

## DS 9: Organic Thin Films II

Time: Monday 15:00–16:45

Location: H11

DS 9.1 Mon 15:00 H11

**Investigation of phase separation in bulk heterojunction organic solar cells** — ●VLADISLAV JOVANOVIĆ, ARNE HENDEL, NIVEDITA YUMNAM, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Performances of bulk heterojunction organic solar cells strongly depend on their ability to dissociate photo-generated excitons. Efficient exciton dissociation is crucial for achieving high short circuit currents and energy conversion efficiencies. A volume distributed junction between donor and acceptor material is needed to obtain efficient dissociation, since exciton dissociation occurs only at their interface. Furthermore, the domain sizes of donor and acceptor material should be at nanometer length scale, so that excitons can reach the interface before they recombine. In this study, a phase separation of bulk heterojunction organic solar cells based on a blend mixture of PTB7 (donor) and PCBM (acceptor) material is investigated. To record the phase separation, an atomic force microscopy (AFM) has been used. The phase image measured by AFM depends on the energy dissipated by a cantilever tip to a material at the surface of a sample. Consequently, the phase contrast observed in the phase image is influenced by different materials present at the sample surface. By identifying the phase of donor and acceptor material, the phase separation and its dependence on preparation conditions can be determined from AFM phase image.

DS 9.2 Mon 15:15 H11

**Charge transport and trap dynamics investigations in organic solar cells via MIS structures** — NIVEDITA YUMNAM, HIPPOLYTE HIRWA, and ●VEIT WAGNER — Jacobs University, Campus Ring 1, 28759 Bremen, Germany

The charge transport in organic bulk heterojunction solar cells is a critical process affecting the performance of the solar cell. Investigating the charge transport dynamics in the solar cell allows determination of the relevant transport parameters. The mobility of the charge carriers can be determined in the short time regime (up to 1ms). While the longer time regime allows to study the density of trap states. For our characterization we have prepared metal insulator semiconductor (MIS) devices based on Si/SiO<sub>2</sub> substrate and bulk heterojunction semiconductor mixture of P3HT and PCBM. The mobility of charge carriers is determined by using MIS-CELIV (metal insulator semiconductor-charge carrier extraction by linearly increasing voltage) [1]. For the investigation of trap states in our device, we have employed our recently developed transient current measurement technique which does not need light illumination [2]. This illumination-free transient current (IFTC) technique offers insights on the capture time of the trapping states, their density of states and the attempt-to-escape frequency of trapped carriers. [1] A.Armin et al., *Advanced Energy Materials*, 2014, 4, 1300954.[2] H.Hirwa, V.Wagner, *Organic electronics*, Vol. 25, 2015, 112\*120

DS 9.3 Mon 15:30 H11

**Investigation of Solution-Processable Electron Injection Layers in Organic Light-Emitting Diodes** — ●FLORIAN ULLRICH<sup>1,2,3</sup>, SEBASTIAN STOLZ<sup>1,3</sup>, MICHAEL SCHERER<sup>1</sup>, MALTE JESPER<sup>4</sup>, MANUEL HAMBURGER<sup>1,4</sup>, GERARDO HERNANDEZ-SOSA<sup>1,3</sup>, and ERIC MANKEL<sup>1,5</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg — <sup>2</sup>University of Heidelberg, Kirchhoff-Institute for Physics — <sup>3</sup>Karlsruhe Institute of Technology, Light Technology Institute — <sup>4</sup>University of Heidelberg, Organisch-Chemisches Institut — <sup>5</sup>TU Darmstadt, Material-Wissenschaft, Surface Science

One crucial obstacle for the realization of efficient organic light-emitting diodes (OLEDs) produced by high-throughput printing technologies is the poor injection of electrons since typical low work-function cathode layers like calcium or barium are highly reactive and cannot be solution-processed.

In this work, we investigate alkali metal stearates as solution processable electron injection layers in OLEDs. We fabricated yellow emitting OLEDs with different concentrations of Cs, Rb and K stearate and studied the influence on device performance, e.g. efficiency and efficacy. Values of about 9 cd/A and 10 lm/W were reached equalling the respective values of reference devices. The results were correlated to topography studies using atomic force microscope. The electronic interaction of the alkali metal stearates with the emitting layer and the

aluminum top contact was examined by various photoelectron spectroscopy measurements.

DS 9.4 Mon 15:45 H11

**Thermoelectric characterization of doped organic semiconductors** — ●BERNHARD NELL and KOEN VANDEWAL — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The introduction of p- and n-doped layers into the device structure of opto-electronic devices plays a crucial role in improving device performance. In this way, the charge carrier extraction or injection from or into the organic photo-active layer is improved and ohmic losses are reduced. Molecular doping of organic host materials increases the conductivity of the transport layers and moves the Fermi level to the appropriate position enabling electron or hole selectivity. In this work, we use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a different degree of fluorination in various amorphous host materials allows us to tune the energy level offsets between host and dopant and study their influence on the Fermi level position and overall doping efficiency systematically.

DS 9.5 Mon 16:00 H11

**Computer simulation of self-assembled monolayers of alkanethiols on liquid mercury** — ●ANTON IAKOVLEV<sup>1</sup>, DMITRY BEDROV<sup>2</sup>, and MARCUS MÜLLER<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — <sup>2</sup>Department of Materials Science & Engineering, University of Utah, Salt Lake City, 84112, UT, USA

The defectless, high-tension surface of liquid mercury facilitates the creation of high-quality self-assembled monolayers (SAMs) of organic molecules. SAMs of alkanethiols on liquid mercury are widely used in organic electronics to study the properties of metal-SAM-metal and metal-SAM-semiconductor junctions, where the liquid mercury is usually utilized as the second electrode. Recent experiments have revealed the coexistence of densely packed standing and flat-lying alkanethiols on the surface of liquid mercury and proposed rectangular unit cells for both, the head groups and tails, in the standing phase. Earlier, an oblique unit cell has also been considered to be a possible arrangement of alkanethiols on liquid mercury. In this report we present the first study of the phase coexistence and structure of SAM of alkanethiols on mercury by means of large-scale Molecular Dynamic simulation. We have developed a model of the SAM of alkanethiol on mercury, that allows us to reproduce the experimentally observed coexistence of the standing and lying molecules and to gain additional insights (eg. tilting of the tails) into the structure of alkanethiol SAMs on mercury. Our results indicate the oblique arrangement of thiols to be the preferred one.

DS 9.6 Mon 16:15 H11

**Tip-induced gating of carbene-based molecular circuits** — GIUSEPPE FOTI and ●HECTOR VAZQUEZ — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In this talk I will discuss N-heterocyclic carbene-based (NHC) molecules on gold [1] and explore their adsorption, mechanical and transmission properties by means of first-principles simulations based on DFT and NEGF.

First, I will examine the adsorption properties of NHCs on Au(111). NHCs bind selectively to the Au atop sites through a strong Au-C bond. I will then address the mechanical properties of NHCs through simulations where the metal-molecule junction is stretched. Upon elongation, the strong Au-C bond induces rearrangements of the Au surface and ultimately a Au-Au bond, and not the Au-C bond, breaks. Finally, I will discuss the conducting properties of NHC-based molecular junctions. We consider several tip structures and find a strong dependence of the position of the NHC molecular levels with the atomic structure of the tip [2]. The LUMO position changes by almost 0.8 eV with tip shape. This is understood in terms of the net charge transfer, electron redistribution and work function for each tip structure. The differences in the LUMO position effectively gate the molecular levels

and result in large conductance variations. These findings open the way to modulating the conductance of NHC-based molecular circuits through the controlled design of the tip atomistic structure.

[1] C.M. Crudden et al., Nature Chemistry 6 409 (2014).

[2] G. Foti and H. Vazquez (under review).

DS 9.7 Mon 16:30 H11

**Magnetic transition metal phthalocyanine thin films, tuning of electronic properties via alkali metal doping —**

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many — <sup>5</sup>Uni Halle, Germany — <sup>6</sup>Uni Bonn, Germany — <sup>7</sup>ISSP RAS, Chernogolovka, Russia — <sup>8</sup>TU Bergakademie, Freiberg, Germany

The evolution of electronic structure of the MTM-Pc\*s intrinsic and with potassium doping has been studied by means of photoemission spectroscopy, near-edge X-ray absorption fine structure and DFT calculations. The DFT calculations and detailed analysis of the core-level spectra permit us to suggest possible lattice sites for the potassium ions. The data disclosed filling of the lowest unoccupied molecular orbital upon doping and associated changes of the core level absorption spectra. None of the films prepared in our studies showed a finite electronic density of states at the Fermi level. This work was supported by the RFBR Grant No. 13 -02-00818 and the BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211