

## CPP 31: Organic semiconductors II

Time: Thursday 9:30–12:45

Location: C 130

## Invited Talk

CPP 31.1 Thu 9:30 C 130

**Large area flexible and stretchable electronics** — ●SIEGFRIED BAUER — Soft Matter Physics, Johannes Kepler University, Altenbergerstrasse 69, A-4040 Linz, Austria

Today's electronics is stiff, usually made of brittle materials. Tomorrow's electronic may be highly flexible and even mechanically deformable to conform to arbitrary forms. Such electronics must be built on a combination of soft and hard materials. Challenges in this field of research are the largely different mechanical properties of the materials used: entropy elastic elastomers and energy elastic solids. New research directions in mechanics emerge leading to new and unexpected electromechanical instabilities. In the presentation, a tour d'horizon through the mechanics of soft materials under extreme conditions of stretch is given. Examples chosen will be based on recent developments in large area flexible and stretchable electronics, such as ultrathin, ultraflexible and ultracompliant organic solar cells, integrated sensors and active matrix arrays. Work supported by the Austrian Science Funds and by the European Research Council under the advanced grant Soft-Map.

CPP 31.2 Thu 10:00 C 130

**Doping as a new approach in promoting charge separation in polymer:fullerene solar cells** — ●DANIEL RIEDEL<sup>1</sup>, FELIX DESCHLER<sup>1</sup>, ENRICO DA COMO<sup>1</sup>, JOCHEN FELDMANN<sup>1</sup>, BERNHARD ECKER<sup>2</sup>, and ELIZABETH VON HAUFF<sup>2</sup> — <sup>1</sup>PhOG, Department of Physics, LMU, Munich — <sup>2</sup>Institute of Physics, University of Freiburg

Charge separation at polymer:fullerene interfaces is the primary process for organic bulk-heterojunction solar cells. Following the ultrafast photoinduced charge transfer, electrons and holes are still bound because of Coulomb interactions, resulting in the formation of charge transfer excitons (CTEs). Those are known to play a crucial role in solar cells being responsible for the open circuit voltage and the short circuit current. In this contribution, we propose a novel strategy to overcome some of the recombination channels due to charge transfer excitons. This new approach considers the modification of the electronic properties of the conjugated polymer by doping with F4TCNQ molecules. The free holes induced by F4TCNQ on the low-bandgap polymer PCPDTBT fill the tail of states in the highest occupied molecular orbital (HOMO) and in addition are expected to screen Coulomb interactions of CTEs at the interface between PCPDTBT and the fullerene derivative PCBM. By the unique combination of time resolved photoluminescence and photoinduced absorption spectroscopy, we demonstrate how doping results in a decreased population of CTEs and enhanced formation of free carriers. The spectroscopy experiments are complemented by measurements on solar cells showing an overall increase of more than 30% in the power conversion efficiency.

CPP 31.3 Thu 10:15 C 130

**Improved performance of organic photovoltaic cells processed on corrugated substrates structured with laser interference patterning** — ●REINHARD SCHOLZ<sup>1</sup>, LARS MÜLLER-MESKAMP<sup>1</sup>, YONG HYUN KIM<sup>1</sup>, SIMONE HOFMANN<sup>1</sup>, KARL LEO<sup>1</sup>, SEBASTIAN ECKARDT<sup>2</sup>, and ANDRÉS FABIÁN LASAGNI<sup>2</sup> — <sup>1</sup>Institut für Angewandte Photophysik, Technische Universität Dresden — <sup>2</sup>Fraunhofer Institut für Werkstoff- und Strahltechnik, Dresden

Due to the short exciton diffusion length in organic semiconductors, bulk heterojunction solar cells consisting of donor-acceptor blends can help to improve the charge separation of the photocarriers. However, in the blends, problems in the formation of continuous percolation pathways towards the electrodes limit the total absorber thickness to rather low values, so that the photovoltaic cells would greatly benefit from an improved light management and an optical concentration in the absorber layer. We successfully use direct laser interference patterning (DLIP) to generate periodic surface structures on different types of substrates. DLIP uses high power laser pulses to ablate the target material directly, without need for classical lithography, resist, and transfer steps, allowing instead scalable structuring at reasonable costs and throughput. Comparing photovoltaic cells grown on corrugated substrates with reference cells grown on a flat surface of the same material, we obtain a relative enhancement of the power conversion efficiency by a factor of 1.21 [1].

[1] L. Müller-Meskamp, Y. H. Kim, T. Roch, S. Hofmann, R. Scholz,

S. Eckardt, K. Leo and A. F. Lasagni, *Adv. Mater.* (2011) *in press*.

CPP 31.4 Thu 10:30 C 130

**Blocking layer influence on Diindenoperylene based photovoltaic devices** — ●ANDREAS STEINDAMM<sup>1,2</sup>, MICHAEL BRENDEL<sup>1,2</sup>, KATHARINA TOPCZAK<sup>1</sup>, and JENS PFLAUM<sup>1,2</sup> — <sup>1</sup>Exp. Phys. VI, Julius-Maximilians-University Würzburg, D-97074 Würzburg — <sup>2</sup>ZAE Bayern e.V., D-97074 Würzburg

Diindenoperylene (DIP) has shown to be a suited donor material in combination with the acceptor C<sub>60</sub> resulting in bilayer photovoltaic cells with open circuit voltages up to 0.9 V. Together with an exceptionally high fill factor of 74 % this yields an overall cell efficiency of around 4 % [1]. However, a severe drawback is the rather poor light absorption of the crystalline DIP layer due to the unfavorable orientation of transition dipoles along the surface normal, i.e. perpendicular to the electric field vector of the incident light. Therefore, harvesting of all photon-generated excitons is essential in these structures to achieve highest photocurrents possible. As a promising concept the application of exciton blocking layers (EBLs) has been suggested and will be addressed in this contribution by means of an intermediate Batho-Phenanthroline (BPhen) EBL between the fullerene acceptor and the metallic cathode. As a main result, a doubling of the short circuit current ( $I_{SC}$ ) could be achieved by implementing the BPhen EBL. To identify the underlying effects, responsible for this enhancement, we employed photoluminescence (PL) quenching measurements which allow for separation of contributions caused by exciton reflection versus those related to metal penetration during deposition.

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

CPP 31.5 Thu 10:45 C 130

**Evidence for non-isotropic emitter orientation in a red phosphorescent OLED and its implications for determining the emitter's radiative quantum efficiency** — ●TOBIAS DANIEL SCHMIDT<sup>1</sup>, MICHAEL FLÄMMICH<sup>2</sup>, JÖRG FRISCHEISEN<sup>1</sup>, DIRK MICHAELIS<sup>2</sup>, NORBERT DANZ<sup>2</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — <sup>2</sup>Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The efficiency of organic light-emitting diodes (OLEDs) is still limited as only a fraction of the consumed electrical power is converted into light and only a small part of this light is finally extracted from the device to air. Especially the radiative quantum efficiency (RQE) of the utilized guest-host system is of interest and should be close to unity in phosphorescent emitter/matrix combinations in order to achieve highly efficient devices. We show that the commonly used red phosphorescent emitter Ir(MDQ)<sub>2</sub>(acac) doped in an  $\alpha$ -NPB matrix exhibits a profound non-isotropic dipole orientation of the emitter molecules. Ignoring this feature leads to a significant overestimation of the RQE or other factors, which determine the external quantum efficiency of a device. Furthermore, we demonstrate the huge potential for efficiency enhancement of mainly parallel dipole emitter orientation in phosphorescent OLED systems.

CPP 31.6 Thu 11:00 C 130

**Tailoring the electronic properties of polypyrrole thin films for acid detection** — ●CÉLINE VERVACKÉ<sup>1</sup>, CARLOS CÉSAR BOF BUFON<sup>1</sup>, PABLO ROBERTO FERNÁNDEZ SILES<sup>1,2</sup>, and OLIVER G. SCHMIDT<sup>1,2</sup> — <sup>1</sup>Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — <sup>2</sup>Material Systems for Nanoelectronics, TU Chemnitz, Reichenhainerstrasse 70, 09107 Chemnitz, Germany

Water acidification is one of the most important environmental issues affecting all ecosystems [1]. In this work we demonstrate the fabrication and characterisation of HCl, H<sub>2</sub>SO<sub>4</sub> and H<sub>3</sub>PO<sub>4</sub> detectors based on chemically grown polypyrrole (PPy) thin films with thickness below 100 nm [2, 3]. In addition, the organic layers are incorporated into self-wound microtubes with diameter of about 15-20  $\mu$ m for lab-on-a-chip integration. In order to allow the acid detection, PPy was successfully discharged in water, minimizing in this way the polymer degradation which is often observed when performed by other means (e.g. chemical and electrochemical reduction) [4]. The investigation of the structural modifications and the electrical properties were conducted by means

of transport measurements, infrared spectroscopy, cyclic voltammetry and current sensing AFM methods.

1. C.D. Evans et al., *Environ. Sci. Technol.* 45, 1887 (2011)
2. C.C. Bof Bufon and T. Heinzel, *Appl. Phys. Lett.* 89, 012104 (2006)
3. C.C. Bof Bufon and T. Heinzel, *Phys. Rev. B* 76, 245206 (2007)
4. C.C. Bof Bufon et al., *J. Phys. Chem. B* 114, 714 (2010)

### 15 min break

CPP 31.7 Thu 11:30 C 130

**Magnetoresistive organic field-effect transistors based on donor/acceptor blends** — ●THOMAS REICHERT, TOBAT P. I. SARAGI, and JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials, Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology, University of Kassel, Heinrich Plett Strasse 40, D 34132 Kassel, Germany

Room temperature magnetoresistive organic field-effect devices operated at low magnetic fields (<100 mT) are presented. They consist of different coevaporated donor/acceptor blends, with a high probability for intermolecular charge-transfer states. No magnetic field-effect is observed in the devices of pristine compounds. In contrast, a significant magnetoresistance effect is obtained in the mixed systems. The sign of magnetoresistance can be tuned by varying the applied drain and gate voltages. The magnetoresistance values also depend on the composition of the donor- and acceptor-molecules. Our results contribute to the elucidation of the origin of magnetoresistance in organic field-effect transistors and open a way to magnetosensitive organic devices without ferromagnetic materials.

CPP 31.8 Thu 11:45 C 130

**Crystal Growth of Organic Compound From The Melt** — ●HUAMIN IRVINE HONG and CHRISTIAN KLOC — School of Materials Science and Engineering Nanyang Technological University Block N4.1 Nanyang Avenue Singapore 639798

In this study, single crystals of anthracene up to few centimeters were developed from the melt based on a self designed, inexpensive and versatile zone refining apparatus. Platelets cut from these crystals by applying thread saw were tested for purity and perfection by Powder X-ray Diffraction (XRD), Laser Desorption Ionization-Time of Flight Mass Spectrometry (LDI-ToF MS), Fourier-Transform Infrared Spectroscopy (FT-IR), Atomic Force Microscopy (AFM) & fluorescence measurement. Based on the purity analysis, impurities within commercial anthracene powder such as Carbazole and 9, 9'-Bianthryl (dimers) have been reduced significantly as indicated by LDI-ToF MS analysis.

In addition, single crystals of Stilbene up to few centimeters (ideal scintillation properties) has been developed applying the same technique. The Stilbene crystal does not show any formation of intrinsic impurities such as dimers as compared to those of anthracene crystal upon zone refinement. Hence, the results indicate that zone refinement can produce high quality organic crystals with desired properties provided that intrinsic impurities (dimers etc) do not form upon the thermal fusion.

CPP 31.9 Thu 12:00 C 130

**Non-empirical Determination of the Fraction of Exact Exchange in Density-functional Theory** — ●VIKTOR ATALLA<sup>1</sup>, MINA YOON<sup>2</sup>, and MATTHIAS SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, Berlin, Germany — <sup>2</sup>Oak Ridge National Laboratory, USA

Calculating the electronic structure of small molecules with density-functional theory (DFT) is challenging because conventional exchange-correlation (XC) functionals typically severely underestimate HOMO-LUMO gaps, which may result in a wrong description for charge trans-

fer between weakly interacting molecules.

Here we consider the PBE0 [1] types of XC functionals using the fraction of exact exchange ( $\alpha$ ) as an adjustable parameter. Employing the  $G^0W^0$  approach we identify the optimum  $\alpha$  ( $\alpha_0$ ) for which the quasi particle correction to the Kohn-Sham HOMO vanishes. We tested this scheme for the G2 datasets of small molecules and find  $\alpha_0$  values in the range of 0.7 – 0.9. The generalized Kohn-Sham HOMO levels at the  $\alpha_0$  have a mean error of  $\sim 0.3$  eV with respect to the experimental vertical ionization potentials.

We apply the scheme for the prototypical donor-acceptor complex TTF/TCNQ and obtain  $\alpha_0 \sim 0.8$ , which gives an electronic level alignment consistent with the experimental value. It follows that this system rather exhibits intra-molecular electron-density rearrangement than charge transfer.

- [1] C. Adamo, V. Barone, *J. Chem. Phys.* 110, 6158 (1999)

CPP 31.10 Thu 12:15 C 130

**Ab initio simulations in aza-bodipy derivatives: How energetic disorder affects the charge carrier mobility in 3D systems** — ●SEBASTIAN RADKE, RAFAEL GUTIERREZ, CAROLINE GOL-LUB, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Potential candidates for low cost large area photovoltaic applications are organic solar cells based on small molecules because they can be produced on flexible substrates at low temperatures. To enlarge their efficiency, organic absorber materials covering the whole sun light spectrum are required. Nevertheless, efficient infrared absorbers for application in organic solar cells are still rare.

Based on first principle methods, we investigate theoretically the electronic structure and the charge transport of a promising near-infrared absorber material, bis-(phenyl)-borondifluoride-azadiisoindomethene. We simulate the charge carrier mobility in terms of disorder kinetic Monte Carlo simulations by means of semi-classical Marcus theory. By using this approach, we are able to analyze the effects of the dynamics of the electronic system parameters, which are sensitively related to the molecular structure as well as to the system morphology, on the anisotropic charge transport in the different materials. Our theoretical investigations enable us to predict and to understand experimental findings on this material and help to develop a materials design not only for the class of aza-bodipy derivatives but also for arbitrary highly ordered molecular systems.

CPP 31.11 Thu 12:30 C 130

**Continuum Solvent Model for extended periodic Systems** — ●MATTHIAS WITTE, UWE GERSTMANN, EVA RAULS, and WOLF GERO SCHMIDT — Universität Paderborn, Germany

Solvent influences play an important role in physical chemistry and are becoming recently a matter of interest for density functional theory (DFT) [1]. In order to increase the applicability to more realistic systems one needs to combine periodic systems and a solvent model. Periodic boundary conditions are still important for condensed matter systems and surfaces. We implemented the continuum solvent model proposed by Fattbert et al. [2] in the plane wave DFT code PWscf [3]. The modified Poisson equation is solved with the Parallel algebraic MultiGrid (PMG) solver [4]. Instead of the suggested zero-Dirichlet boundary conditions we use a different approximation using the screened Hartree potential. With this approach we studied various physical properties, like e.g. the optical absorption of small model systems in solution and their dependence of the surrounding medium. First test calculations show good agreement with theoretical data.

- [1] J. Tomasi et al., *Chem. Rev.* 105 (2005) 2999  
 [2] J.L. Fattbert et al., *Int. J. Quantum Chem.*, 23 (2002) 662  
 [3] P. Giannozzi et al., *J. Phys.: Condens. Matter* 21 (2009) 395502  
 [4] M.J. Holst et al., *J. Comput. Chem.* 14 (1993) 105