

CPP 3: Charge Transfer Effects in Molecular Materials I (joint session CPP/HL/BP/DS)

Related to SYCT organized by Frank Schreiber (Tübingen) and Wolfgang Brütting (Augsburg).

Time: Monday 12:15–13:30

Location: H1

CPP 3.1 Mon 12:15 H1

Thermally Activated Intermixing in Pentacene - Perfluoropentacene Heterostructures — •TOBIAS BREUER and GREGOR WITTE — Molekulare Festkörperphysik, Philipps-Universität Marburg, Renthof 7, 35032 Marburg

We report on the thermal stability of pentacene (PEN, C₂₂H₁₄) and perfluoropentacene (PFP, C₂₂F₁₄) heterostructures. We show that the thermal stability of the heterostructure compared to the single compounds is significantly enhanced by about 20 K. By varying preparation methods and stoichiometric ratios of the heterostructures we show that the stabilization is restricted to heterostructures with stoichiometric ratio of 1:1. Moreover, the thermal stabilization strongly depends on the preparation method, especially the deposition sequence of both materials in subsequent stacks. While PFP as bottom and PEN as top layer yield stabilized layers, no such effect is found for PEN as bottom layer and PFP on top. This asymmetry of intermixing and corresponding morphological information obtained by means of AFM measurements as well as optical absorption spectra as benchmark for hetero-interaction are discussed. The results are compared to additional preparation methods of heterostructures like co-evaporation and post-deposition-annealing.

CPP 3.2 Mon 12:30 H1

Mixing-induced anisotropic correlations in molecular crystalline systems: Rationalizing the behavior of organic semiconductor blends — •KATHARINA BROCH, ANTJE AUFDERHEIDE, JIŘÍ NOVÁK, ALEXANDER HINDERHOFER, RUPAK BANERJEE, ALEXANDER GERLACH, and FRANK SCHREIBER — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Binary mixtures of organic semiconductors (OSCs) have recently become an important field of research, as they find applications in optoelectronic devices [1]. In these systems, the mixing (intermixing vs. phase separation) and ordering behavior is crucial, since it affects the optical and electronic properties including the degree of charge-transfer (CT). We present a comprehensive study of binary mixtures of the three prototypical OSCs pentacene (PEN), perfluoropentacene (PFP) and diindenoperlyene (DIP) in all possible combinations [1,2,3]. Using X-ray reflectivity and grazing incidence X-ray diffraction we investigate the structural properties of the mixed films as well as their impact on the optical spectra obtained by spectroscopic ellipsometry. For PEN:DIP we find an anisotropic ordering behavior, comparable to that observed in some liquid crystals, which is fundamentally new for OSCs [2]. The influence of steric compatibility and the strength of the intermolecular interactions on the mixing and ordering behavior in the different blends will be discussed by extending a conventional mean-field model [1]. [1] A. Hinderhofer and F. Schreiber, *Chem.Phys.Chem.*, **13**, 628 (2012); [2] A. Aufderheide et al., *Phys.Rev.Lett.*, **109**, 156102 (2012); [3] J. Reinhardt et al., *J.Phys.Chem. C*, **116**, 10917 (2012)

CPP 3.3 Mon 12:45 H1

Screening Effects on Excitation Energy Transfer in Supramolecular Complexes in a Mixed Quantum Classical Description — •JÖRG MEGOW¹, THOMAS RENGER², and VOLKHARD MAY¹ — ¹Humboldt-Universität zu Berlin, Deutschland — ²Johannes Kepler Universität Linz, Österreich

Excitation energy transfer (EET) within the supramolecular complex P16 (sixteen pheophorbide a molecules covalently linked to a DAB-dendrimer) is studied using a mixed quantum classical methodology [1,2] that takes the screening of excitonic coupling into account. The excitonic coupling between two chromophores is calculated as Coulomb-coupling between transition partial charges. This treatment neglects the screening effects due to interaction with the solvent molecules.

The Poisson-TrEsp (transition charges from electrostatic potentials) method [3], developed in the group of Renger, allows the calculation of screening factors that correct the excitonic coupling between two chromophores dependent on their distance, mutual orientation and conformation. A new method is proposed that allows to obtain the orientation and conformation dependence of the Poisson-TrEsp screening factors in a mixed quantum-classical description by introducing a novel fitting procedure. While all screening ansatzes result in a deceleration of the EET, the new approach results in a considerable acceleration of the EET compared to standard screening approaches.

[1] J. Megow et al., *ChemPhysChem* **12**, 645 (2011) [2] J. Megow et al., *Chem. Phys.* **377**, 10 (2010) [3] J. Adolphs et al., *Photosynth. Res.* **95** (2008)

CPP 3.4 Mon 13:00 H1

In operando STXM investigations of charge carriers in SAM-FET devices — •ANDREAS SPÄTH¹, THOMAS SCHMALTZ², BENJAMIN WATTS³, MARCUS HALIK², and RAINER H. FINK¹ — ¹FAU Erlangen-Nürnberg, Physical Chemistry II, Erlangen, Germany — ²FAU Erlangen-Nürnberg, Polymer Sciences, Erlangen, Germany — ³Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

Based on previous work on pentacene based organic FETs [1], we present first results of zone plate scanning transmission soft x-ray microspectroscopy (STXM) on novel organic devices based on self assembled monolayers (SAMs). STXM combines high lateral resolution and spectroscopic sensitivity. Electron detection is used to achieve surface sensitivity, thus offering access to monolayer films. The SAMs implement all functionalities of the FET, i.e. gate dielectric and organic semiconductor [2]. STXM analysis within the active channel during operation of the SAMFET shows small variations in the electronic structure which are interpreted in terms of field induced shifts of the electronic levels and/or local charges. The unique combination of STXM and AFM provided by the NanoXAS beamline at the Swiss Light Source enables us to monitor both, the morphological homogeneity of the SAM film and modifications in the electronic structure. Thus, a more detailed insight into the correlation of morphological and electronic properties of these ultrathin devices can be achieved. The project is funded by the BMBF (contract 05K10WEA).

[1] C. Hub, et al., *J. Mater. Chem.* **20**, 2010, 4884

[2] A. Rumpel, et al., *Langmuir* **27**, 2011, 15016

CPP 3.5 Mon 13:15 H1

Scanning Kelvin Probe Microscopy on FIB-milled Cross Sections of Organic Solar Cells — •REBECCA SAIVE^{1,2,3}, CHRISTIAN MÜLLER^{1,2,3}, MICHAEL SCHERER^{1,2,3}, DOMINIK DAUME^{1,2,3}, MICHAEL KRÖGER^{1,3}, and WOLFGANG KOWALSKY^{1,2,3} — ¹InnovationLab GmbH, Heidelberg, Germany — ²Kirchhoff-Institut für Physik, University Heidelberg, Germany — ³Institut für Hochfrequenztechnik, Technische Universität Braunschweig, Germany

Scanning Kelvin probe microscopy (SKPM) is a promising tool to analyze charge carrier transport paths in electronic devices. Conventional SKPM is limited to analysis of charge transport parallel to the device surface, e.g. within planar field-effect transistors, whereas the transport in vertical devices e.g. bulk heterojunction solar cells is not accessible to further characterization. Therefore we introduce a method to directly measure at the cross sections of organic devices by milling with a focused ion beam (FIB) and adjacent SKPM characterization. By this method we can reveal a spatially resolved potential distribution and therefore identify charge injection and charge transport barriers. In this work, we could correlate microscopic measurement results like the work function difference between the contact materials to macroscopic device characteristics received by J-V measurements and impedance spectroscopy.