

## HL 100: Organic Electronics and Photovoltaics III (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Friday 9:30–12:00

Location: H40

HL 100.1 Fri 9:30 H40

**Influence of order and disorder on some photovoltaic properties of AnE-PV polymers - a DFT study** — ●CHUAN-DING DONG and WICHARD J. D. BEENKEN — Institut für Physik und Institut für Micro- und Nanotechnologie, Technische Universität Ilmenau, Germany

Recently, the copolymer poly(p-anthraceneethynylene-alt-poly(p-phenylenevinylene) (AnE-PV) has turned out to be a promising model for the effect of order and disorder in polymer-based solar cells.[1] By substituting linear octyl or branched 2-ethyl-hexyl sidechains to the conjugated backbone, the structure of AnE-PV can be tuned from order to disorder. Using Grimme's correction for dispersion in our DFT calculations, we will show that the van-der-Waals interaction between the sidechains influences the planarity of the conjugated backbones significantly. Consequently, we found order-dependent shifts of the respective absorption spectra, which are in agreement with the experimental data. Furthermore, we will demonstrate the effect of the alternative sidechain substitution on the stacking of AnE-PV copolymers to semi-crystalline aggregates, which is crucial for the efficiency of polymer solar cells.

[1] Kästner, C.; Egbe, D.; Hoppe, H.: *J. Mater. Chem. A* **3**(2015)395.

HL 100.2 Fri 9:45 H40

**Influence of surface characteristics on electronic properties of polymer thin films** — ●PHILIPP EHRENREICH, SUSANNE BIRKHOLO, ALEXANDER GRAF, EUGEN ZIMMERMANN, HAO HU, KWANG-DAE KIM, and LUKAS SCHMIDT-MENDE — Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany

Many applications in polymer electronics demand not only for a loss-free charge percolation pathway towards electrodes, but also a highly delocalized pi-orbital system for efficient charge generation after exciton dissociation. The latter is especially important for the development of all-polymer solar cells, in order to compete with fullerene-based devices. Within this work the influence of surface characteristics on structural, or rather electronic properties of polymer thin films is investigated by means of an H/J-aggregate analysis on the model polymer Poly(3-hexylthiophene).

HL 100.3 Fri 10:00 H40

**Quantum Molecular Dynamical Calculations of Poly(3,4-ethylenedioxythiophene) and its derivatives** — ●AMINA MIRSAKIYEVA, HÅKAN W. HUGOSSON, and ANNA DELIN — KTH Royal Institute of Technology, Department of Material and Nanophysics, SE-16440, Sweden

Organic thermoelectrics (TE) are materials with the ability to produce an electrical current from a temperature gradient (the so-called Seebeck effect) and the advantages of organic compounds, such as less toxicity. Organic TE are based on conductive polymers where the conjugation between double and single bonds creates the  $\pi$ -bonds overlapping and consequently allows charge carriers transport along the polymer backbone. Up to this date, the most studied organic TE material is poly(3,4-ethylenedioxythiophene) (PEDOT). Its transparency, high stability in the oxidized state and ability to form water-soluble polyelectrolytes bring it to the leading position in industry. The success of PEDOT makes also its selenium (PEDOS) and tellurium (PEDOTe) derivatives promising thermoelectric materials. Here, we present theoretical calculations of PEDOS and PEDOTe. We determined structures of the polymer chains of PEDOS and PEDOTe, investigated HOMO and LUMO and calculated point-charge distributions along the polymer backbone. Our analysis aims at finding the localization of a polaron, i.e. the electronic excitation resulting in localized structural changes and charge accumulation. Such a deeper atomistic understanding of the processes inside thermoelectric materials will hopefully allow an improvement of the thermoelectric qualities of conductive polymers.

HL 100.4 Fri 10:15 H40

**How Morphology Affects the Charge Transport: A Case Study for C60** — ●SEBASTIAN SCHELLHAMMER<sup>1,2,3</sup>, FRANK ORTMANN<sup>1,2</sup>, and GIANAURELIO CUNIBERTI<sup>1,2,3</sup> — <sup>1</sup>Institute for Ma-

terials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — <sup>3</sup>Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

The performance of organic electronic devices is significantly influenced by the morphology of the individual layers. However, theoretical studies can cover mostly only highly ordered or completely amorphous systems.

We present a computational algorithm for the construction of arbitrarily ordered films ranging from amorphous to polycrystalline and highly crystalline. We demonstrate its application for a systematic study of the electron mobility in C60 systems depending on the degree of ordering which is based on a full parameterization of the electronic properties. Additionally, we present a generalization for other molecular materials such as pentacene as well as organic blends.

HL 100.5 Fri 10:30 H40

**Intermolecular hopping transfer between DPP-based donor-acceptor polymers: A first principle study** — ●FLORIAN GÜNTHER<sup>1,2</sup>, SIBYLLE GEMMING<sup>1,3</sup>, and GOTTHARD SEIFERT<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — <sup>2</sup>Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — <sup>3</sup>Institute of Physics, Technical University Chemnitz, Germany

Diketopyrrolopyrrole (DPP) based materials have recently been considered as promising candidates for novel organic electronics. Here, we report about our investigation on intermolecular charge transfer between DPP-based polymers. We utilize Marcus transfer theory and evaluate the required quantities, the reorganisation energy and the coupling, by density functional-based tight binding (DFTB) calculations. Due to its computational efficiency as well as the opportunity to tune some calculation features, the DFTB method is well suited for this purpose. In doing so, the coupling elements have been calculated for various stacking formations. In order to derive a single quantity, which can be used for calculate the transfer rates, an energy-weighted statistical approach has been utilised.

The obtained values allow to analyse the charge carrier mobilities in dependence of isomeric effects as the orientation of the individual units, of the molecular structure as functionalization, or the meaning of stacking properties as parallel and anti-parallel.

15 min. break

HL 100.6 Fri 11:00 H40

**Comparison of electrostatic, inductive and dispersive excitation energy shifts for the example of a molecular crystal** — ●JÖRG MEGOW — University of Potsdam, Germany

The description of dispersive excitation energy shifts is necessary whenever different molecules within a supramolecular aggregate experience a different environment. A new approach that is based on an extended dipole approximation for higher transition densities in the sum over states expression [1] allowed for an appropriate description of gas-to-crystal-shifts in thin 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) films [2]. It was also possible to explain the splitting of the main bands in the UV/Vis spectrum of double-walled tubular cyanine aggregates [3] as well as the line shift and broadening of the measured UV/Vis spectrum of pheophorbide *a* dendrimers [4]. For the example of a PTCDI crystal the different contributions to the overall site energy shifts are calculated while approximating the sum over states expressions for the energy shifts due to dispersion and inductive polarization, respectively. It is shown that the dispersive site energy shift dominates the site energy shifts due to electrostatic interaction and inductive polarization.

[1] A. Stone, *The theory of intermolecular forces*, Oxford University Press (2013); [2] J. Megow, T. Körzdörfer, T. Renger et al., *J. Phys. Chem. C* **119**, 5747-5751 (2015); [3] J. Megow, M. I. S. Röhr, M. Schmidt am Busch et al., *PCCP* **17**, 6741-6747 (2015); [4] J. Megow, *ChemPhysChem* **16**, 3101-3107 (2015)

HL 100.7 Fri 11:15 H40

**Efficient first-principles based screening for high charge carrier mobility in organic crystals** — ●CHRISTOPH SCHÖBER, KARSTEN REUTER, and HARALD OBERHOFER — Technische Universität München

In organic electronics, charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. We developed a fast and efficient protocol with a descriptor based on electronic coupling values to assess the expected performance of organic materials for application in organic electronic devices. Applying this protocol to experimental structures of organic crystals obtained from the Cambridge Structural Database (CSD), we screened about 40000 structures employing only first principle methods. Out of the 28000 successfully calculated structures we selected 2000 candidates with above- average electronic couplings for additional calculations and in-depth analysis using statistical methods and automated classification based on chemical structure. This allowed us not only to identify a number of specific crystals with exceptionally high electronic coupling values and therefore promising properties, but also possible lead structures which can be the basis for in-depth theoretical and experimental studies of new classes of materials for organic electronics.

HL 100.8 Fri 11:30 H40

**In-situ x-ray investigation of the structure formation of metal films on photoactive polymers** — ●FRANZISKA C. LÖHRER<sup>1</sup>, VOLKER KÖRSTGENS<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>2</sup>, ALEXANDER HINZ<sup>3</sup>, OLEKSANDR POLONSKYI<sup>3</sup>, THOMAS STRUNSKUS<sup>3</sup>, FRANZ FAUPEL<sup>3</sup>, STEPHAN V. ROTH<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1</sup> — <sup>1</sup>TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — <sup>2</sup>Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany — <sup>3</sup>CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany

Photoactive polymers have received high attention in recent years due to a large variety of different applications in molecular electronics. Although organic materials are used in the active layers of these devices, typically in many cases the electrodes are still made from metals. Thus,

the polymer-metal interfaces are inherently present in all these novel devices. Our work takes a deeper look at the morphology of interfaces between photoactive layers and metal contacts deposited on top of them. We investigate morphological changes during sputter deposition of metal films (electrodes) onto photoactive films using in-situ GISAXS. Probing the sputter process in-situ allows highly time resolved insights into the deposition behavior of the metal depending on the polymer layer's properties. The deposition behaviors of gold and aluminium are compared, as both metals are frequently used as electrodes. The photoactive films consist of the low band gap polymer PTB7 as well as of PTB7:PCBM blends. The final film morphology is characterized via SEM and XRR after sputter deposition.

HL 100.9 Fri 11:45 H40

**Charge-Transfer - Solvent Interaction Predefines Doping Efficiency in p-Doped P3HT-Films** — ●LARS MÜLLER<sup>1,2,6</sup>, DIANA NANOVA<sup>1,2,6</sup>, TOBIAS GLASER<sup>2,6</sup>, SEBASTIAN BECK<sup>2,6</sup>, ANNEMARIE PUCCI<sup>2,6</sup>, ANNE K. KAST<sup>3,6</sup>, RASMUS R. SCHRÖDER<sup>3,4,6</sup>, ERIC MANKEL<sup>5,6</sup>, ROBERT LOVRINCIC<sup>1,6</sup>, and WOLFGANG KOWALSKY<sup>1,2,6</sup> — <sup>1</sup>IHF, TU Braunschweig — <sup>2</sup>KIP, Heidelberg University — <sup>3</sup>BioQuant, Heidelberg University — <sup>4</sup>CAM, Heidelberg University — <sup>5</sup>Surface Science Division, TU Darmstadt — <sup>6</sup>InnovationLab, Heidelberg

Doping of organic semiconductors is a prerequisite for the production of efficient devices such as organic light emitting diodes. Numerous recent publications reveal new insights on doping mechanisms and charge transfer, emphasizing the need for further investigations, especially on polymer systems. In this work, we study p-type doping of poly(3-hexylthiophene) (P3HT) with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), spin coated from the solvents chlorobenzene or chloroform. We find that films prepared from chloroform show a higher conductivity than films prepared from chlorobenzene. To clarify this unintuitive behavior, electron diffraction is used to reveal differences in the structural order within films from the two solvents. Additionally, UV-Vis and infrared spectroscopy help to expand the view to electronic properties such as vibrational or polaronic absorptions. It turns out that structural order and electronic properties in doped films are predefined by the interaction of the solvent with charge-transfer complexes already in solution.