hysteresis in an accessible temperature region. We report the synthesis and characterization of a spin crossover coordination polymer exhibiting such attributes. By differential scanning calorimetry and magnetic measurements, Mössbauer spectroscopy, and X-ray powder diffraction, we revealed a wide and stable hysteresis of the spin transition between $T_{1/2, up} = 371 K$ and $T_{1/2, down} = 323 K$, which can additionally be tracked using photoluminescence spectroscopy due to a change in emission color.

CPP 46.50 Wed 11:00 Poster A

Phosphorescence Lifetime of a Brominated Diphenylphosphine-Alkyl Naphthaleneimide Luminescence Turn-On Dyad in Different Atmospheres — SEBASTIAN FEULNER¹, ●LOTHAR KADOR¹, PAUL M. REICHSTEIN², and WERNER REICHSTEIN³ — ¹University of Bayreuth, Institute of Physics, 95440 Bayreuth, Germany — ²University of Bayreuth, Macromolecular Chemistry I, 95440 Bayreuth, Germany — ³University of Bayreuth, Bayreuth Materials Center (BAYMAT), 95440 Bayreuth, Germany

We have studied a brominated diphenylphosphine-alkyl naphthalene-imide luminescence turn-on dyad which, in its oxidized form, emits strong fluorescence and moderate phosphorescence when excited with UV light at 365 nm. In ambient air, the phosphorescence is partly quenched by triplet-triplet annihilation (TTA) with molecular oxygen. At lower pressure, TTA is reduced and, therefore, the contribution of the phosphorescence to the total luminescence and the phosphorescence lifetime increase. The phosphorescence signal and the phosphorescence lifetime were studied in the frequency domain with modulated UV excitation at air pressures between 1 bar and vacuum. Both quantities increase strongly below 100 mbar. The phosphorescence was also investigated in pure oxygen and pure argon atmosphere at 1 bar. As expected, oxygen causes slightly stronger phosphorescence quenching than air. Surprisingly, in argon the phosphorescence is significantly weaker than in vacuum. The experimental data are interpreted in the so-called polar-plot (or Cole-Cole plot) representation.

CPP 46.51 Wed 11:00 Poster A

Calculation of electron-phonon coupling constants in

π -conjugated molecules from first principles — ●IRINA PETRESKA^{1,2} and GERTRUD ZWICKNAGL² — ¹Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University in Skopje, 1000 Skopje, Republic of Macedonia — ²Institut für Mathematische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Electron-phonon coupling constants for a class of π -conjugated molecules will be calculated using excited states and vibrational spectra obtained from first principles. Electronic excitations will be evaluated in the frame of configuration interaction (CI) picture, as well as the time-dependent density functional theory (TD-DFT). Hamiltonian matrix involving electronic and vibronic energies obtained from CI and TD-DFT calculations will be then composed, which will enable evaluation of the electron-phonon coupling constants. The obtained results could be further used to parametrize the extended Hubbard-like Hamiltonians in order to treat the inelastic transport regime in π -conjugated molecules.

CPP 46.52 Wed 11:00 Poster A

Singlet And Triplet Dynamics of Covalently Bound Ditetracene in Various Environments — ●MAXIMILIAN FRANK¹, ULRICH MÜLLER¹, LENA ROOS², ANKE KRUEGER², and JENS PFLAUM^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Institute of Organic Chemistry, Julius Maximilian University of Würzburg, 97074 Würzburg — ³Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Singlet fission significantly affects the performance of many organic photovoltaic cells and light-emitting diodes. In this process a singlet state decays into two triplet states which strongly depends on the relative orientation of the participating chromophores. As tetracene constitutes a model system showing efficient, thermally activated singlet fission, we study covalently bound ditetracene to determine the influence of the rotation angle between the two tetracene molecules on this process. Therefore, ditetracene and tetracene doped into different host systems like a disordered PMMA matrix or a single anthracene crystal are optically analysed by means of photon-correlation studies together with lifetime measurements at room temperature. By comparing this data with that of a tetracene single crystal or the molecules in solution we are able to identify two different excitonic species in ditetracene and to show how the influence of the environment and temperature affects their photophysical characteristics such as the spectral intensity distribution, fluorescence lifetime and quantum efficiency. This project was funded by the DFG in the framework of the GRK 2112.

CPP 46.53 Wed 11:00 Poster A

Synthesis of a series of brominated TPB molecules to increase the phosphorescence — ●ANNA HAFT¹, FELIX FRIES¹, RAMUNAS LYGAITIS², OLAF ZEIKA¹, and SEBASTIAN REINEKE¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Nöthnitzer Str. 61, 01187 Dresden — ²Kaunas University of Technology, K. Donelaičio g. 73, 44249 Kaunas

Biluminescent emitter molecules are able to show phosphorescence and fluorescence efficiency at room temperature. N,N,N',N'-tetraphenyl-[1,1'-biphenyl]-4,4'-diamine (TPB) is one of these special emitters. By adding heavy atoms like bromine it is possible to increase the ratio of phosphorescence to fluorescence by increasing the intersystem crossing through intramolecular heavy atoms.

To investigate this effect, a series of TPB derivatives was synthesized successfully. The pure TPB was obtained using the Ullmann reaction. A bromination in para position in case of mono to tetra brominated species was achieved via an electrophilic substitution with N-bromosuccinimide. The materials were investigated in form of a host:guest system embedded in a rigid matrix of poly(methyl methacrylate) PMMA with respect to the internal conversion rates, where the increased phosphorescence-to-fluorescence ratio with increasing heavy atom decoration was confirmed.

CPP 46.54 Wed 11:00 Poster A

Macroscopic anisotropic optical properties by wrinkling instabilities — ●ANIK KUMAR GHOSH¹, BERNHARD ALEXANDER GLATZ¹, SVEN WIESSNER^{1,2}, AMIT DAS¹, TOBIAS A. F. KÖNIG^{1,2}, and ANDREAS FERY^{1,2} — ¹Leibniz-Institut für Polymerforschung Dresden e. V., Germany — ²Cluster of Excellence Centre for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, Germany

Polymeric wrinkled structures are exquisite, concerning their apparent advantages with reverence to their flat counterparts. Their repeating sinusoidal geometry is the result of an energetic instability induced by a mechanical mismatch between two layers that is easy to handle, reproducible and very robust. A well-known way to gain such structures represents the oxidation of a pre-strained polydimethylsiloxane (PDMS) slab by plasma treatment [Microchimica Acta, 2009, 165, 249 and Soft Matter, 2015, 11, 3332]. It creates in situ a glassy layer on top, while the consequent strain relaxation of the two-layer system results in a mechanical buckling instability that forms permanent wrinkles. In our setup, we move onward by fabricating blazed grating structures via angle-dependent thin metal film deposition on top of the PDMS wrinkles. This enables them for enhanced light-matter interactions, subsequently a gateway towards high-performance optoelectronic devices, non-linear optical phenomena which further results in a key point to build a cost-efficient class of photonic structures. Supported by finite-difference time-domain simulations, we further discuss the grating efficiency of the anisotropic structure.

CPP 46.55 Wed 11:00 Poster A

Optical and structural properties of diindenoperylene and perylene-tetracarboxylic-diimide on ZnO and SiO₂ — ●CLEMENS ZEISER, ALEXANDER HINDERHOFER, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

In recent years, heterostructures of donor and acceptor compounds have attracted significant attention due to their applications in organic devices [1]. We studied blends of diindenoperylene and perylene-tetracarboxylic-diimide (PTCDI) deposited by organic molecular beam deposition on SiO₂ as an inert and on ZnO as a strongly interactive substrate. Uniaxial absorption spectra of films on silicon oxide measured by spectroscopic ellipsometry could be explained with the molecular structure determined by synchrotron x-ray diffraction. Using differential reflectance spectroscopy, also thickness dependent absorption spectra of films deposited on ZnO and SiO₂ have been examined. We find changes in the vibronic progression of flat-lying monolayer spectra which could be assigned to molecular interactions with the ZnO surface [2]. Furthermore, also the changing absorption spectra of the following layers could be explained by molecular coupling and morphologic influences.

- [1] A. Hinderhofer, ChemPhysChem 2012, 13, 628-643
[2] P. Winget et. al., Adv. Mater. 2014, 26, 4711-4716

CPP 46.56 Wed 11:00 Poster A

Investigation of opto-electronic properties of ZnPc:F₄ZnPc OLEDs — ●SIMON WIEGAND¹, THOMAS FERSCHKE¹, GABRIEL FREIHERR VON EYB¹, SEBASTIAN HAMMER¹, 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

To analyze the electrically driven generation of excitonic and possible charge transfer states we fabricated organic light emitting diodes (OLEDs) comprising an emission layer (EML) made out of co-evaporated neat and partially fluorinated zinc phthalocyanin, ZnPc and F₄ZnPc, respectively. By means of electroluminescence (EL), photoluminescence (PL) and I(V) characteristics, we studied the optoelectronic properties of these OLEDs. The additional variation of the EML thickness provides access to the microscopic mechanisms, such as local space charging or an unbalanced injection of electrons and holes, governing the radiative as well as non-radiative relaxation of excited states. Furthermore, guided by a recent publication of our group [1] we intend to utilize plasmonic emission enhancement by using suited electrode materials and electrode geometries matching the spectral characteristics of our ZnPc:F₄ZnPc OLEDs.

- [1] V. Kolb, et al., Opt Express, 2017, 25(6), 6678-6689

CPP 46.57 Wed 11:00 Poster A

Study on conductive silver nanowire networks in 3D printed polymers — ●LEWIS AKINSINDE¹, TOMKE GLIER¹, FERDINAND OTTO¹, CALVIN J. BRETT^{2,3}, MILENA LIPPMANN³, STEPHAN V. ROTH^{3,4}, and MICHAEL A. RÜBHAUSEN¹ — ¹Institut für Nanostruktur und Festkörperphysik, Universität Hamburg — ²Department of Fluid Physics, Royal Institute of Technology (KTH), Stockholm, Sweden — ³Photon Science, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — ⁴Royal Institute of Technology (KTH), Stockholm, Sweden

Nowadays, increasing attention has been devoted to transparent con-

ductive films because of their various applications in Solar cells and OLEDs. 3D printing is an alternative promising fabrication process. The embedding of silver nanowires in a UV sensitive polymer matrix enables 3D printable conductive objects. Hence silver nanowires were synthesized via the polyol method resulting in an average diameter of approximately 130 nm and a length up to 100 μm . With optimization through dry etching sheet electrical resistance could be reduced to ca. 1.5 Ω/square . This is highly competitive with existing candidates such as indium tin oxide (ITO). As a next step layer systems consisting of UV cured 1,6-Hexanediol diacrylate (HDDA) and silver nanowires were prepared. The structure and morphology of the silver nanowire incorporated thin films were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), conductivity measurements and spectroscopic measurements. Inner film morphology was studied using grazing incidence small-angle X-ray scattering (GISAXS)

CPP 46.58 Wed 11:00 Poster A

Flexible Modulation of Electronic Band Structures of Wide Band Gap GaN Semiconductors Using Bioinspired, Non-Biological Helical Peptides — •SVEN MEHLHOSE¹, NATALYA FRENKEL¹, WASIM ABUILLAN¹, SARA LIPPERT³, GESCHE MÜNTZE³,

MARTIN EICKHOFF³, SHUNSAKU KIMURA², and MOTOMU TANAKA¹ — ¹Physical Chemistry of Biosystems, Institute of Physical Chemistry, Heidelberg University, D69120 Heidelberg, Germany — ²Department of Material Chemistry, Graduate School of Engineering, Kyoto University, 6158510 Kyoto, Japan — ³Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee, D28359 Bremen

We show the modulation of the electronic band profiles of wide band gap GaN semiconductors by the macromolecular dipole potentials exerted from ordered monolayers of synthetic, non-biological aldehyde terminated helical peptides deposited on wet chemically oxidized GaN surfaces functionalized with aminosilanes. The selective coupling of either N- or C-terminal to the amino-terminated surface enables one to control the direction of the dipole moment. After confirming the formation of highly ordered peptide monolayers, the impact of macromolecular dipole potentials was quantified by electrochemical impedance spectroscopy. The same functionalization steps were transferred to GaN/AlGaIn/GaN high electron mobility transistor structures. Stable and quantitative modulation of the current-voltage characteristics of the two-dimensional electron gas by the deposition of bio-inspired peptides is a promising strategy for the macromolecular dipole engineering of GaN semiconductors.