

## DS 1: Organic Electronics and Photovoltaics

Time: Monday 9:30–13:00

Location: H 2032

DS 1.1 Mon 9:30 H 2032

**Metal-organic interfaces: from molecular self-assembly to electronic transport through ultrathin functional monolayers** — ●FLORIAN VON WROCHEM — Sony Deutschland GmbH, Stuttgart

The continuous development of organic electronic devices, combined with the advances in spectroscopy and electrical characterization, dramatically extended our understanding of the physical and chemical processes occurring at metal/organic interfaces. Here, an overview of experimental and theoretical efforts aiming towards the selective modification of interfaces is given. Various anchor groups designed to connect organic materials to metal electrodes are presented (e.g. thiolates, dithiocarbamates, mercuryls and stannyls) and their potential for optimizing the charge injection as well as the morphological, chemical, and electronic nature at the contact is illustrated. On this basis, functional molecular building blocks are grafted to the surface by self-assembly, providing rectification, switching, or chemical selectivity. Once the key parameters for interface formation and fabrication are under control, a huge number of potential applications emerge, ranging from optoelectronics to organic printed circuits. As one example, electrostatic dipole layers for tuning the injection barrier between metals and organic semiconductors are presented, which may find applications in organic light emitting diodes, field effect transistors, and solar cells. When further reducing device dimensions towards the nanoscale, organic monolayers might foster the development of molecular electronics, as illustrated here by highly robust metal-molecule-metal junctions based on FeII-terpyridine molecular wires or by optically switchable protein layers.

DS 1.2 Mon 9:45 H 2032

**Grain boundaries in CuInSe<sub>2</sub> and CuGaSe<sub>2</sub> solar cell materials: New insights from hybrid functional calculations** — HOSSEIN MIRHOSSEINI, ●JANOS KISS, and CLAUDIA FELSER — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

Polycrystalline thin-film solar cells based on CuIn<sub>1-x</sub>Ga<sub>x</sub>Se (CIGSe) are an economically viable alternative to the Si based technology. During the deposition of the polycrystalline light absorber layer grain boundaries (GBs) are formed in the CIGSe material, and the effect of these GBs upon the structural and electronic properties of the thin-film solar cells are not yet fully understood. Different atomic structures of the GBs in CIGSe have been reported experimentally. The outcomes of the theoretical calculations, however, are diverse and sometimes inconsistent due to the limitation of the functionals, which fail to properly describe the band gap of thin film solar cell materials. Employing a state of the art method using the HSE hybrid functional, which is known to predict the atomic and electronic structure of solar cell materials rather well, we have looked at the behavior and properties of GBs in CuInSe<sub>2</sub> and CuGaSe<sub>2</sub>. In the framework of our investigation, we have studied the atomic relaxation and electronic structure of various GBs and also considered the effect of the impurity segregation close to the GBs.

DS 1.3 Mon 10:00 H 2032

**Relationship between the chemical structure of low band gap polymers and self-organization properties** — ●MILUTIN IVANOVIC<sup>1</sup>, U MUT AYGÜL<sup>1</sup>, ULF DETTINGER<sup>1</sup>, AURELIEN TOURNEBIZE<sup>1</sup>, DAVID BATCHELOR<sup>2</sup>, STEFAN MANGOLD<sup>2</sup>, HEIKO PEISERT<sup>1</sup>, and THOMAS CHASSÉ<sup>1</sup> — <sup>1</sup>) University of Tuebingen, Institute of Physical and Theoretical Chemistry, 72076 Tuebingen, Germany — <sup>2</sup>Karlsruhe Institute of Technology (KIT), ANKA Synchrotron Radiation Facility, 76344 Eggenstein-Leopoldshafen, Germany

A possible approach to improve the efficiency of donor-acceptor based bulk heterojunction (BHJ) of OPV cells is the use of low band gap (LBG) polymers as donor materials. Basic electronic processes in OPV cells are however strongly influenced by the morphology and the ability for self-organization of the polymers in the thin-films. We utilize NEXAFS spectroscopy to study the molecular orientation of novel LBG polymers (PCPDTTBTT, PCPDTTBT and PCPDTzTBTT) for OPVs in thin films. The influence of post-processing annealing as well as of blending with Phenyl-C61-butyrac acid methyl ester (PCBM) on the orientation is investigated. The studied LBG polymers are characterized by a variation of (hexyl-) thiophene groups compared to related LBG polymers recently studied.[1,2]. Acknowledgments: This

research is funded by the European Union Seventh Framework Programme (FP7/2011 under grant agreement ESTABLIS n° 290022). References: 1.\*Aygül, U. et al. J. Phys. Chem. C 2012, 116, 4870-4874. 2.\*Aygül, U. et al. Sol. Energ. Mat. Sol. Cells 2014, 128, 119-125.

DS 1.4 Mon 10:15 H 2032

**Organic ambipolar field-effect transistors: *In situ* electrical investigation of MnPC-OFETs** — ●FRANZISKA LÜTTICH, OVIDIU D. GORDAN, and DIETRICH R. T. ZAHN — Semiconductor Physics, Technische Universität Chemnitz, Chemnitz, Germany

On the way to low-cost and flexible applications organic semiconducting materials are promising. Devices like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs) can be produced e.g. on flexible and elastic substrates and with chemical variation of side groups or substitution of metal centers their properties like optical absorption and charge carrier mobilities can be influenced.

Here we present a temperature dependent study on Manganese Phthalocyanine (MnPc)-OFETs, which reveal an ambipolar behaviour. In order to investigate the electrical properties of MnPc we used OFET "end-of-line" substrates from Fraunhofer IPMS with a 100 nm thick thermal silicon dioxide layer as dielectric. The investigated bottom-contact OFETs were fabricated under high vacuum conditions ( $p < 4 \cdot 10^{-7}$  mbar) by evaporating MnPc on top of the pre-structured substrates. The electrical DC characteristics were measured *in situ* as a function of temperature. This procedure enables us to determine the activation energies for the hole and electron transport. The influence of ambient atmosphere was also investigated and revealed strong impact on the electrical performance. The topography was determined using an Atomic Force Microscope (AFM).

DS 1.5 Mon 10:30 H 2032

**Photoelectron spectroscopy studies on efficient air-stable molecular n-dopants** — ●MARTIN SCHWARZE<sup>1</sup>, MAX L. TIETZE<sup>1</sup>, PAUL PAHNER<sup>1</sup>, BEN NAAAB<sup>2</sup>, ZHENAN BAO<sup>2</sup>, BJÖRN LÜSSEM<sup>1</sup>, DANIEL KASEMANN<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Department of Chemical Engineering, Stanford University, Stanford, California 94305, United States

Understanding the working mechanism of electrical doping in organic semiconductors is essential for the optimization of organic semiconductor devices such as organic light emitting diodes or organic solar cells. A defined doping concentration allows for the control of the Fermi-level position as well as the adjustment of the conductivity of transport layers. In comparison to molecular p-doping of organic semiconductors, n-doping creates the additional problem of air instability. To successfully transfer an electron to the lowest unoccupied molecular orbital (LUMO) of the matrix material, dopants exhibiting shallow highest molecular orbitals (HOMO) are necessary, rendering them prone to reactions with e.g. oxygen. In this study, three different types of n-dopants are compared: air stable cationic DMBI dopants, halogen-free DMBI dimers, and the established but air sensitive Cr<sub>2</sub>(hpp)<sub>4</sub>. Fermi-level shift and conductivity of co-evaporated Bis-Hf1-NTCDI layers at different doping concentrations as well as stability during air exposure are investigated by UPS and electrical measurements.

DS 1.6 Mon 10:45 H 2032

**Mode-selective vibrational manipulation of charge transport in  $\pi$ -conjugated molecular materials** — ●ROBERT LOVRINCIC<sup>1,2</sup>, ARTEM A. BAKULIN<sup>3,4</sup>, YU XI<sup>1</sup>, OLEG SELIG<sup>3</sup>, HUIB J. BAKKER<sup>3</sup>, YVES L. A. REZUS<sup>3</sup>, PABITRA K. NAYAK<sup>1</sup>, ALEXANDR FONARI<sup>5</sup>, VEACESLAV COROPCEANU<sup>5</sup>, JEAN-LUC BREDAS<sup>5,6</sup>, and DAVID CAHEN<sup>1</sup> — <sup>1</sup>Department of Materials & Interfaces, Weizmann Institute of Science, Israel — <sup>2</sup>IHF, TU Braunschweig & Innovationlab, Germany — <sup>3</sup>FOM Institute AMOLF, The Netherlands — <sup>4</sup>Cavendish Laboratory, University of Cambridge, UK — <sup>5</sup>School of Chemistry and Biochemistry, Georgia Institute of Technology, USA — <sup>6</sup>Solar & Photovoltaics Center, King Abdullah University, Saudi Arabia

The soft character of organic materials leads to strong coupling between molecular nuclear and electronic dynamics. This coupling opens the way to control charge transport in organic electronic devices by directing molecular vibrational motions. However, despite encouraging

theoretical predictions, experimental realization of such control has remained elusive. Here we demonstrate experimentally that photoconductivity in a model organic optoelectronic device can be controlled by the selective excitation of molecular vibrations. Using an ultrafast infrared laser source to create a coherent superposition of vibrational motions in a pentacene/C<sub>60</sub> photoresistor, we observe that excitation of certain modes in the 1500–1700 cm<sup>-1</sup> region leads to photocurrent enhancement. The effect depends on the nature of the vibration and its mode-specific character can be well described by the vibrational modulation of intermolecular electronic couplings.

DS 1.7 Mon 11:00 H 2032

**Investigation of charge transfer in organic semiconductors using infrared spectroscopy** — ●TOBIAS GLASER<sup>1,2</sup>, SEBASTIAN BECK<sup>1,2</sup>, and ANNEMARIE PUCCI<sup>1,2,3</sup> — <sup>1</sup>Universität Heidelberg, Kirchhoff-Institut für Physik — <sup>2</sup>InnovationLab GmbH, 69115 Heidelberg — <sup>3</sup>Universität Heidelberg, Centre for Advanced Materials

Charge transfer in organic semiconductors is used in various ways to increase the performance of organic electronic devices. For example electrochemical doping is used to increase the conductivity in charge transport layers. Additionally, charge injection layers are used to decrease injection barriers between electrodes and organic transport layers. In both cases molecular charge transfer plays an important role, but the basic mechanisms are still subject of heated debate. Due to strong relaxation effects upon molecular charging, infrared (IR) spectroscopy is very well suited to investigate charge transfer in organic semiconductors. Neutral and charged molecules can be distinguished by their different specific vibrational features in spectra of doped layers as well as for interfaces. In this study we investigated charge transfer in thin layers of commonly known transport materials such as 4,4'-bis(N-carbazolyl)-1,1'-biphenyl (CBP) doped with inorganic and organic dopants such as MoO<sub>3</sub> or F4TCNQ and at interfaces of organic semiconductors. By quantitative analysis of the experimental spectra the doping efficiency and the degree of charge transfer can be determined for the doped layers. Whereas, for interfacial charge transfer, the formation of a space charge region can be mapped. Financial support by BMBF (project MESOMERIE) is gratefully acknowledged.

DS 1.8 Mon 11:15 H 2032

**Structure and Photovoltaic Performance of Chiral Anilino Squaraines** — ●MANUELA SCHIEK<sup>1</sup>, MATTHIAS SCHULZ<sup>2</sup>, STEFANIE BRÜCK<sup>1</sup>, MARTIN SILIES<sup>3</sup>, HEIKO KOLLMANN<sup>3</sup>, CHRISTOPH LIENAU<sup>3</sup>, ARNE LÜTZEN<sup>2</sup>, and JÜRGEN PARISI<sup>1</sup> — <sup>1</sup>Energy and Semiconductor Research Laboratory, University of Oldenburg, Germany — <sup>2</sup>Kekule-Institute for Organic Chemistry and Biochemistry, University of Bonn, Germany — <sup>3</sup>Ultrafast Nano-Optics, University of Oldenburg, Germany

Small molecular semiconductors such as squaraines are advantageous compared to polymeric materials because they allow a more direct control of the structure on the molecular level and consequently solid state properties. Especially the implementation of chiral side chains introduces new functionalities such as circular dichroism. Different 1,3-bis(N,N-substituted-2,6-dihydroxy-anilino)squaraines with varying terminal N-substitution, in some cases including a stereogenic center, are investigated as single crystals, in thin films and blended with a fullerene acceptor as active layer in bulk heterojunction organic solar cells.

DS 1.9 Mon 11:30 H 2032

**Charge separation and C<sub>60</sub> crystallinity in bulk heterojunction solar cells: the decisive role of device architecture** — ●FELIX SCHELL<sup>1,2</sup>, MICHAEL SCHERER<sup>1,3</sup>, DIANA NANOVA<sup>1,2,3</sup>, ANNE KATRIN KAST<sup>2,4</sup>, WOLFGANG KOWALSKY<sup>1,2,3</sup>, RASMUS R. SCHRÖDER<sup>1,4,5</sup>, and ROBERT LOVRINCIC<sup>1,3</sup> — <sup>1</sup>InnovationLab GmbH, Heidelberg — <sup>2</sup>Kirchhoff-Institute for Physics, Heidelberg University — <sup>3</sup>Institute for High-Frequency Technology, TU Braunschweig — <sup>4</sup>CellNetworks, BioQuant, Heidelberg University — <sup>5</sup>Center for Advanced Materials, Heidelberg University

The crucial influence of C<sub>60</sub> crystallinity on the charge separation in organic solar cells (OSC) has been realized very recently. Here, we show the importance of the device architecture on C<sub>60</sub> crystallisation in the bulk-heterojunction (BHJ). Active layer morphology of small molecule BHJ OSC and its influence on device performance are studied by means of energy-filtered transmission electron microscopy (EFTEM) and electrical characterization. The influence of substrate temperature during deposition and of pure sublayers is assessed. BHJs fabricated at room temperature are found to be finely mixed and amorphous, whereas the

corresponding films deposited onto heated substrates show pronounced phase separation. Despite these clear morphological changes, substrate heating does not increase efficiency of OSCs in a non-inverted device architecture. Improvements found in literature for inverted cells can be attributed to stronger acceptor crystallization, present, if deposited onto a pure C<sub>60</sub> layer but not with an F<sub>4</sub>ZnPc substrate, leading to more efficient exciton dissociation.

DS 1.10 Mon 11:45 H 2032

**Influence of DMSO-treatment on morphology, composition and performance of PEDOT:PSS layers in organic photovoltaic cells** — SIDHANT BOM, ●TORSTEN BALSTER, MARLIS ORTEL, and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

PEDOT:PSS layers in organic solar cells are used as hole transport (HTL) and electron blocking layers. Therefore the morphology and composition of the layer and the interface have a great influence on the performance of organic photovoltaic devices.

Additional post-deposition treatment of the PEDOT:PSS layers (HTL) in P3HT/PCBM solar cells were studied in this work. For this purpose, pristine PEDOT:PSS layers were spin coated with dimethyl sulfoxide (DMSO) after annealing. Pristine and treated layers were characterized by means of electrical characterization, atomic force microscopy (AFM) and x-ray photoelectron spectroscopy (XPS).

The additional post-deposition DMSO treatment induces an increase in power conversion efficiency by more than 50%. In addition, the open circuit voltage and the short-circuit current were enhanced, whereas the fill factor remained constant. This behavior is explained by modification of the PEDOT:PSS-semiconductor interface. On the one hand smoothing of the interface by reduction of large PSS particles visible in AFM occurs. On the other hand XPS data show a reduction of PSS-sulphur species. Less PSS at the interface should improve the charge carrier injection properties, as observed experimentally.

DS 1.11 Mon 12:00 H 2032

**Charge transfer, optical and transport properties in pure organic heterostructures** — ●LIEBING SIMON, HAHN TORSTEN, and KORTUS JENS — Institute of Theoretical Physics, TU Bergakademie Freiberg, Leipziger Strasse 23, 09599 Freiberg

We will present theoretical investigation on pure charge transfer materials within the density functional theory framework (DFT). Starting from the recently fabricated picene-F<sub>4</sub>TCNQ [1] we explore the electronic and optical properties of novel representatives of this new class of materials. These representatives are formed of polycyclic hydrocarbons and TCNQ derivatives and we compare our results with experimental spectroscopic data.

The picene-F<sub>4</sub>TCNQ system shown pronounced diode transistor behavior [2]. By means of DFT/NEGF (non equilibrium green function formalism) [3,4] we obtain the IV-characteristics of selected model devices for these systems. The formation of hybrid orbitals together with intrinsic charge transfer seems to be the origin of the novel electronic and transport properties [5].

[1] Mahns, B. et. al. *Crystal Growth & Design* (2014). [2] Hahn T., Liebing S., and Kortus J., *Nanoscale* 6, 14508 (2014). [3] Pederson, M. et. al. *Phys. Status Solidi b* 217, 197. (2000) [4] Enkovaara, J. et al. *Journal of Physics: Condensed Matter* 22, 253202 (2010). [5] Lindner S. et. al. *Phys. Rev. Lett.* 109, 027601 (2012).

DS 1.12 Mon 12:15 H 2032

**Single molecule circuits with N-heterocyclic carbene linkers** — ●HECTOR VAZQUEZ — Inst. of Physics, Academy of Sciences of the Czech Rep., CZ

In single molecule circuits, where an electrical current flows through a molecule, conducting molecules often have terminal linker groups which bind to the metallic electrodes [1]. These chemical link groups strongly influence the conducting properties, often acting as bottlenecks for electron transmission and result in low-transmission resonances localized at the interface. Therefore, identifying adequate chemical linker groups is essential for achieving ideal mechanical and conducting properties in molecular circuits.

Recently, SAMs of N-heterocyclic carbenes on gold were shown to have very high thermal and oxidative stability [2], making N-heterocyclic carbenes potentially very useful linkers for single molecule transport. In this talk, I will present results from first-principles simulations based on DFT-NEGF for the electronic and conducting properties of carbene-terminated molecules. I will show results for the adsorption properties of N-heterocyclic carbenes on gold. I will also

present transmission calculations of carbene-terminated molecules and discuss these results in the context of other metal-molecule links with Au-C bonds [3].

[1] F. Schwarz and E. Loertscher, *J. Phys. Condens. Matter* 26 474201 (2014).

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

[3] W. Chen et al., *J. Am. Chem. Soc.* 133 17160 (2011).

DS 1.13 Mon 12:30 H 2032

**Charge and spin transfer materials for molecular electronic and spintronic applications** — •TORSTEN HAHN, SIMON LIEBING, and JENS KORTUS — TU Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg

The combination of different functionalized metal phthalocyanines was found to lead to novel charge- and spin transfer compounds [1,2]. The recently synthesized picene / F4TCNQ charge transfer salt [3] also shows promising physical properties and the theoretical modeling predicts the material to act as a molecular diode with high rectification ratio [4]. Based on density-functional theory calculations we show that in case of the metal phthalocyanines as well as for the picene / F4TCNQ system hybrid states formed by the donor / acceptor system are playing the key role to determine the spectroscopic and quantum transport properties. We further conclude that the tuning of quantum transport properties through hybrid states is a general concept which opens a new route towards functional materials for molecular electronics.

[1] R. Friedrich et al., *Phys. Rev. B* 87, 115423 (2013). [2] R. Friedrich, B. Kersting, and J. Kortus, *Phys. Rev. B* 88, 155327 (2013).

[3] Mahns, B. et. al., *Cryst. Growth and Design* 14, 1338-1346 (2014).

[4] T. Hahn, S. Liebing, and J. Kortus, *Nanoscale* 6, 14508 (2014).

DS 1.14 Mon 12:45 H 2032

**Device-like calcium corrosion test for ultra-barrier materials** — •FREDERIK NEHM<sup>1</sup>, HANNES KLUMBIES<sup>1</sup>, JOHN FAHLTEICH<sup>2</sup>, FELIX DOLLINGER<sup>1</sup>, KARL LEO<sup>1</sup>, and LARS MÜLLER-MESKAMP<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, TU Dresden, Dresden, Deutschland — <sup>2</sup>Fraunhofer FEP, Dresden, Deutschland

The continuous progress of organic electronics demands for flexible moisture barriers with water vapor transmission rates (WVTRs) below  $10^{-4} \frac{g(H_2O)}{m^2d}$  and quick, reliable measurement techniques for such WVTRs. The electrical calcium corrosion test is an extremely sensitive technique used widely in research groups. However, setups differ strongly as do their accuracy and background rates. We report on common issues and show how we manage them in our setup. Barrier corrosion because of direct water condensation on its surface is prevented by a glued-on PET film and Ca-induced stress is mitigated by organic decoupling layers. We demonstrate the effectiveness of our approach with studies on sputtered Zinc-Tin-Oxide and atomic layer deposited (ALD) alumina moisture barriers in different aging climates. Single barriers show a linear WVTR increase with rising absolute humidity at given temperature. Below  $40^\circ C$ , this is even valid independent of temperature. A divergence at higher temperatures probably originates from the actual barrier layer, since this effect cannot be observed for the pure substrate. Also, nanolaminates using ALD alumina, titania and alkoxide, and multilayer barriers with polymer interlayers with WVTRs down to at least  $2 \cdot 10^{-5} \frac{g(H_2O)}{m^2d}$  in  $38^\circ C$ , 90% relative humidity environments are investigated.