

HL 65: Poster: Organic electronics and photovoltaics (CPP; jointly with HL, O)

Time: Wednesday 16:30–18:30

Location: Poster C

HL 65.1 Wed 16:30 Poster C

Templating effects of 6T layers for organic DIP layers — •CHRISTOPHER LORCH, ALEXANDER HINDERHOFER, RUPAK BANERJEE, CHRISTIAN FRANK, JOHANNES DIETERLE, ALEXANDER GERLACH, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany

Recently, the donor-acceptor combination of the two compounds, α -sexithiophene (6T) [1] and diindenoperylene (DIP) [2], respectively, has shown an extraordinarily high open circuit voltage in organic solar cells with a planar heterojunction (PHJ) architecture [3].

Synchrotron based real-time *in situ* X-ray diffraction experiments were performed to study the temperature-dependent growth characteristics of 6T. Furthermore, the influence of the structural properties of the 6T layer on the top DIP layer were investigated. In this contribution, the following points are discussed: i) Dependence of the ratio of lying and standing domains in the top DIP layer on the corresponding ratio in the bottom 6T layer. ii) The thickness dependence of the DIP layer structure. iii) Possible reorganization effects in the bottom layer during the growth of the top layer. iv) The dependence of top layer structure on the temperature.

[1] W. Steinkopf *et al.*, Justus Liebig's Ann. Chem. 546, 180-199 (1941)

[2] A. C. Dürr *et al.*, Phys. Rev. Lett. 90, 016104 (2003)

[3] U. Hörmann *et al.*, Phys. Status Solidi RRL 5, 241-243 (2011)

HL 65.2 Wed 16:30 Poster C

Solution processing of self-assembled monolayers as charge injection layers in organic FETs. — •MILAN ALT^{1,4}, JANUSZ SCHINKE^{2,4}, KAJA DEING^{3,4}, ULI LEMMER¹, and NORMAN MECHAU^{1,4} — ¹Karlsruher Institute of Technology — ²TU Braunschweig — ³Merck KGaA, Darmstadt — ⁴InnovationLab, Heidelberg

All-solution processed organic field effect transistors (OFETs) are expected to play a key role in the mass production of organic electronic devices via high throughput printing techniques. In this study we focus on solution processing of self-assembled monolayers (SAMs) for enhancement of charge carrier injection at the metal-semiconductor interface. One necessity in order to make SAMs printable is an understanding of molecular assembly in dependency to process parameters like accumulation time and molecular concentration in the solution. We used well established benchmark materials to investigate the functionality of different benzyl-mercaptop and alkanethiol SAMs in OFETs. The methodic evaluation of OFET devices, in which the transistor effectively serves as a characterization tool, revealed an expected correlation between metal work function shift and device threshold voltage. More interestingly, an optimum ratio of accumulation time/SAM concentration has been identified. In contrast, investigations of SAM accumulation on crystalline Au 111 surfaces in literature reveal a saturation of work function shift when approaching a closed monolayer. This demonstrates that understanding of SAM growth mechanisms gained on single crystalline surfaces cannot naturally be transferred to assembly on printed or evaporated metal contacts.

HL 65.3 Wed 16:30 Poster C

Photophysical Processes in Polymer:PDI Solar Cells — •DOMINIK GEHRIG, VALENTIN KAMM, HANNAH MANGOLD, IAN HOWARD, GLAUCO BATTAGLIARIN, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max-Planck-Institute for Polymer Research, Mainz, Germany

We present the implementation of different polymers as donors in combination with new PDI-based acceptors in organic solar cells. Increasing the absorption of the photoactive layer is a rational strategy that could give rise to an enhanced photon harvesting and hence an improvement of the photocurrent. The contribution of PDI to the photocurrent generation can be proved by EQE measurements. Additionally exciton and charge carrier dynamics as well as loss mechanisms are investigated by sub-picosecond to millisecond pump-probe transient absorption spectroscopy (TA) and time-resolved photoluminescence (TRPL) spectroscopy. The former tracks the dynamics of non-radiative species whereas the latter enables the observation of emissive decay channels. Supplementary experiments like the evaluation of the morphology by AFM and charge transport experiments by the time-of-flight (TOF) technique and space-charge-limited-current (SCLC) measurements deliver additional information which allow to derive mean-

ingful structure-property-relations.

HL 65.4 Wed 16:30 Poster C

Increased conductivity of PEDOT:PSS for application in organic solar cells: electrical and morphological investigations — •CHRISTOPH HELLER¹, CLAUDIA M. PALUMBINY¹, VOLKER KÖRSTGENS¹, YUAN YAO¹, WEIJIA WANG¹, STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹Lehrstuhl für Funktionelle Materialien, Physik-Department, Technische Universität München, James-Frank-Str. 1, 85748 Garching, Germany — ²HASYLAB at DESY, Notkestrasse 85, 22603 Hamburg, Germany

Poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) is commonly used as a transparent electrode for flexible electronic devices. Its conductivity plays a crucial role for the device performance.

In our study, the conductivity of PEDOT:PSS films has been increased via a post treatment method reaching the conductivity order of indium tin oxide (ITO) which is commonly used as an electrode in organic solar cells. Among other techniques the effect of the post treatment has been investigated using advanced scattering methods such as grazing incident small angle x-ray scattering (GISAXS). Furthermore, the influence of doping PEDOT:PSS, different post treatments, the treatment time and the effect of the number of post treatments have been investigated focusing on conductivity and morphological changes. The results are very promising for using post treated PEDOT:PSS as an electrode in ITO-free organic solar cells.

HL 65.5 Wed 16:30 Poster C

Low-bandgap DPP-type Polymers for OPVs: Relation between Device Performance and Photophysical Properties — •JULIAN OCHSMANN¹, MATHIEU TURBIEZ², DEEPAK CHANDRAN³, IAN HOWARD¹, KWANG-SUP LEE³, and FRÉDÉRIC LAQUAI¹ — ¹Max Planck Institute for Polymer Research, Mainz, Germany — ²BASF, Basel, Switzerland — ³Hannam University, Seoul, Korea

Low-bandgap polymers are promising materials to serve as electron donors in the photoactive layer of bulk heterojunction solar cells. In combination with a suitable electron acceptor such as PC70BM the photoactive layer covers a broad absorption range spanning from the visible to the near-infrared spectral region leading to increased photon harvesting and thus a higher photocurrent compared to mid-bandgap polymers such as P3HT.

In this study the photovoltaic performance of several low-bandgap polymers based on the diketopyrrolopyrrole (DPP) unit was evaluated in Organic Photovoltaic Cells (OPVs) prepared with different solvent mixtures. Depending on the polymer structure and preparation conditions maximum power conversion efficiencies between 1.6 and 5 % could be reached. The photophysical properties of the photoactive layers of the OPVs were investigated by steady-state photoinduced absorption and broadband transient absorption pump-probe spectroscopy (TA) to get further insight into the exciton and polaron dynamics as well as into the efficiency-limiting mechanisms of the devices.

HL 65.6 Wed 16:30 Poster C

Investigation of Polyethylenimine and Polyethylenimine-ethoxylated as electron injection layers in solution processed organic light-emitting diodes. — •SEBASTIAN STOLZ^{1,4}, INGO RINGLE², ERIC MANKEL^{3,4}, JANUSZ SCHINKE⁴, MICHAELA AGARI², GERARDO HERNANDEZ-SOSA^{1,4}, WOLFRAM JAEGERMANN^{3,4}, ULI LEMMER¹, and NORMAN MECHAU^{1,4} — ¹Light Technology Institute, Karlsruhe Institute of Technology — ²Pre-development, Heidelberger Druckmaschinen AG — ³Materials Science Institute, Technische Universität Darmstadt — ⁴InnovationLab GmbH, Heidelberg

One obstacle for inexpensive solution processed organic light-emitting diodes (OLEDs) is the current use of low work-function metals like calcium or barium as cathode materials. These metals are highly reactive, which is why they cannot be easily solution processed but have to be prepared in UHV. In this work, we investigate two organic polymers, Polyethylenimine (PEI) and Polyethylenimine-ethoxylated (PEIE), which are known to reduce the work-function of various metals, for their applicability as electron injection layers. Therefore, both polymers are dissolved in 2-Methoxyethanol with varying concentrations and are then spin coated on top of Aluminum substrates. The concentration dependent change in work-function is determined

by kelvin probe measurements and ultraviolet photoemission spectroscopy. Furthermore, OLEDs using PEI, or PEIE respectively, as electron injection layer are prepared by spin coating. Compared to reference devices with calcium as electron injection material, these OLEDs show comparable turn on voltages and luminance values of more than 50%.

HL 65.7 Wed 16:30 Poster C

Surface morphology of P3HT, PCBM and blends of both — •MARTIN DEHNERT¹, MARIO ZERSON¹, SVEN HÜTTNER², ZHUXIA RONG², ULLRICH STEINER², and ROBERT MAGERLE¹ — ¹Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Chemnitz, Germany — ²Cavendish Laboratory, JJ Thomson Avenue, Cambridge, U.K.

We investigate the surface morphology of thin films of pure poly(3-hexylthiophene) (P3HT), [6,6]-phenyl C61-butyric acid methyl ester (PCBM) and blends of P3HT and PCBM using atomic force microscopy (AFM) operated in multi-set point intermittent contact (MUSIC) mode. This allows for depth-resolved mapping of the mechanical properties of the top surface layer of the specimen. AFM images of pure P3HT and PCBM before and after annealing show the crystallisation behaviour of the pure materials at the film surface. Blends of P3HT and PCBM with different composition were used for investigating the morphology, the nanomechanical properties, and the composition of the top surface layer. Our results indicate that for large range of blend compositions the volume ratio of P3HT and PCBM is constant within the top surface layer. Furthermore, we observe crystallisation of PCBM in films annealed at 175°C. We discuss the impact of the surface morphology of P3HT:PCBM blends and the crystallisation of PCBM on the efficiency and lifetime of organic solar cells.

HL 65.8 Wed 16:30 Poster C

Probing charge carrier dynamics in organic solar cells based on merocyanines — •STEVEN GRAF¹, MARTIN LENZE¹, JULIAN KRUMRAIN¹, DIRK HERTEL¹, KLAUS MEERHOLZ¹, and FRANK WÜRTNER² — ¹Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic photovoltaics offer a very promising green energy alternative. Highly efficient organic solar cells can be produced by cost-effective methods such as coating from solution (SOL) or depositing under high vacuum conditions (VAC). In our approach we investigate merocyanines (MC), a class of low-molecular-weight colorants, as donor material in organic BHJ solar cells. These molecules are processable via both deposition techniques showing remarkable power conversion efficiencies (PCE) beyond 4% for SOL- and 6% for VAC-processed devices. Towards even higher PCEs it is mandatory to obtain a better insight into fundamental charge carrier processes such as generation, transport and recombination. We use steady state and time resolved photoluminescence spectroscopy to examine charge-transfer (CT) states in pure and blended merocyanine thin films. The role of these CT states in solar cells is further studied by field and temperature dependent measurements of the external quantum efficiency (EQE). By varying processing conditions as well as blend compositions the influence of morphology on the solar cells is illustrated. The investigations are supported by temperature and electric field dependent studies of charge recombination and transport via photo-CELIV technique.

HL 65.9 Wed 16:30 Poster C

Influence of different alkyl side chains on merocyanine dye performance in organic solar cells — •JULIAN KRUMRAIN¹, ALHAMA ARJONA ESTEBAN², STEVEN GRAF¹, MARTIN LENZE¹, DIRK HERTEL¹, FRANK WÜRTNER², and KLAUS MEERHOLZ¹ — ¹Department für Chemie, Universität zu Köln, Luxemburger Straße 116, 50939 Köln (Germany) — ²Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg (Germany)

In recent years, organic photovoltaics have attracted great attention as an alternative energy source due to their reduced cost and easier processability, compared to inorganic materials. Specifically, small-molecule dyes have achieved great strides in recent years reaching power conversion efficiencies up to 7%. These dyes have advantages over polymers, most notably their simplified, large-scale syntheses and purification. Furthermore small molecules can be processed either by solution or vapor-deposition processes. We have investigated organic solar cells based on merocyanine (MC) dyes as an electron donor material in vacuum-deposition processed bulk-heterojunctions (BHJ). In order to get a better understanding of the influence of side chains on

the MC dyes in BHJ, we have synthesized MC dyes with different alkyl side chain lengths. We have carried out temperature and light intensity dependent current-voltage measurements as well as atomic force microscopy studies. It becomes apparent that the BHJ morphology is strongly influenced by the side chain length. The short-circuit current density decreases enormously for increasing side chain length in complete contrast to the solubility of the MC dyes.

HL 65.10 Wed 16:30 Poster C

Absorption and exciton management in DIP/C₆₀ bilayer photovoltaic cells — •A. STEINDAMM^{1,2}, M. BRENDL^{1,2}, K. TOPCZAK¹, and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The combination of the promising material Diindenoperylene (DIP) with the acceptor C₆₀ has led to overall efficiencies up to 4 % in organic photovoltaic cells (OPVCs) [1]. A drawback in performance is found in the rather poor light absorption of the crystalline DIP layer due to its unfavorable orientation of transition dipoles perpendicular to the electric field vector of incident light. Therefore we pursued different approaches for increasing the current density. First, the orientation of the individual DIP molecules was altered by varying the growth conditions in order to increase light absorption. Second, the interface effects of an Bathophenanthroline (BPhen) exciton blocking layer (EBL) on the exciton management in DIP/C₆₀ were investigated by a complementary study of current density, external quantum efficiency, and photoluminescence quenching for various EBL thicknesses. These investigations reveal exciton losses by contact metal quenching in both active layers if no EBL is applied. In contrast, an optimal trade-off between exciton blocking, suppression of metal penetration, and electron transport is achieved for a 5 nm thick BPhen layer yielding an improvement of power conversion efficiency by more than a factor of 2 [2]. Financial support by BMBF (GREKOS) and DFG (SPP1355) is acknowledged.

[1] A. Opitz, et al., IEEE J. Sel. Top. Quant. El. 16, 1707 (2010)

[2] A. Steindamm, et al., Appl. Phys. Lett. 101, 143302 (2012)

HL 65.11 Wed 16:30 Poster C

The effect of fluorination on the performance of F_nZnPc/C₆₀ organic photovoltaic cells — •M. BRENDL^{1,2}, A. STEINDAMM^{1,2}, F. STAUB¹, and J. PFLAUM^{1,2} — ¹Exp. Phys. VI, University of Würzburg, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

The material class of phthalocyanines has proven to be a suited donor material in small molecule organic photovoltaic cells (OPVCs). Planar heterojunctions based on zinc phthalocyanine (ZnPc) in combination with the acceptor C₆₀ show high short circuit currents (*j*_{sc}) of 6.3 mA/cm² and fill factors (FF) of 51 % [1]. However, due to the small effective band gap *E*_{g,eff} of only 1 eV between ionisation potential of the donor and electron affinity of the acceptor, the correlated open circuit voltage (*V*_{oc}) is limited to 0.5 V. As a possible approach energy levels of Pcs can be modified by substituting hydrogen atoms. With increasing degree of fluorination the position of the HOMO and LUMO levels are shifted to lower energies. In this contribution we investigated the impact of *E*_{g,eff} on *V*_{oc} for a varying degree of fluorination (*n* = 0, 4, 8, 16) in F_nZnPc/C₆₀ OPVCs. First results revealed a significant *V*_{oc} improvement of 20 % to 0.6 V for F₄ZnPc based cells compared to ZnPc, while *j*_{sc} and FF ideally remained unaffected. However, the gain in *V*_{oc} is smaller than expected by the difference in ionisation potential which accounts for 0.2 - 0.4 eV. This discrepancy will be analyzed in our studies and will lead to a deeper insight into the origins of *V*_{oc} and its correlation to the energetics on the molecular entities. Financial support by the BMBF (project GREKOS) and by the DFG (program SPP1355). [1] Z. R. Hong, et al., Appl. Phys. Lett. 2007, 90, 203505

HL 65.12 Wed 16:30 Poster C

Surface Structure of organic solar cells based on PBDTTT-C and PC70BM — •MARIO ZERSON¹, ANDREAS ZUSAN², CARSTEN DEIBEL², and ROBERT MAGERLE¹ — ¹Chemische Physik, Technische Universität Chemnitz, Chemnitz, Germany — ²Experimental Physics VI, Julius-Maximilians-University of Würzburg, Würzburg, Germany

We study the surface structure of organic heterojunction solar cells based on blends of poly[4,8-bis-(2-ethylhexyloxy)-benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-(4-(2-ethylhexanoyl)-thieno[3,4-b]thiophene)]-2,6-diyl (PBDTTT-C) and Phenyl-C70-butyric acid methyl ester (PC70BM) with a weight ratio of 1:1.5. The additive diiodooctane (DIO) is used with ratios between 0% and 10% to increase the compatibility of the two components. We investigate the

surface structure of the devices with amplitude modulation atomic force microscopy (AFM). Conventional AFM height and phase images are complemented with data obtained from maps of amplitude-phase-distance (APD) curves. This allows us to determine the unperturbed (true) surface and the mechanical properties of the soft surface layer of the specimen. The AFM height and phase images of PBDTTT-C:PC70BM blends produced with different ratio of DIO indicate, that the additive plays a fundamental role in the structure formation process. Blends with DIO ratios between 1,8% and 5% show the best power conversion efficiency (PCE) up to 6,9%. We discuss the structure and the structure of the interface between donor and acceptor components in view of their impact on charge carrier dynamics and solar cell performance.

HL 65.13 Wed 16:30 Poster C

Triplet Excitons and Cations in DCV4T-Me:C₆₀ blends with different mixing ratio — •DANIEL SCHÜTZE¹, CHRISTIAN KOERNER¹, ROLAND FITZNER², EGON REINOLD², PETER BÄUERLE², KARL LEO¹, and MORITZ RIEDE¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — ²Institut für Organische Chemie II und Neue Materialien, Universität Ulm, Germany

Dicyanovinyl end-capped oligothiophenes (DCVnT) have demonstrated their ability of achieving high power conversion efficiencies of up to 6.9% in a bulk heterojunction solar cell¹. Besides that, they act as a model system because of the possibility of changing properties by varying the length of backbone or side chains.

In this work, we use DCV4T with two methyl side chains at the first and the last thiophene ring. By photoinduced absorption spectroscopy (PIA) measurements we probe the long-living (μ s-ms) excited states (triplet excitons, cations) after photoexcitation of our samples. With PIA, their generation and recombination behavior can be investigated. Here, we report our results obtained on a series of DCV4T-Me:C₆₀ blends with varying mixing ratio from 3:1 to 1:2. We found strong influence of the mixing ratio on the generation rate of triplet excitons and also an influence in the generation rate and the activation energy of free charge carriers with increasing temperature. The results are compared to solar cells containing identical blend layers as active layer to investigate the dependence of the photo current on the mixing ratio.

¹ Fitzner et al., J. Am. Chem. Soc. 2012, 134, 11064 (2012)

HL 65.14 Wed 16:30 Poster C

Nucleation and Growth of Copper Phthalocyanine from Solution — •FATEMEH GHANI and HANS RIEGLER — Max Planck Institute f. Colloid & Interfaces, Potsdam-Golm, Germany

Silver nanoparticles are usually synthesized by physical vapor deposition or through complicated methods like ion implantation or wet chemistry. A self-assembly method is of interest due to its simplicity and cost-efficiency [202]. By combining physical vapor deposition and solvent treatment (spin casting), we applied a simple hybrid method to produce appropriate silver nanoclusters for organic solar cells. Through evaporation of the silver film (~ 5 nm), nanoclusters (of ~ 4 nm height and ~ 25 nm widths) cover the surface. By spin casting the solvent, a thin liquid film covers the evaporated film. The silver clusters redistribute in the solution film and by evaporation of the solvent, they aggregate in larger clusters (~ 20 nm height and ~ 45 nm width). The process is influenced via physical parameters of growth from solution like evaporation rate and liquid film concentration. We show that the size of the clusters can be controlled by the thickness of the deposited film, type of solvent, and spin casting speed. We applied this method to increase the efficiency of a hybrid solution processed and vacuum deposited unsubstituted copper phthalocyanine/fullerene organic solar cells.

HL 65.15 Wed 16:30 Poster C

Charge generation in solid-state dye-sensitized solar cells using peryleneimide sensitizers — •YOOJIN KIM, MICHAEL MEISTER, IAN HOWARD, FELIX HINKEL, GLAUCO BATTAGLIARIN, CHEN LI, KLAUS MÜLLEN, and FRÉDÉRIC LAQUAI — Max Planck Institute for Polymer, Mainz, Germany

Solid-state dye-sensitized solar cells (DSCs) have attracted a lot of attention owing to their advantages compared to liquid-electrolyte DSCs such as ease of fabrication and the absence of corrosive electrolytes that are typically used in liquid-electrolyte cells. However, fast charge recombination between electrons in the titania nanoparticle films and dye/hole conductor cations, incomplete pore-filling, and the decreased thickness of titania films necessary for efficient charge extraction cur-

rently limit the power conversion efficiency. In this contribution we compare the charge generation and recombination processes in a series of peryleneimide-sensitized DSCs studied by steady-state photoinduced absorption (PIA) and ultrafast broadband transient absorption spectroscopy (TAS) covering the sub-picosecond to millisecond timerange. By fitting the dynamics to a photophysical model we extract the parameters relevant for the photovoltaic efficiency such as the yield of electron injection and the recombination rate constants which allows us to derive meaningful structure-property relations.

HL 65.16 Wed 16:30 Poster C

Sequentially solution-processed bulk-heterojunction CuPc/PCBM - bilayer for organic solar cells — •MARKUS REGNAT, FATEMEH GHANI, and HANS RIEGLER — Max Planck Institut of Colloids and Interfaces, Potsdam-Golm, Germany

Copper Phthalocyanine (CuPc) is a commonly used electron donor material in vacuum-processed organic solar cells (OSC) due to its suitable electronic properties, chemical stability and low material cost. Recent studies have revealed appropriate solvents for CuPc [1] and thus also opened a way for cost-efficient wet-deposition techniques, like spin casting or dip coating. Based on this, a working hybrid solution/vacuum processed OSC with a CuPc film prepared by wet-processing (spin cast) could be obtained [2]. The nanostructures of the CuPc film have an important influence on the efficiency of the OSC. A systematic study reveals the impact of various process parameters on nucleation and growth of wet-processed CuPc films and allows the optimization of the nanostructures. By using appropriate orthogonal solvents, even both essential optoelectronic layers (CuPc, PCBM) can now be sequentially wet-deposited for a bulk-heterojunction CuPc/PCBM - bilayer OSC.

[1] Ghani, F.; Kristen, J.; Riegler, H., Solubility properties of unsubstituted metal phthalocyanines in different types of solvents, J. Chem. (2012)

[2] Fatemeh Ghani; Ivelin Bochukov; Konstantinos Fostiropoulos; Hans Riegler, Hybrid solution/vacuum-processed bilayer heterojunction organic solar cells: Structural characterization and performance, Thin Solid Films (2012)

HL 65.17 Wed 16:30 Poster C

Preferential orientation of molecular dipoles in amorphous vacuum deposited films studied by surface potential measurements — •CHRISTIAN WEIGEL, SAMI HAMWI, and WOLFGANG KOWALSKY — Institut fuer Hochfrequenztechnik, TU Braunschweig

Amorphous thin films of semiconducting small molecules are commonly used in organic optoelectronic devices to avoid detrimental effects of grain boundaries in polycrystalline thin films. Studies of surface potential development with film thickness have shown that sublimation of common OLED molecules such as Tris(8-hydroxyquinolino) aluminum (Alq3) or 1,3,5-tris(2-N-phenylbenzimidazolyl)benzene (TPBi) results in amorphous films with a preferential orientation of the molecular dipoles. Kelvin probe measurements provide a sensitive tool to detect a shift in the average molecular dipole orientation by as little as 5 degrees from the isotropic case. The detected shift in surface potential is characteristic for each molecules and is found in the order of several volts per 100 nm, comparable to operating voltages of organic electronic devices. The recorded increase in surface potential is largely independent of material or preparation of the substrate upon which the amorphous film is grown (barring the different interface dipoles between substrate and film), so that anisotropy at the organic film to vacuum interface drives the preferential orientation. Upon optical excitation, the measured potential vanishes, presumably due to mobile charges screening the dipole field.

HL 65.18 Wed 16:30 Poster C

Encapsulation of small molecule organic devices by a functional thin top layer of tetratetracontane — •FLORIAN STAUB¹, ANDREAS STEINDAMM^{1,2}, MICHAEL BRENDL^{1,2}, and JENS PFLAUM^{1,2} — ¹Experimental Physics VI, Julius-Maximilians-University, 97074 Würzburg — ²ZAE Bayern, 97074 Würzburg

Providing long-term stability for organic devices is still a challenging task due to the sensitivity of molecular materials as well as organic/metal interfaces on water incorporation and oxidation processes. The straight-chain alkane tetratetracontane (TTC) is capable to protect organic devices from those degradation mechanisms by forming closely packed and highly crystalline films [1]. TTC is transparent in the visible range, highly hydrophobic and chemically inert and therefore suited to conserve the opto-electronic properties of the underlying films. In this contribution we apply nanometer thick top layers

of TTC by thermal vacuum deposition onto planar heterojunction organic photovoltaic cells (OPVCs) based on zinc phthalocyanine (ZnPc) and diindenoperylene (DIP) in combination with the acceptor C₆₀, respectively. For ensuring best comparability, encapsulated and bare cells are prepared under identical conditions on the same substrate. We investigate the degradation mechanisms by measuring the external quantum efficiency and the IV-characteristics over time under exposure to various environmental conditions (vacuum, nitrogen, air). The occurring changes in the opto-electronic device performance will be discussed in relation with structural data obtained by AFM and X-ray diffraction. [1] M. Göllner et al., Adv. Mater. 2010, 22, 4350-4354

HL 65.19 Wed 16:30 Poster C

Brightly Blue and Green Emitting Copper Compounds for Singlet Harvesting in OLEDs — ●MARKUS LEITL¹, FRITZ-ROBERT KÜCHLE², LARS WESEMAN², and HARTMUT YERSIN¹ — ¹Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany — ²Institut für Anorganische Chemie, Universität Tübingen, D-72076, Germany

In this contribution, a series of four Cu(I) complexes is presented. All substances exhibit high emission quantum yields of up to 65 % at relatively short emission decay times of several μ s. The emission wavelength varies from the blue (460 nm) to the green (505 nm). This is induced by defined modifications of the chemical structure. Detailed photophysical investigations reveal that the energy separation $\Delta E(S_1 - T_1)$ between the triplet state T_1 and the singlet state S_1 is small and lies in the range of 500 cm^{-1} . As a consequence, emission at ambient temperature originates dominantly (> 99 %) from the S_1 state which is thermally populated from the energetically lower lying T_1 state. For this reason, the emission at ambient temperature represents a thermally activated delayed fluorescence (TADF). It is proposed to utilize this property for collecting both singlet and triplet excitons in the lowest excited singlet state for light generation in OLEDs. This effect represents the singlet harvesting mechanism.

HL 65.20 Wed 16:30 Poster C

Interface trap density investigation by impedance spectroscopy of MIS structures for different surface treatments — ●HIPPOLYTE HIRWA, STEVE PITTNER, and VEIT WAGNER — Jacobs University Bremen, Campusring 1, D-28759 Bremen, Germany

For high performance electronic devices, reliability and stability are crucial parameters. Since reliabilities and stabilities issues in field effect transistors are mainly related to the semiconductor-gate insulator interface properties, a MIS (Metal-insulator-semiconductor) capacitor structure can be equally used for investigation of interface traps. We report on impedance measurements carried out on MIS capacitors fabricated using silicon oxide as insulator prepared under 3 different surface treatments and poly(3-hexylthiophene) as semiconductor. The conductance technique was used to extract the interface trap density. For this a proper equivalent circuit for our MIS structures had to be chosen. The results reveal first the formation of a double layer with 2 different conductivities in the semiconductor layer, secondly the presence of interface trap states and finally they show that the interface states density and energy distribution is related to the sample surface treatment.

HL 65.21 Wed 16:30 Poster C

Combined photoemission and X-ray absorption study of the 'rods-in-belt' supramolecular complexes containing gold-copper and gold-silver clusters — ●ANNA MAKAROVA^{1,2}, ELENA GRACHOVA², DMITRY KRUPENYA², JULIA SHAKIROVA², IGOR KOSHEVOY³, ECKART RÜHL⁴, CLEMENS LAUBSCHAT¹, SERGEY TUNIK², and DENIS VYALIKH¹ — ¹Technische Universität Dresden, Dresden, Germany — ²St.-Petersburg State University, St.-Petersburg, Russia — ³University of Joensuu, Joensuu, Finland — ⁴Freie Universität Berlin, Berlin, Germany

Recently created self-assembled Au(I)-Cu(I) and Au(I)-Ag(I) 'rods-in-belt' supramolecular complexes display intriguing phosphorescence properties. Another important issue is the tunability of their electronic structure, and consequently their photophysical properties through modification of the ligand environment that opens great perspectives for their implementation in light-emitting devices and in bio-imaging. It is believed that high structural ordering and self-assembling properties of such objects can open a new avenue for the design of artificial nanostructures that may potentially be ideal building blocks for next generation electronics. Nonetheless, the electronic structure of these materials has not been investigated experimentally by now. We have demonstrated that photoemission and X-ray absorption techniques can be successfully applied for systematic investigation of the series of these unique complexes. It has been shown that the all complexes inside the series exhibit similar electronic structures, however, the electronic states near the HOMO reveal notable differences.

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A multiscale modeling study of loss processes in block-copolymer-based solar cell nanodevices — ●SERGII DONETS, ANTON PERSHIN, and STEPHAN BAEURLE — University of Regensburg, Institut of Physical and Theoretical Chemistry, D-93053

Flexible photovoltaic devices possess promising perspectives in optoelectronic technologies, where high mobility and/or large-scale applicability are important. However, their usefulness in such applications is currently still limited due to the low level of optimization of their performance and durability. For the improvement of these properties a better understanding and control of small-scale annihilation phenomena of the elementary particles involved in the photovoltaic process, such as exciton loss and charge carrier loss, are necessary. Here, we explore the causes for their occurrence with a novel field-based solar-cell algorithm on the example of self-organizing nanostructured block-copolymer systems, which possess a broad variability in their chemical and physical characteristics, and explore new routes to optimize their performance. From our calculations, we deduce that in the regime from low up to intermediate chi-parameters the charge transport efficiency (CTE) and internal quantum efficiency (IQE) of both block-copolymer systems increase up to a maximum, characterized by a minimum in the number of charge losses due to charge recombinations. In the regime of high chi-parameters they form nanostructures with a large number of bottlenecks and dead ends, leading to a large number of charge losses due to charge recombination, charge trapping and an impaired exciton dissociation.