HL 48: Organic semiconductors II (joint session HL/CPP)

Time: Wednesday 15:00–17:30 Location: POT 112

Invited Talk HL 48.1 Wed 15:00 POT 112

Ultrafast nonadiabatic dynamics and intermolecular conical intersections in organic photovoltaic materials — •Antonietta De Sio — Institut für Physik, Universität Oldenburg

Conjugated polymer and molecular aggregates, used as photoactive materials in organic optoelectronic devices, are large supramolecular assemblies which often present complex energy landscapes and many vibrational degrees of freedom. Coupling of electronic and nuclear motion in molecules may lead to special topologies of potential energy surfaces, such as conical intersections (CoIns). At CoIns, strong vibronic couplings drive ultrafast and efficient nonadiabatic transitions between electronic states and may thus profoundly influence the ultrafast pathways of energy flow and motion of charges. CoIns are of key importance in many photochemical and biological intramolecular processes. So far, however, not much is known about their possible occurrence and relevance for intermolecular excitations in functional condensed-phase assemblies. Here we discuss how ultrafast two-dimensional electronic spectroscopy (2DES) can provide detailed insight into vibronic couplings and nonadiabatic dynamics in technologically relevant organic materials. Specifically, high-time resolution 2DES allows us to experimentally reveal the ultrafast, sub-50-fs passage of a coherent vibrational wavepacket through an intermolecular CoIn in molecular aggregate thin films used in organic photovoltaics. Our results suggest that vibronic couplings and CoIns may help to efficiently steer the energy flow in functional nanostructures, thus opening up new opportunities for controlling transport in organic-based devices.

HL 48.2 Wed 15:30 POT 112

Photoemission Spectroscopy of Organic Charge Transfer Interfaces — •Robert Kuhrt, Martin Hantusch, and Martin Knupfer — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

Understanding physical processes at interfaces involving organic semiconductors plays a key role in optimizing the performance of electronic devices such as solar cells, where absorber and transport layers form interfaces involving metals as well as organic semiconductors. Furthermore, charge transfer between organic molecules might result in interesting properties such as metallic conductivity or correlated electronic states like superconductivity.
In this contribution, we present photoemission spectroscopy studies of various interfaces involving the strong electron acceptor hexafluorotetracyanonaphthoquinodimethane (F6TCNNQ). We compare the electronic properties of organic based donor, acceptor systems. Significant changes are observed in both the core levels and the valence orbitals at the interface, indicating a charge transfer between the materials. Origin and character of the charge transfer as well as the influence of substrate and film structure are discussed.
Acknowledgement: Financial support by the DFG (KN393/25; KN393/26) is gratefully acknowledged.

HL 48.3 Wed 15:45 POT 112

Vacuum processed single crystalline organic semiconductor thin films for high-performance electronic and optoelectronic device applications — •Shu-Jen Wang[1,2], Michael Sawatzski[1], Ilia Lashkov[1], Yulia Krupskaya[2], Hans Kleemann[1], Bernd Büchner[2], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), TU Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research (IFW), Germany

Organic semiconductors enable many technologically important applications such as organic light emitting diodes, solar cells and flexible circuits due to their unique physical properties and chemical structure tunability. Conventional amorphous organic semiconductors show low carrier mobility as their charge transport is limited by their structural order. Therefore, charge transport in organic semiconductors can generally be improved by higher degree of structural order and crystallinity. In this presentation, we will show efficient conversion of vacuum processed amorphous thin films to single crystalline thin films through annealing with appropriate surface treatment. We will also show functional devices such as field-effect transistors and light emitting diodes built on the single crystalline thin films and discuss their potential for high performance circuit and optoelectronics applications.

30 min. break.

HL 48.4 Wed 16:30 POT 112

Coherent Real-Space Charge Transport Across a Donor-Acceptor Interface Mediated by Vibronic Couplings — Ziyao Xu[1], Yi Zhou[1], Lynn Gross[2], Antonietta De Sio[3], ChiYung Yam[4], Thomas Frauenheim[2], GuanHua Chen[1], and •Christoph Lienau[3] — [1]Department of Chemistry, University of Hong Kong — [2]BCCMS, University of Bremen — [3]Institut für Physik, Universität Oldenburg — [4]Beijing Computational Science Research Center

Growing experimental and theoretical evidence suggests that vibronic couplings (VCs), couplings between electronic and nuclear degrees of freedom, play a fundamental role for the ultrafast excited-state dynamics in organic donor-acceptor materials. While VC has been shown to support charge separation at donor-acceptor interfaces, so far, little is known about its role for the real-space transport of charges in these systems. Here we theoretically study charge transport in thiophene-fullerene stacks using time-dependent density functional tight-binding theory combined with Ehrenfest molecular dynamics for open systems. Our results reveal coherent oscillations of the charge density between neighboring donor sites, persisting for ~200 fs and promoting charge transport within the polymer. At the donor-acceptor interface, vibronic wave packets are launched, propagating coherently over distances of >3 nm into the acceptor region. This supports previous experimental observations of long-range ballistic charge motion in organic photovoltaic systems and highlights the possibility of VC engineering as a concept for tailoring the functionality of organic devices

HL 48.5 Wed 16:45 POT 112

Light-assisted charge propagation in organic semiconductor networks on hexagonal boron nitride — Matkovic Aleksandar[1], Genser Jakob[1], •Kratzer Markus[1], Lüftner Daniel[2], Chen Zhongrui[3], Siri Olivier[3], Puschnig Peter[2], Becker Conrad[3], and Teichert Christian[1] — [1]Institute of Physics Montanuniversität Leoben Franz Josef Strasse 18, Leoben 8700, Austria — [2]Institute of Physics Karl-Franzens-Universität Graz NAWI Graz Universitätsplatz 5, Graz 8010, Austria — [3]Aix Marseille University CNRS CINaM UMR 7325 Campus de Luminy 13288, Marseille cedex 09, France

Electrostatic force microscopy is utilized to track charge propagation in organic semiconductor nanoneedles. As model system, crystalline dihydrotetraazaheptacene needles epitaxially grown on ultrathin hexagonal boron nitride was investigated. Due to light exposure, the specific resistivity of the crystallites changed by two orders of magnitude. Exploiting the highly anisotropic optical properties of the organic nanoneedles, selective charge propagation along the crystallites was achieved by matching the incident light's polarization direction with the direction of the molecular backbones in the crystals. Thus, it was possible to guide charge propagation along desired paths in self-assembled crystallite networks. This way, polarized light can be used as a "light gate" to control charge propagation.

HL 48.6 Wed 17:00 POT 112

Electron paramagnetic resonance in OLEDs based on dual-emitting host-guest systems — •Felix Braun[1], Tobias Grünbaum[1], Wolfram Ratzke[1], Sebastian Bange[1], Sigurd Höger[2], and John M. Lupton[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg, Germany — [2]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Straße 1, 53121 Bonn, Germany

OLEDs exhibit strong sensitivity to magnetic fields due to spin-dependent electron-hole recombination. Employing the dual-emitting host-guest system CBP:DB, we can optically assess the spin-permutation symmetry of charge-carrier pairs by their magnetic-field dependent electroluminescence.

We monitor the interconversion between singlet-like and triplet-like populations under electron paramagnetic resonance (EPR) conditions and observe the anticipated anticorrelation in the behaviour of singlet-like and triplet-like carrier pairs. Furthermore, using a deuterated counterpart of the dual-emitting system, we can verify the influence of the hyperfine fields on the linewidth of the EPR signal. We anticipate

that altering the spatial distribution of hyperfine interactions between host and guest will allow us to pinpoint the molecular site on which a charge-carrier pair is formed by analysing the EPR linewidth. With the spin-sensitivity introduced by the dual emitter, we even hope to determine whether, e.g., a singlet-like carrier pair preferentially forms on the guest emitter or on the host matrix.

HL 48.7 Wed 17:15 POT 112

Reverse Dark Current in Organic Photodetectors — •Jonas Kublitski[1], Andreas Hofacker[1], Christina Kaiser[2], Donato Spoltore[1], Hans Kleemann[1], Axel Fischer[1], Koen Vandewal[3], and Karl Leo[1] — [1]IAPP - TU Dresden, Germany — [2]Swansea University, UK — [3]IMO - Hasselt University, Belgium

Photodetectors (PDs) find broad applications in many fields of optics. While inorganic PDs are widely used, they lack in easy processability and narrow-band detection. Organic PDs can fulfill these demands, providing many further advantages in comparison to inorganic PDs. The limiting factor of OPDs is their low detectivity, mostly caused by high dark current (J_D) at reverse bias. Traps and sub-gap states are often observed in organic materials. Here, we investigate their effect on J_D. We observe that J_D follows a trend with the energies of the sub-gap CT states (E_{CT}). Furthermore, in specific donor:C_{60} blends, we find trap concentrations of around 10^{16} cm^{-3} with an energy of around 0.5 eV below the transport level of C_{60}. We intentionally vary the trap concentration in these blends and observe that*J_D scales accordingly. Dark current-voltage simulations show that the expected value of*J_D increases four orders of magnitude and rules the dark JV characteristics, when traps are included. The dependence of J_D on reverse bias can be understood as an enhanced detrapping by means of Poole-Frenkel effect. These results point out to a physical process that might be general in donor:acceptor structures, explaining the high*J_D commonly observed in OPDs. Moreover, optimized devices show J_D as low as 500 pA cm^{-2} at -1 V, and on/off ratio of 10^7.