

CPP 50: Poster: Organic Electronics and Photovoltaics, Molecular Excitations

Time: Wednesday 18:30–21:00

Location: P3

CPP 50.1 Wed 18:30 P3

Solid state structure and charge transfer properties of D-A-D conjugated blocks: A joint experimental-theoretical approach — DEYAN RAYCHEV^{1,2}, YEVHEN KARPOV¹, ANTON KIRIY¹, JÖRG GRENZER³, JENS-UWE SOMMER^{1,2}, and OLGA GUSKOVA^{1,2} — ¹Leibniz-Institute of Polymer Research Dresden, Hohe Str. 6 01069 Dresden — ²Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden — ³Helmholtz-Zentrum Dresden-Rossendorf e. V., Bautzner Landstraße 400 01328 Dresden

The performance of molecular materials in organic electronics dramatically depends on their electronic properties and solid-state structure. In this work, we have investigated donor-acceptor-donor (D-A-D) conjugated molecules having central benzothiadiazole A-unit in order to understand the structure-property correlation by selecting thiophene or furan D-flanks. We have found, that the electronic and photophysical behavior is not affected, but the conformational and charge transfer properties exhibit a significant alteration upon varying a flank [1]. A joint theoretical packing prediction and experimental powder X-ray diffraction analysis showed differences in the solid-state structure and intermolecular interactions of D-A-D molecules. As a result, the difference in the solid-state packing defines the mobility of electrons and/or holes within the organic molecular stacks. The financial support from the ESF Group "CoSiMa" at DCMS, TU Dresden is highly appreciated.

[1] D. Raychev, O. Guskova, G. Seifert and J.-U. Sommer, *Comp. Mater. Sci.*, 2017, 126, 287-298.

CPP 50.2 Wed 18:30 P3

Self-organization of liquid spread polymers for organic photovoltaics studied by 2d polarization microscopy — DANIELA TÄUBER¹, WANZHU CAI², OLLE INGANÄS², and IVAN SCHEBLYKIN¹ — ¹Chemical Physics, Lund University, Lund, Sweden — ²Biomolecular and Organic Electronics, Linköping University, Linköping, Sweden

Large-area self-assembly of functional conjugated polymers holds a great potential for practical applications of organic electronic devices. We obtain well aligned films of poly[2,3-bis(3-octyloxyphenyl)quinoxaline-5,8-diyl-alt-thiophene-2,5-diyl] (TQ1) by the floating film transfer method. Thereby, a droplet of a TQ1 solution is injected on top of the surface of an immiscible liquid substrate, at the meniscus formed at the edge of a Petri dish, from where the polymer solution and film then spreads in one direction. Characterization of the TQ1 film by the recently developed two-dimensional polarization imaging (2D POLIM) reveals large, mm sized domains of oriented polymer chains. The irregular shape of the contact line at the droplet source induced the appearance of disordered stripes perpendicular to the spreading direction. A correlation of polarization parameters measured by 2D POLIM revealed the microstructure of such stripes, providing valuable information for further improvement and possible upscaling of this promising method.

CPP 50.3 Wed 18:30 P3

Imidazo[1,5-a]pyridines as Light Emitting Materials — JASMIN MARTHA HERR^{1,3}, GEORG ALBRECHT^{2,3}, JULIA SCHULZE¹, DERCK SCHLETTWEIN^{2,3}, and RICHARD GÖTTLICH^{1,3} — ¹Justus-Liebig-University Giessen, Institute of Organic Chemistry — ²Justus-Liebig-University Giessen, Institute of Applied Physics — ³Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Imidazo[1,5-a]pyridines display blue photoluminescence, tunable by introducing functional groups, and can be used as ligands to form coordination complexes. The goal of this work is the preparation and electro-optical characterization of imidazo[1,5-a]pyridine solutions and thin films as a prerequisite to their further investigation as stable blue-light emitting building blocks for OLEDs. We synthesized 1,3-disubstituted imidazo[1,5-a]pyridines with different substituents. The influence of these substituents on the electro-optical properties was measured in solution via UV-Vis spectroscopy, fluorescence spectroscopy and cyclic voltammetry as part of our research. For the application of imidazo[1,5-a]pyridines as emitting OLED building blocks, the electro-optical properties of the material in solid state have to be characterized. Therefore, we used spin-coating to fabricate thin films on different substrates and with different solvents.

CPP 50.4 Wed 18:30 P3

Thin Films of Imidazo[1,5-a]pyridines as Building Blocks of New Electro-Optic Devices — GEORG ALBRECHT^{1,3}, JASMIN MARTHA HERR^{2,3}, FRIEDER MÜNTZE^{1,3}, RICHARD GÖTTLICH^{2,3}, and DERCK SCHLETTWEIN^{1,3} — ¹Justus-Liebig-University Giessen, Institute of Applied Physics — ²Justus-Liebig-University Giessen, Institute of Organic Chemistry — ³Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Imidazo[1,5-a]pyridines display blue photoluminescence, tunable by introducing functional groups, and can be used as ligands to form coordination complexes. The goal of this work is the preparation and electro-optical characterization of imidazo[1,5-a]pyridine thin films as a prerequisite to their further investigation as stable blue-light emitting building blocks for OLEDs. Suitable candidates for thin film preparation were chosen among 1,3-disubstituted imidazo[1,5-a]pyridines and deposited by spin-coating and physical vapor deposition. The optical absorbance of the samples was measured during film growth or subsequent to preparation by UV-Vis spectroscopy and morphological information was obtained by atomic force microscopy. The stability of samples was studied by storing the thin films either in the dark or under illumination and subsequent measurements of optical absorption. Cyclic voltammetry was used to obtain the redox potentials.

CPP 50.5 Wed 18:30 P3

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

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

CPP 50.6 Wed 18:30 P3

Investigation of ZnO scattering layers for OLED applications — DOMINIK SCHULLERER, LORENZ BIESSMANN, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Organic light emitting diodes (OLED) are reaching inner quantum efficiencies close to 100%, but the overall efficiency of conventional devices is limited to about 20% mainly by the photon extraction. One approach to overcome this issue is the implementation of an additional scattering layer into the device. A standard OLED is used to study the impact of such layer. This layer can either be created by a direct surface structuring or the introduction of an additional transparent layer. ZnO is a suitable choice for the latter due to its transmittivity in the entire visible spectrum, caused by its direct optical bandgap of 3.3eV. This layer is deposited on a glass substrate. The micro- and nano-structure of ZnO can be adjusted by combining a structure-giving diblock copolymer with sol-gel chemistry. It is investigated how different structuring, which is analyzed by scattering techniques and electron microscopy, can influence the external quantum efficiency and the macroscopic properties of the OLEDs over the entire spectral range.

CPP 50.7 Wed 18:30 P3

Investigation of an n-type conducting polymer for potential use in all-polymer thermoelectric generators — REGINA MICHAELA KLUGE, NITIN SAXENA, and PETER MÜLLER-BUSCHBAUM — Technische Universität München, Physik-Department, LS Funk-

tionelle Materialien, 85748 Garching, Germany

Thermoelectric generators pose a promising approach in renewable energies, as they are able to convert waste heat into electricity. In order to build high efficiency devices, suitable thermoelectric materials are needed. Unfortunately, state-of-the-art thermoelectric materials have the drawback of using toxic or less abundant constituents, making it necessary to look for alternatives. One promising approach is to use conjugated polymers. They have the encouraging ability of easy and various types of scalable solvent processes like roll-to-roll printing. Although they are still less efficient than their inorganic counterparts, their easy synthesis, flexibility and eco-friendliness make them a valuable alternative. For building a thermoelectric generator, p- and n-type materials have to be combined. However, in the past effort was focused on the electronic and thermal transport properties of p-type conjugated polymers. Therefore, we investigate the thermoelectric properties of an n-type polymer P(NDI2OD-T2). Its successful application to transistors and solar cells encourages an auspicious try to build an all-polymer thermoelectric generator.

CPP 50.8 Wed 18:30 P3

Solvent Induced Galvanoluminescence of Metal-Organic Framework Electroluminescent Diodes — ●HAONAN HUANG¹, MICHELLE BEUCHEL², DAGO DE LEEUW², and KAMAL ASADI² — ¹Max Planck Institute for Solid State Research, D-70569 Stuttgart — ²Max Planck Institute for Polymer Research, D-55128 Mainz

Alternating current (AC) electroluminescent diodes were fabricated from MOF-5, a metal organic framework consisting of tetrahedral $[Zn_4O]^{6+}$ units linked by 1,4-benzenedicarboxylate ligands. An additional insulating layer was incorporated to prevent formation of electrical shorts. The electroluminescence spectrum was dramatically redshifted with respect to the photoluminescence spectrum. By deliberately varying trapped solvent molecules, we demonstrate that the light emission does not originate from MOF-5 but is due to galvanoluminescence, emission of weak optical radiation in the visible region that occurs during anodic oxidation of the Al top electrode in contact with electrolytes.

CPP 50.9 Wed 18:30 P3

Comparison of theoretical and actual benefit of birefringent layers in OLEDs — ●MARKUS SCHMID, THOMAS LAMPE, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

One of the main factors influencing the efficiency of OLEDs is the microcavity formed by the organic layers enclosed between the electrodes. From a theoretical point of view it was shown that the inclusion of a birefringent material as transport layer at the reflective cathode can improve the outcoupling efficiency of such devices [1]. The main reason for this is reduced coupling to surface plasmons at the organic-metal interface due to the effects of the anisotropic material.

In this work we present an OLED-layout using a birefringent electron transport layer and a reference device with isotropic optical constants. However, the main challenge is that most optically anisotropic organics like TCTA or Spiro-2CBP are hole-conductors not suitable for electron-transport. Additionally the use of electron injection layers would prevent the beneficial effects of the anisotropic material. In order to reach the necessary electric properties we doped the organic material. Making use of electrical and optical simulations as well as a heteroleptic phosphorescent emitter, we achieved a highly efficient OLED with a birefringent layer in contact to the reflective cathode. The devices even show an external quantum efficiency close to their theoretical limit of about 21%.

[1] CALLENS, MICHIEL K. ET AL.: Anisotropic materials in OLEDs for high outcoupling efficiency. *Optics express* 23, p.21128–21148 (2015).

CPP 50.10 Wed 18:30 P3

Molecular Dynamics Simulations of Perylene Bisimide Dimers — ●SEBASTIAN JOHANNES MÜLLER, AXEL BOURDICK, and STEPHAN GEKLE — Universität Bayreuth

Investigating the stacking mechanism of two perylene bisimide dimers by means of free energy calculations with the molecular dynamics implementation Gromacs shall explain the great difference in their suitability for organic solar cells. The dimers consist of two perylene molecules linked by a short alkane chain whose length differs by one carbon atom. We clarify how different configurations in the stacked state affect the π - π -stacking ability and further show that the dimer with the longer link gains more free energy during a stacking process

and has more stable stacked states and configurations than the other.

CPP 50.11 Wed 18:30 P3

Proton Beam Writing in Alq3 — ●CLEMENS BECKMANN, ALRIK STEGMAIER, ULRICH VETTER, and HANS HOFSSÄSS — II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Proton Beam Writing (PBW) is a direct-write lithography process for nano- and microfabrication of two- or three-dimensional structures [1]. The straight path and low proximity effect of MeV protons in matter allow for the fabrication of structures with high aspect ratio and vertical smooth sidewalls. PBW has been widely studied in resists for lithography and conventional semiconductors like Si and GaAs [1,2]. In this work we focus on PBW in organic semiconductors, which are the key materials in the fast growing field of organic optoelectronics. We will discuss possible ways for structuring of tris(8-hydroxyquinoline)aluminum (Alq3) and present experimental results on the irradiation of Alq3 thin films with high energy protons.

[1] Watt et al, *Materials Today* 10 6 (2007)

[2] Schulte-Borchers et al, *J. Micromech. Microeng.* 22 (2012)

CPP 50.12 Wed 18:30 P3

Influencing emitter orientation in solution processed guest-host-systems — ●PHILIPPE LINSMAYER, THOMAS LAMPE, and WOLFGANG BRÜTTING — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The beneficial horizontal alignment of the transition dipole moments in heteroleptic Ir-complexes is dominated by the interaction at the aromatic film surface during the step-by-step layer deposition in thermally evaporated films. In order to probe weaker molecular interactions besides these effects, we studied phosphor alignment in solution processed guest-host systems. While this approach is not giving the possibility for horizontal alignment of the transition dipole moments, it reveals the influence of the processing parameters like dopant concentration, glass-transition temperature of the host and impact of thermal annealing in solution processed films. For the experiments a common heteroleptic Ir-complex was doped into four different host materials with varying glass transition temperatures. After deposition the films were treated with thermal annealing near the glass transition temperature. The results indicate dependence of the resultant emitter orientation on several parameters which can be attributed to different molecular interactions inside the guest-host system.

CPP 50.13 Wed 18:30 P3

controlling excitons in exciplex host systems for efficient white OLEDs — ●YUAN LIU, SIMONE LENK, KARL LEO, and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

White organic light-emitting diodes (WOLEDs) are highly attractive for flexible displays and lighting panels due to their ultrathin form factor, low cost, good color quality, and high power efficiency. Here, an exciplex system consisting of mCP and B3PYMPM is demonstrated to achieve high efficiency blue and white OLEDs. Employing Iridium(III) bis[(4,6-difluorophenyl)pyridinato-N, C2*] picolinate (FIrpic) as emitter, an external quantum efficiency (EQE) of 19.1% is realized by optimizing the hole and electron transporting layer. Triplet-triplet annihilation and triplet-polaron quenching models are utilized to understand the efficiency roll-off of the devices. Based on optimized blue OLEDs, an efficient WOLED with maximum 19.5% EQE (50.6 lm/W) has been realized by carefully controlling exciton generation and transfer processes. At the practical brightness of 1000 cd/m², it still keeps 18.8% EQE (42.7 lm/W). Adopting a glass half sphere as a light outcoupling technology, the luminous efficacy of the WOLED reaches a maximum of 84.9 lm/W with Commission Internationale de L'Eclairage coordinates of (0.452, 0.457) and a color rendering index of 81. Further, the influence factors of color stability and efficiency roll-off in exciplex-based WOLEDs are investigated in detail.

CPP 50.14 Wed 18:30 P3

Efficient Deep-blue Pyridimidine-based TADF Emitters Using a Highly Twisted Molecular Skeleton — ●RYUTARO KOMATSU¹, TATSUYA OHSAWA², HISAHIRO SASABE^{1,2,3}, KOHEI NAKAO¹, YUYA HAYASAKA¹, and JUNJI KIDO^{1,2,3,4} — ¹Department of Organic Materials Science, — ²Faculty of Engineering, — ³Research Center for Organic Electronics (ROEL), — ⁴Frontier Center for

Organic Materials (FROM), Yamagata University, 4-3-16 Jonan, Yonezawa, Yamagata, 992-8510, Japan

The development of efficient deep-blue emitters is one of the key issues in organic light-emitting devices (OLEDs). As a promising technology that realizes 100% conversion from electrons to photons, thermally activated delayed fluorescence (TADF) emitters have attracted considerable attention. However, only a few efficient deep-blue TADF emitters have been reported to date. Here, we molecularly manipulated the electronic excited state energies of pyrimidine-based TADF emitters to realize deep-blue emission. We then systematically investigate the relationships among the chemical structure and optical properties. The resultant novel pyrimidine emitters called Ac-XMHPMs (X = 1, 2, and 3) contain different numbers of bulky methyl substituents at acceptor moieties, increasing the excited singlet and triplet state energies. Among them, Ac-3MHPM, with a high triplet state energy of 2.95 eV exhibits a high peak external quantum efficiency (EQE) of 18% and an EQE of 10% at 100 cd/m² with Commission Internationale de l'Éclairage chromaticity coordinates of (0.16, 0.15). These efficiencies are among the highest values to date for deep-blue TADF-OLEDs.

CPP 50.15 Wed 18:30 P3

Influence of sidechains on the aggregation behavior of polythiophenes — ●KONSTANTIN SCHÖTZ¹, TOBIAS MEIER¹, DOMINIC RAITHEL², DANIEL SCHIEFER³, MICHAEL SOMMER³, FABIAN PANZER¹, RICHARD HILDNER², and ANNA KÖHLER¹ — ¹Experimental Physics II, Universität Bayreuth — ²Experimental Physics IV, Universität Bayreuth — ³Department for Macromolecular Chemistry, Albert-Ludwigs-Universität Freiburg

Polythiophenes are known to often undergo a phase transition from a high energy coiled phase to a low energy aggregated phase upon cooling or spin coating. The properties of these aggregates have strong impact on the performance of devices like OFETs or solar-cells. It is known that these properties and the characteristics of the aggregate formation depend on different parameters like chain length, polydispersity or concentration of the solution. We measured temperature dependent absorption and emission on various polythiophenes that differ in their sidechain architecture. We show that the electronic structure and thus the character of the formed aggregates depend strongly on the type of the sidechains.

CPP 50.16 Wed 18:30 P3

Thermally Activated Delayed Fluorescence studied by Electroluminescence Detected Magnetic Resonance — ●SEBASTIAN WEISSENSEEL¹, NIKOLAI BUNZMANN¹, BENJAMIN KRUGMANN¹, JEANNINE GRÜNE¹, STEFAN VÄTH¹, ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The mechanism of thermally activated delayed fluorescence (TADF) in organic light emitting diodes (OLEDs) raised many questions with respect to the spins of the emitting exciplex states. In particular, whether the TADF mechanism is a spin-dependent process and, if yes, what is the mechanism of the triplet-singlet Up to now spin-sensitive measurements for OLED devices are scarcely presented in literature. Here, we investigate TADF OLEDs by electroluminescence detected magnetic resonance (ELDMR) in devices based on 4,4',4''-Tris(N-3-methylphenyl-N-phenylamino)triphenylamine (m-MTDATA): Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB) exciplexes. The triplet states of this system energetically split in an external magnetic field. Microwave radiation, applied by a stripline, is absorbed at a resonant magnetic field and enhances the intensity of electroluminescence. Modifying experimental conditions, e.g. resonance frequency, temperature or microwave power, leads to detailed knowledge of the spin system and the underlying mechanism of the reverse intersystem crossing. This information will assist designing new cost-effective OLED materials.

CPP 50.17 Wed 18:30 P3

Towards high-mobility polymorphs in organic semiconductors — ●DANIEL R. REITERER, SIMON ERKER, EGBERT ZOJER, and OLIVER T. HOFMANN — Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria

An important aspect for the application of organic semiconductors in practical devices is their charge-carrier mobility. However, in organic molecules the mobilities are often small. One of the reasons is that organic molecules tend to crystallize in polymorphs with a small band

dispersion and that polymorphs with large dispersion tend to be energetically unfavorable. This is because increasing the intermolecular wave-function overlap, which would increase the band dispersion, also increases Pauli-repulsion. In this work, we discuss various strategies to mitigate or circumvent this effect in order to achieve high-mobility (high dispersion) polymorphs of organic semiconductors. For the example of pentacene we show that high-dispersion polymorphs can be stabilized when the antibonding states in the valence band are depleted. This can be achieved via doping or, to a lesser extent, via contact with passivated metal surfaces. Another possible strategy that we demonstrate here is the use of antiaromatic molecules such as cyclooctatetraene (COT).

CPP 50.18 Wed 18:30 P3

Degradation in polymer-fullerene bulk heterojunction solar cells due to charge carrier recombination — ●ELIUTER NDERIMO, ARNE MÜLLER, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic solar cells have become an increasingly important form of solar cells in recent years. The prolonged illumination of solar cells under sunlight usually leads to a slow reduction of their efficiency. Studying their degradation allows us to accurately predict their power delivery over time. In this work we will focus on the recombination dynamics of PTB7:PCBM bulk-hetero junction solar cells under prolonged illumination. We show that the change in efficiency of the solar cells over time due to charge carrier recombination is a dominating factor of degradation. This is done by applying different potential biases to the cell under continuous AM1.5G equivalent illumination. The lifetime of the solar cell is decreased by a factor of 10 if the charges recombine in the semiconductor bulk (Voc condition) instead of being extracted (Jsc condition). Other means of degradation, such as oxygen and water vapour interference, were minimized by encapsulation. From dark measurements the pure degradation by recombination is extracted and supports the observed effect under illumination.

CPP 50.19 Wed 18:30 P3

Synthesis and characterisation of the new emitters for OLED applications — ●RAMUNAS LYGAITIS^{1,2}, OLAF ZEIKKA¹, REINHARD SCHOLZ¹, LUDWIG POPP¹, PAUL KLEINE¹, SIMONE LENK¹, and SEBASTIAN REINEKE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Deutschland — ²Kaunas University of Technology, Kaunas, Lithuania

Organic light-emitting diodes (OLEDs) are a sustainable, low cost light source used in displays and other applications. Quite big step in progress was made when phosphorescent materials containing Ir(III), Pt(III), or other heavy metals were used in order to harvest both singlet and triplet excitons by means of enhanced intersystem crossing. Today, one of the issues which prevent current iridium-based, phosphorescent emitters widely used in the lighting markets, is that iridium is the fourth rarest naturally-occurring element on the planet, so the usage of this element in large scales could be very risky. Therefore new iridium-free emitters harvesting both singlet and triplet excitons are of big interest. Here, we present the synthesis and characterisation of the series of carbazole-based derivatives containing electron accepting trifluoromethyl groups which support certain intermolecular charge transfer. The newly synthesised derivatives were characterised by means of absorption spectroscopy, steady-state and time-resolved fluorescence spectroscopy, and cyclic voltametry. The collected data prove that our new materials could be regarded as potential TADF emitters as well OLEDs have been prepared with reasonable efficiencies.

CPP 50.20 Wed 18:30 P3

Tuning organic solar cells via doping with inorganic nanoparticles — ●SEBASTIAN GROTT, NURI HOHN, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Organic solar cells have attracted increased attention due to their advantages in tunable characteristics, low-cost manufacturing processes and flexibility, which opens up a promising alternative for conventional photovoltaics. Recently the most widely investigated bulk heterojunction donor-acceptor system of P3HT:PCBM was doped with iron oxide nanoparticles, resulting in an increase of efficiency.[1] Based on this approach, we investigate the effect of doping P3HT:PCBM active layers with alternative inorganic nanoparticles. We study the influence of different inorganic nanoparticle concentrations on current density-voltage characteristics and the absorbance. These optoelectronic properties

are compared with structure information determined with scattering methods. [1] D. M. González, V. Körstgens, Y. Yao, L. Song, G. Santoro, S. V. Roth, P. Müller-Buschbaum, *Adv. Energy Mater.* 2015, 5, 1401770.

CPP 50.21 Wed 18:30 P3

Investigation of Spin States Involved in Thermally Activated Delayed Fluorescence by Magnetic Resonance Methods — •BENJAMIN KRUGMANN¹, NIKOLAI BUNZMANN¹, SEBASTIAN WEISSENSEEL¹, JEANNINE GRÜNE¹, ANDREAS SPERLICH¹, and VLADIMIR DYAKONOV^{1,2} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) can exhibit a maximum internal quantum efficiency (IQE) of 100% instead of the 25% IQE that classical fluorescence emitters reach. The TADF mechanism is believed to include thermally induced reverse intersystem crossing (RISC) between slightly energetically split triplet and singlet states of exiplexes. Here, we present measurements based on bilayer 4,4',4''-Tris[phenyl(m-tolyl)amino]triphenylamine:Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (m-MTDATA:3TPYMB) OLEDs. We are using the spin sensitive method of electroluminescence detected magnetic resonance (ELDMR), in which spin states are energetically separated by an external magnetic field. Additionally, we apply microwaves to excite transitions between triplet states at resonance, where the emission of electroluminescence is elevated. By investigation of the resonant peak at different parameters we can draw conclusions about the spin dependent mechanisms involved in the TADF process.

CPP 50.22 Wed 18:30 P3

Charge carrier dynamics in bilayer coupled organic-inorganic nanostructures — •FLORIAN GRASSL¹, ALEXANDER HOFMANN¹, EDUARD MEISTER¹, ALEXANDER ANDRÉ², MICHELLE WEBER², 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]. Here we focus on out-of-plane charge carrier dynamics of COIN layers in diodes and solar-cells. Using three different techniques of fabricating COIN layers from PbS nanocrystals with Cu-phthalocyanine as organic linker molecules, we elucidate the influence of preparation conditions on carrier transport and device performance. Additionally we compare different organic and inorganic hole injection layers and the impact of the COIN production process on their electrical properties.

[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.chem.mater.5b03821

CPP 50.23 Wed 18:30 P3

Structuring of insoluble polythiophene for organic solar cells — •EVA MARIA KRATZER, JENNY LEBERT, and EVA MARIA HERZIG — TU München, Munich School of Engineering, Herzig Group, 85748 Garching

Polythiophene, an insoluble semiconducting material, can be used as donor material in organic polymer solar cells. However, to cheaply process this material from solution the insolubility needs to be taken into account. Therefore, it is synthesized *in situ* from the soluble monomer to make it processable in solution. Advantages of the polythiophene are the low costs and the high availability of the used material for the synthesis. An important property for organic solar cells fabrication is a high degree of interfacial control between the donor and acceptor material for efficient charge separation.

In this work, we exploit the insolubility of the polythiophene thin films for processing of structured multilayers. Different approaches are shown to achieve well-defined, structured donor-acceptor interfaces. The structured multilayers are investigated regarding their geomet-

ric from on various length scales and the resulting influence on the electronic properties is systematically analyzed with microscopy, spectroscopy and scattering.

CPP 50.24 Wed 18:30 P3

Hybrid quantum dots: poly(3-hexylthiophene) solar cells — •WEI CHEN^{1,2} and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching, Germany — ²Department of Electrical and Electronic Engineering, Southern University of Science and Technology, 518055 Shenzhen, China

Blends of semiconducting polymers and inorganic semiconductor nanocrystals, like quantum dots (QDs), have started to attract intensive interests because of their inexpensive costs and the ability of being solution processed. Both facts render them very promising candidates for next generation organic photovoltaics. Hybrid bulk heterojunction (BHJ) solar cells integrated with CuInSexS2-x (CISS) QDs and poly(3-hexylthiophene) (P3HT) are under investigation. CISS QDs are used as acceptor in our BHJ solar cell schematic, due to their strong optical absorption, tunable band-gap reaching to near infrared and long exciton lifetime, while P3HT is employed as donor material. The surface engineering of the QDs is investigated as a key factor to increase the exciton diffusion length and therefore improve the performance of solar cell devices. The QDs- P3HT active layers with 120 nm thickness are fabricated by blending using the spin-coating method. Different blend ratios are compared.

CPP 50.25 Wed 18:30 P3

Coupling of organic light emitting diode emission to planar waveguides — •TONI BÄRSCHNEIDER¹, SIMONAS KROTKUS², SIMONE LENK¹, SEBASTIAN REINECKE¹, and KARL LEO¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Germany — ²School of Physics and Astronomy, St Andrews, United Kingdom

Organic light-emitting diodes (OLEDs) are cheap, bright, and easy-to-fabricate light sources which can be deposited on arbitrary substrates. For these reasons, successful OLED integration on the planar waveguide structure is advantageous for a wide range of applications, including point-of-care sensing and optical circuits. However, due to the optical absorption of the electrodes, efficient coupling of OLED emission into the thin waveguide core lying beneath is one of the major challenges. One promising approach is to make use of evanescent coupling, which relies on the overlap between emission and waveguide mode. However, there are number of possible improvements in efficiency and composition of light. Here especially, one targets blue light emission for compatibility with common analytes as well as light that is TM polarized. In this work, we investigate the waveguide coupling of a blue OLED to a 70 nm TiO₂ layer. A p-i-n device design enables optical optimization guided by numerical calculations, while the use of the thin metal electrode is shown to be beneficial for an efficient light incoupling. A highly transparent, easy and effective ALD encapsulation is used to carry out measurements under ambient conditions.

CPP 50.26 Wed 18:30 P3

Investigations on Band Structure Engineering in Organic Semiconductors — •KATRIN ORTSTEIN¹, MARTIN SCHWARZE¹, and KARL LEO^{1,2} — ¹Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Germany — ²Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

In modern electronics, it is essential to create almost arbitrary band structures by adjusting the energy bands and the band gap. Until now, a possibility of band structure engineering in organic semiconductors has not been possible, since they usually exhibit localized electronic states instead of energy bands. In a recent publication [1], we showed that it is possible to continuously shift the ionization energy of organic semiconductors over a wide range by mixing them with halogenated derivatives. This tuning mechanism is based on long-range interactions of excess charges with the mean quadrupole field in the thin film.

In this work, we further investigate this phenomenon using ultraviolet photoelectron spectroscopy measurements and set the focus on the range of these charge-quadrupole interactions. For this purpose, we study blended layers composed of C₆₀, ZnPc and F₈ZnPc and additionally probe stepwise the electronic levels at their flat interfaces.

[1] Schwarze et al., *Science* 352, 1446 (2016)

CPP 50.27 Wed 18:30 P3

A Novel Approach to Align Small Molecules Thin Films by Light-Directed Molecular Self-Assembly — ●ANDIKA ASYUDA, LINUS PITHAN, ANTON ZYKOV, ANDREAS OPITZ, and STEFAN KOWARIK — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany

For the functionality of organic thin film devices, several film's structural properties, such as surface morphology, polymorphism, and molecular alignment, are known to be highly important. Recently light-directed molecular self-assembly (LDSA) was shown to promote a growth of aligned tetracene film(1). The versatility of this technique motivates us to closely investigate various related aspects, such as its implication on transport properties due to an optimization in molecular alignment. In this contribution we presented the state of art of LDSA toward a realisation of organic transistor with an increased mobility, due to an enhanced crystallinity and anisotropy in a molecular thin film.

1. L. Pithan, P. Beyer, L. Bogula, A. Zykov, P. Schäfer, J. Rawle, C. Nicklin, A. Opitz, and S. Kowarik, *Adv. Mater.* 2017, 1604382

CPP 50.28 Wed 18:30 P3

Fabrication of organic nanowires by melt infiltration of a discotic liquid crystal: A combined X-ray diffraction and optical birefringence study — ●KATHRIN SENTKER¹, ARDA YILDIRIM², ANDREAS SCHÖNHALS², and PATRICK HUBER¹ — ¹Institut für Werkstoffphysik und -technologie, Technische Universität Hamburg-Harburg — ²Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin

Discotic liquid crystals (DLC) can exhibit a liquid crystalline phase with their molecules oriented along one specific direction forming hexagonal arranged columns. Embedded in nanoporous membranes the columns orient perpendicular (radially) or parallel (axially) with respect to the pore axis. Due to their hydrophilic nature porous membranes enforce face-on anchoring leading to a radial orientation. Axially oriented columns ensure high conductivity in the stacking direction due to overlapping pi - electrons yielding interesting applications in e.g. organic semiconductor-based devices. Optical birefringence measurements show that we successfully realized an axial orientation by embedding the DLC HAT6 in an alumina membrane with a pore size of 25 nm. We suspect that anions introduced into the membrane lattice from the manufacturing process react with the DLCs changing the anchoring condition of the membrane. This enforces edge-on-orientation leading to an axial orientation of columns. XRD experiments giving detailed information about the translational order support the findings from optical measurements.

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Measuring C60 diffusion in the low bandgap copolymer PCDTBT — ●DENYS PRIADKO¹, THOMAS MÜLLER¹, CHRISTINA SALLER², TOBIAS HAHN¹, JULIAN KAHLE¹, STEFFEN TSCHUEUSCHNER¹, PETER STROHRIEGL^{2,3}, and ANNA KÖHLER^{1,3} — ¹Experimental Physics II, University of Bayreuth, 95440, Bayreuth, Germany — ²Macromolecular Chemistry I, University of Bayreuth, 95440, Germany — ³Bayreuth Institute of Macromolecular Science (BIMF), University of Bayreuth, 95440, Bayreuth, Germany

Although diffusion of fullerenes in blend or bilayer heterostructures has a strong impact on the efficiency and long-term stability of organic solar cells and other organic electronic devices, little is known about the diffusion coefficient of fullerenes in different materials. We have recently shown that the C60 diffusion in the high bandgap homopolymer polyfluorene can be reduced by a factor of 1000 by crosslinking the polymer. We have now extended our approach to the low bandgap copolymer PCDTBT. We study how crosslinking PCDTBT suppresses the diffusion of C60 into it compared to inserting a LiF layer between the PCDTBT and the C60.

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Charge stability on polypropylene electrets with surfaces treated in orthophosphoric acid — ●JINGWEN WANG and DMITRY RYCHKOV — University of Potsdam, Potsdam, Germany

It is known that both, physico-chemical surface modification and thermal treatment, can lead to enhanced electret properties of dielectric polymers. To further investigate the influence of surface modifications on charge storage in polypropylene (PP) electrets, a combined thermal and chemical treatment with orthophosphoric acid (H₃PO₄) is applied to PP films. Charged samples are then studied by means of thermally-stimulated discharge (TSD) experiments, contact-angle measurements

and Fourier-transform infrared (FTIR) spectroscopy. From the results, it can be concluded that additional deeper traps have been formed along with the treatment-induced conformation variations on the surface of the PP films. The new traps significantly improve the surface charge-stability of PP electrets.

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Fluorescence Lifetime Imaging Microscopy on Different Samples of the Conjugated Polymer P3HT — ●VIKTOR MESSERER¹, LOTHAR KADOR¹, RICHARD HILDNER², HANNES WELZ³, and HANS-WERNER SCHMIDT³ — ¹University of Bayreuth, Institute of Physics and BIMF, 95440 Bayreuth, Germany — ²University of Bayreuth, Experimental Physics IV, 95440 Bayreuth, Germany — ³University of Bayreuth, Macromolecular Chemistry I, 95440 Bayreuth, Germany

A custom-built fluorescence lifetime imaging microscope operating in the frequency domain (FD-FLIM) was used for mapping the fluorescence lifetimes of different samples of the conjugated polymer poly(3-hexylthiophene) (P3HT). Excitation was performed with a diode laser ($\lambda = 488$ nm) amplitude-modulated at frequencies between 104 and 160 MHz. Thin films of P3HT which contain a small amount of a tailored supramolecular nucleating agent to allow for the formation of highly ordered P3HT nanofibers were investigated. Neat P3HT was used as a reference. The fluorescence lifetime is obtained from the modulation amplitude of the fluorescence and its phase shift with respect to the excitation. The measured lifetimes are distinctly below 100 ps with the longest values found in the vicinity of the nucleating fibers. This result is ascribed to improved order of the H-aggregated P3HT nanofibers.

CPP 50.32 Wed 18:30 P3

In-situ polymerized PEDOT: Tos thin films for thermoelectric applications — ●MUBASHAR RAFIQ, NITIN SAXENA, and PETER MÜLLER-BUSCHBAUM — TU München, Physik-Department, LS Funktionelle Materialien, James-Frank-Str. 1, 85748 Garching

Thermoelectric materials are an efficient tool to convert waste heat into electrical energy in an environment-friendly manner. These materials make use of the Seebeck effect for the transformation of heat into electrical energy. PEDOT: TOS thin films show higher Seebeck coefficients and conductivities as compared to PEDOT: PSS, and these quantities play a key role for the figure of merit ZT. To improve these quantities an in-situ polymerized PEDOT: TOS is studied with respect to adding additives and performing pre- and post- treatments of thin films with different chemicals. Measurements of above mentioned quantities are carried out by four probe method and thermo voltage setup. Moreover, we are trying to deduce how these quantities could be affected by polymerization, polymer chain length, morphology, crystallinity and structural changes. For this purpose we use UV-Vis, AFM and x-ray scattering methods.

CPP 50.33 Wed 18:30 P3

Substrate Influence on the Formation of 2D-Polymeric Phthalocyanine Sheets — ●CLEMENS GEIS^{1,2}, THI HAI-QUYEN NGUYEN^{1,2}, PASCAL SCHWEITZER^{1,2}, and DERCK SCHLETTWEIN^{1,2} — ¹Justus-Liebig-University Giessen, Institute of Applied Physics — ²Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Phthalocyanines can be synthesized as two-dimensional polymeric sheets. Interest in their electrical properties and, e.g., in their use as electrode materials in catalysis is rising. Compared to monomeric phthalocyanines, the sheet polymers are characterized by an enhanced mechanical and chemical stability. The synthesis of those networks critically depends on the control of various reaction parameters. This work focuses on the influence of the substrate during a two-step reaction of 1,2,4,5-tetracyanobenzene with copper under vacuum conditions. Diffusion effects, side reactions and alloying within the substrate can hinder or even disrupt the formation of the phthalocyanine network and, hence, lead to undesired results. Spectroscopic methods were used to define and control the influence of the substrate on the growth of the 2D phthalocyanine network.

CPP 50.34 Wed 18:30 P3

Current-Voltage Characteristics of Polymeric Phthalocyanine Thin Films — ●THI HAI QUYEN NGUYEN^{1,2}, CLEMENS GEIS^{1,2}, and DERCK SCHLETTWEIN^{1,2} — ¹Justus-Liebig-University Giessen, Institute of Applied Physics — ²Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

Polymeric phthalocyanines as organic semiconductors have shown a wide range of electrical conductivity. In this work, polymeric copper phthalocyanine (CupPc) thin films were prepared by a reaction of tetracyanobenzene (TCB) with thin copper films on insulating substrates. In order to allow electrical measurements in a two-point-probe geometry electrodes of Au or Ni were vapor-deposited either directly on the substrate before film preparation or onto the prepared film subsequent to its growth. Conductivities of the organic films were determined from the current-voltage curves. The film thickness was measured with the help of a confocal laser scanning microscope and a scanning electron microscope. A more detailed examination of the cross-section of the samples revealed that either sponge-like or compact films could be formed dependent on the reaction temperature. Excess metallic copper remaining in the films after the reaction showed a strong influence on the electrical measurements as seen by thorough variation of the copper film thickness. Using X-ray diffraction the existence of metallic copper in the sample was analyzed and the presence of polymeric phthalocyanines was clearly validated.

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Development of a Procedure for the Synthesis of Two-Dimensional Polymeric Phthalocyanines Under High Vacuum Conditions — ●PASCAL SCHWEITZER^{1,2}, CLEMENS GEIS^{1,2}, and DERCK SCHLETTWEIN^{1,2} — ¹Justus-Liebig-University Giessen, Institute of Applied Physics — ²Justus-Liebig-University Giessen, Laboratory for Materials Science (LaMa)

As two-dimensional polymeric structures are of special interest in current research and phthalocyanine-based molecules can be used in various application fields the setup of a well-controlled synthesis route is needed. High vacuum conditions provide a well-defined reaction environment. A possible synthesis route to polymeric phthalocyanine sheets consists in the reaction of 1,2,4,5 tetracyanobenzene with a metal or metal salt. To achieve control over the reaction and, hence obtain optimized products, the understanding of the reactant behavior under high vacuum conditions is essential. Critical points that have to be considered are the sticking of the molecules on the substrate and the quartz microbalance during the PVD process, compound vapor pressure as well as side-reactions even during heating of the source.

CPP 50.36 Wed 18:30 P3

Absorption Tails of Donor:C₆₀ Blends Provide Insight into Thermally Activated Charge-Transfer Processes and Polaron Relaxation — ●JOHANNES BENDUHN¹, SEBASTIAN SCHELLHAMMER², FORTUNATO PIERSIMONI³, DIETER NEHER³, DONATO SPOLTRE¹, FRANK ORTMANN², and KOEN VANDEWAL¹ — ¹IAP, TU Dresden — ²Institute for Materials Science and cfaed, TU Dresden — ³University of Potsdam

In organic semiconductors, the transfer of a localized charge carrier causes a deformation of the molecular structure, quantified by the intra-molecular relaxation energy. Such structural relaxation occurs upon forming intermolecular charge-transfer (CT) states at organic

electron donor (D)-acceptor (A) interfaces. D-A complexes show weak absorption at photon-energies below the optical gap of both the donor and the C₆₀ acceptor, which is the result of an optical transition from the neutral ground state to the ionic CT state. We show that temperature-activated intra-molecular vibrations of the ground state play a major role in determining the line-shape of such CT absorption bands, allowing to extract values for the relaxation energy. Those experimental values for 20 donor:C₆₀ CT complexes correlate with values calculated within density functional theory. These results provide an experimental method for determining the polaron relaxation energy in solid-state organic D-A blends and show the importance of a reduced relaxation energy for thermally activated CT processes.

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Direct Observation of Intraband Relaxation and Exciton Dispersion Relation in Perylene-diimide H-aggregates — ●WOUTER KOOPMAN¹, STEFANO TOFFANIN², and MICHELE MUCCINI² — ¹Universität Potsdam, Potsdam, Deutschland — ²CNR-ISMN, Bologna, Italien

The excited state properties of organic molecular solids are determined by the aggregation behavior of the constituent molecules. In extreme cases of J- and H-aggregates super-radiance or a complete suppression of photoluminescence can be observed. Here we report the direct observation of the intraband relaxation of H-aggregate excitons in a PTCDI-C13 thin film, by time resolved photoluminescence spectroscopy.

CPP 50.38 Wed 18:30 P3

Analysis of charge transfer states at organic single crystal interfaces — ●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

The formation, dissociation and recombination of charge transfer (CT) states at organic-organic interfaces are vital for the performance of organic opto-electronical devices. However, the energy and dynamics of CT-states strongly depend on the position of the participating molecular frontier orbitals as well as on their respective spatial arrangement.

Therefore, we have chosen chemically and structurally well-defined hetero-interfaces, comprised of organic single crystal surfaces and vacuum deposited molecular adsorbant layers, to analyze the efficiency of CT-state generation and the effective amount of transferred charge. For this purpose, various optical techniques such as locally resolved Raman spectroscopy are applied. In case of the latter, the amount of transferred charge is estimated by the linear frequency shift of selected molecular vibrational modes [1].

The methodical and analytical procedure is demonstrated for the model system Rubrene/C₆₀ at different temperatures and crystallographic orientations.

[1] Matsuzaki, S. et al., *Solid State Commun.* **33**, 403 (1980)