

CPP 38: Organic Electronics and Photovoltaics I

Time: Tuesday 9:30–10:45

Location: ZEU 255

CPP 38.1 Tue 9:30 ZEU 255

Exploring the Design Space of Organic Semiconductors — ●CHRISTIAN KUNKEL, JOHANNES T. MARGRAF, KARSTEN REUTER, and HARALD OBERHOFER — Chair for Theoretical Chemistry, Technical University Munich

Improving charge carrier mobilities of organic semiconductors is usually tackled by empirical structural tuning of promising compounds. Computational methods can greatly accelerate such local exploitation of knowledge –namely by exploration–, providing an overview of the problem-specific design space. Here, we intend to provide such an overview for organic semiconductors. In a first approach, we apply data mining strategies to an in-house database of >64.000 organic molecular crystals, annotated with charge-transport descriptors (electronic coupling and the reorganization energy) that are calculated from first principles. Analysing the design space regions in this dataset by a chemical space network hints at already explored or promising regions. From the dataset, we further derive general design principles by evaluating the performance of molecular scaffold and sidegroup clusters of compounds. For these, we find certain scaffolds (sidegroups) to consistently improve charge-transport properties. Functionalizing promising scaffolds with favorable sidegroups then results in molecular crystals with improved charge-transport properties. Secondly, we test algorithms for chemical space exploration, that demonstrate a high efficiency in the detection of useful candidate compounds. Both approaches highlight the usefulness of data-based strategies for a targeted design of organic electronics materials.

CPP 38.2 Tue 9:45 ZEU 255

Thiophene based Semiconductors for Organic Solar Cells — ●ROY SCHAFFRINNA^{1,2}, MARTINA SCHWAGER², JULIAN E. HEGER¹, NIAN LI¹, CALVIN J. BRETT³, MATTHIAS SCHWARTZKOPF⁴, STEPHAN V. ROTH⁴, and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²Hochschule München, Fakultät für Angewandte Naturwissenschaften und Mechatronik, 80335 München — ³Königliche Technische Hochschule, Mechanik-Department, Teknikringen 8, SE-100 44 Stockholm — ⁴Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg

Polythiophene homo- and copolymer derivatives are synthesized by chemical oxidative polymerization and are characterized with optical spectroscopy and grazing-incidence small-angle X-ray scattering (GISAXS). The molecules differ in their inner morphological behavior but also in their optoelectronic properties, which are both designable during polymerization. The organic materials are electrically conductive due to their extended conjugated π -electron system and therefore require neither heavy metals / heavy metal complexes nor dopants for charge transport and can be easily deposited via spin-coating from the liquid phase. The synthesized electron donors are used together with the polymer acceptor PNF222 as active layer in fullerene free full organic solar cells. The devices are fabricated at air conditions, are resistant to illumination and the electrodes require no evaporation of metals from the gas phase.

CPP 38.3 Tue 10:00 ZEU 255

Factors Determining Charge Transfer Energetics for Organic Photovoltaics — SHAHIDUL ALAM^{1,2}, ULRICH S. SCHUBERT^{1,2}, and ●HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), FSU Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), FSU Jena, Germany

Recently, non-fullerene acceptors have received increasing attention for use in polymer-based bulk-heterojunction organic solar cells, as they have demonstrated considerably improved photovoltaic performances over classical polymer-fullerene blends. One part of the success of these materials has been attributed to an increased con-

tribution to the overall absorption of the solar cells, thanks to relatively low bandgaps in these materials. Another part may be related to lower energy or voltage losses through closer adaptation to today's common donor polymers for organic photovoltaics. Since we like to learn more about the general applicability of non-fullerene acceptors as well as about the energy level alignment at the donor-acceptor heterojunction, we studied the latter and consequences thereof for three different donors in conjunction with classical fullerene-derivatives [6,6]-phenyl-C61/C71-butyric acid methyl ester (PCBM/PC70BM) and the exemplari non-fullerene-acceptor 2,2*-[6,6,12,12-Tetrakis(4-hexylphenyl)-6,12-dihydrodithieno[2,3-d:2*,3*-d*]-s-indaceno[1,2-b:5,6-b*]dithiophene-2,8-diyl]bis[methylidyne(3-oxo-1H-indene-2,1(3H)-diylidene)]bis[propanedinitrile] (ITIC). We find that rather specific properties of ITIC control the solar cell performance and limit its general application.

CPP 38.4 Tue 10:15 ZEU 255

Bimodal Electronic Interactions in Molecular-doped Conducting Polymers — ●VANDANA TIWARI^{1,2}, AJAY JHA¹, HONG-GUANG DUAN¹, MICHAEL THORWART³, and R. J. DWAYNE MILLER^{1,4} — ¹MPSD, Hamburg — ²Department of Chemistry, University of Hamburg (UH), Germany — ³I. Institut für Theoretische Physik, UH, Germany — ⁴University of Toronto, Canada

Doping is an extremely important process where intentional insertion of impurities in semiconductors controls their electronic properties. Unraveling the favorable electronic interaction between dopant and polymer is the key to the success of molecular doping in organic semiconductors. Here we use two-dimensional electronic spectroscopy to explore the electronic dynamics of F4TCNQ-doped conducting polymers, P3HT and PBTTT in precursor solution mixtures. The electronic interactions among the ion-pairs formed in precursor solutions are captured in the form of off-diagonal peaks connecting the electronic states of polymer and dopant radicals. This electronic interaction represents a well resolved electrostatically bound state, as opposed to a random distribution of ions. We have theoretically modeled our system to simulate the experimental data and achieve a quantitative picture of the Coulombic interaction between cation and anion radicals in solution. Our study reveals the heterogeneous electronic interactions that possibly serve as a seed for the structures in the spin-cast films. This new insight will help pave the way towards rational tailoring of the electronic interactions to improve doping efficiencies in processed organic semiconductor thin films.

CPP 38.5 Tue 10:30 ZEU 255

Excitation lifetime reduction in ensembles of oligoacene molecules attached to argon clusters — ●MATTHIAS BOHLEN, MORITZ MICHELBAACH, RUPERT MICHIELS, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, D-79104 Freiburg

The energy conversion efficiency of solar cells is generally limited by the Shockley-Queisser limit [1]. One way to circumvent this limit is through the use of organic photovoltaics (OPV), for which specific charge and energy transfer processes can lead to higher conversion efficiencies. Polyaromatic hydrocarbons, such as oligoacene molecules are promising candidates for OPV applications. In addition to that, these molecules exhibit interesting quantum effects, such as singlet fission, triplet-triplet annihilation or superradiance. Recently anthracene, tetracene and pentacene molecules attached to the surface of neon clusters have been shown to provide interesting model systems for detailed studies of such effects [2]. We have extended these measurements by spectroscopy of oligoacenes deposited onto the surface of argon clusters. The results indicate similar processes as observed for neon clusters, but different magnitudes and timescales of the effects.

[1] W. Shockley and H. J. Queisser, *J. Appl. Phys.* 32, 510 (1961)[2] S. Izadnia et al., *J. Phys. Chem. Lett.* 8,2068 (2017)