CPP 56: Focus: Exploitation of Anisotropy in Organic Semiconductors II (joint session CPP/HL)

Time: Wednesday 9:30–11:15 Location: ZEU 222

Invited Talk CPP 56.1 Wed 9:30 ZEU 222

Structural and photophysical properties of blends of weakly interacting organic semiconductors — •Katharina Broch[1], Clemens Zeiser[1], Giulio Cerullo[2], Roel Tempelaar[3], and Christopher Bardeen[4] — [1]Institute for Applied Physics, University of Tübingen, Germany — [2]Department of Physics, Polytechnic University of Milan, Italy — [3]Department of Chemistry, Northwestern University, USA — [4]Department of Chemistry, University of California at Riverside, USA

Blends of organic semiconductors are functional parts in many organic electronic devices and their structural, electronic and photophysical properties have been studied in great detail. So far, research focussed mainly on electron donating and accepting organic semiconductors due to their relevance for devices. However, also blends of weakly interacting compounds can be interesting from the viewpoint of a fundamental understanding of mixing behavior [1,2], or as tool to study the details of complex photophysical processes [3,4]. Anisotropies in structure formation and their impact on photophysical properties will be discussed using the example of acene blends.

[1] J.-O. Vogel et al., J. Mater. Chem. 20 (2010); [2] A. Aufderheide et al., Phys. Rev. Lett. 109 (2012); [3] D. Lubert-Perquel et al., Nat. Commun. 9, 4222 (2018); [4] K. Broch et al., Nat. Commun. 9, 954 (2018)

CPP 56.2 Wed 10:00 ZEU 222

Influence of alkyl chain variation on co-crystal formation and molecular charge transfer — •Nadine Russegger, Oleg Vladimirov, Alexander Hinderhofer, and Frank Schreiber — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground state and in the excited state.

In this work, the charge transfer effect of weakly interacting organic semiconductor mixtures is comprehensively investigated depending on the influence of alkyl chain variation with different acceptor molecules. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different alkyl chain length in the imide position as acceptor molecules (PDIF-CN_2, PDI-C3, PDI-C5, and PDI-C8-CN_2).

For a full structural overview of the resulting molecularly mixed cocrystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption, photoluminescence as well as *in-situ* differential reflectance spectroscopy. For the various equimolar mixed systems of DNTT as well as DIP and different perylene-diimide derivatives charge transfer effects were estimated [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the chain length and their configuration of the different mixed systems.

[1] V. Belova et al., *J. Am. Chem. Soc.*, **2017**, 139, 8474-8486.

CPP 56.3 Wed 10:15 ZEU 222

Favored face-on crystal orientation in poly(3-(6-bromohexyl)-thiophene) on graphene as a result of modified interfacial interactions — •Oleksandr Dolynchuk[1], Philip Schmode[2], Matthias Fischer[1], Mukundan Thelakkat[2], and Thomas Thurn-Albrecht[1] — [1]Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — [2]Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate could be advantageous for inducing molecular orientation in semicrystalline conjugated polymers whose charge transport properties are anisotropic. Although a preferred face-one molecular orientation was shown in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to vacuum and graphite. Here it is shown that modification of the chemical structure of P3HT side chains can alter the surface interactions and result in fully face-on oriented crystals. Specifically, we present a comparative study of the substrate induced orientation in thin films of poly(3-(6-bromohexyl)-thiophene) (P3BrHT) and P3HT on graphene. The crystal orientation in films of both polymers was explored by surface-sensitive grazing incidence XRD. The results indicated that P3BrHT on graphene had solely face-on oriented crystals in films up to 26 nm, whereas P3HT showed the mixed face-on and edge-on crystal orientation with edge-on crystals formed at the top surface that supports our assumption about competing interfacial orientations.

CPP 56.4 Wed 10:30 ZEU 222

Determining Anisotropic Effects in Strongly Coupled Metal Organic Hybrid Structures — •Maximilian Rödel[1], Thomas Stark[2], Markus Hecht[3], Jochen Manara[2], Matthias Stolte[3], Frank Würthner[3], and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [3]Institut für Organische Chemie &Center for Nanosystems Chemistry (CNC), Julius Maximilian University of Würzburg, 97074 Würzburg

Coupling phenomena in metal organic hybrid structures enable unique possibilities to tune the properties of opto-electronic devices. Furthermore, the strong coupling between surface plasmons and excitons in organic semiconductors leads to novel hybrid states, which are termed plexcitons. By means of surface plasmon resonance spectroscopy we investigate these plexcitonic states in liquid-crystalline perylene bisimide (PBI) thin films exhibiting J-type coupling deposited on gold surfaces processed via doctor blading from solution. These new states show a characteristic coupling strength of ≈110 meV. Alignment of hydrogen-bonded PBI molecules and, thus, their transition dipoles results in long-range ordered films with a pronounced spatially anisotropy of structural and optical characteristics. A ratio of 2.78 can be evaluated between strongest and weakest coupling strength of the anisotropic system. Understanding the correlation between molecular order and optical properties will enable new device concepts utilizing the presented opto-electronic directionality in future applications.

CPP 56.5 Wed 10:45 ZEU 222

Anistropic Charge Transfer Formation at Crystalline Pentacene/Perfluoropentacene Interfaces — •Sebastian Hammer[1], Clemens Zeiser[2], Katharina Broch[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Institute for Applied Physics, University of Tübingen, 72076 Tübingen — [3]ZAE Bayern, 97074 Würzburg

Strongly bound charge transfer (CT) states critically influence the performance of devices based on donor/acceptor (D/A) heterojunctions such as light emitting diodes or photovolatic cells. Whereas the excited states in the archetypical CT system Pentacene:Perfluoropentacene (P:PFP) have been vastly studied in thin films [1][2], the role of molecular orientation on CT formation and energetics has not been evaluated to the same extent, so far. Utilizing heteroepitaxial growth of PFP on P (001) single crystals surfaces we were able to prepare long-range ordered D/A heterojunctions in an edge-on molecular configuration as confirmed by XRD. Optical analyses by temperature dependent cw-fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy on the PFP/P interfaces revealed no indication for CT formation in case of edge-on molecular orientation, in contrast to the face-to-face geometry. By means of bilayer as well as heterojunction diode structures we demonstrate that by controlling the molecular orientation at the PFP/P interface, thus, utilizing the anisotropic CT characteristics, the overall performance can be significantly improved.

[1] K. Broch et al., *Phys. Rev. B* **83**, 245307 (2011)

[2] T. Breuer, G. Witte, *J. Chem. Phys.* **21**, 138 (2013)

CPP 56.6 Wed 11:00 ZEU 222

On the Origin of Electronic Gap States in Molecular Semiconductor Thin Films — •Alexander Hinderhofer[1], Jan Hagenlocher[1], Satoshi Kera[2], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, 72076 Tübingen, Germany — [2]Institute for Molecular Science, Myodaiji, 444-8585, Japan

Electronic gap states within the HOMO-LUMO gap of molecular semiconductors play a key role in the energy level alignment of organic-organic and organic-inorganic interfaces and therefore are a defining parameter for device functionality and efficiency. The density of gap states originates from structural defects acting as dopants and it can be varied by different film preparation methods, e.g. by temperature variation during film deposition.

We present a systematic study of anisotropic structural parameters in thin films, including grain size, strain, dislocation density, mosaicity and coherently ordered domain size (in-plane and out-of-plane) studied by X-ray scattering and atomic force microscopy. The structural properties of several molecular semiconductors (Pentacene (PEN), Perfluoropentacene (PFP), 6-Phenacene (6Phen), etc.) are correlated with their electronic gap state density studied by ultra-low background ultraviolet photoelectron spectroscopy (UPS). We discuss which types of structural parameters have the strongest impact on the gap state density. Finally, we present examples of the energy level alignment in organic-organic heterojunctions controlled by their gap state density.