

CPP 23: Organic Semiconductors (joint session CPP/DS/HL, organized by HL)

Time: Tuesday 9:30–13:15

Location: POT 251

CPP 23.1 Tue 9:30 POT 251

Femtosecond time-resolved spectroscopy of an acceptor-donor-acceptor oligomer film — ●EPHRAIM SOMMER¹, ANTONIETTA DE SIO¹, ELENA MENA-OSTERITZ², PETER BÄUERLE², and CHRISTOPH LIENAU¹ — ¹Institut für Physik, Carl-von-Ossietzky Universität Oldenburg — ²Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Conjugated oligomers are gaining increasing popularity for application in organic solar cells as photoactive materials thanks to their high production reproducibility and device efficiencies [1]. However, a detailed understanding of the initial charge transfer in such systems is missing. Recently, in polymer based active materials it was found that coherent vibronic coupling plays an important role in this process [2]. This raises the question whether this also holds for oligomers. To answer this, we investigate a novel A-D-A-type oligomer by pump-probe and 2D electronic spectroscopy with femtosecond time resolution. Upon selective excitation of the donor unit, we observe strong peak-shifts of the exciton signals as a most dominant feature at early times. Moreover, the signal shows long lived vibrational oscillations. Such a peak shift cannot be explained within a vibronically coupled dimer model including only one dominant vibrational mode like in [2]. Our preliminary results suggest that the photoinduced charge transfer may occur via a conical intersection between the donor and acceptor potential energy surfaces. We will discuss theoretical modelling aimed at validating this idea.

[1] R. Fitzner et al., *Adv. Funct. Mater.*, 12, (2015)[2] A. De Sio et al., *Nat. Commun.*, 7, (2016)

CPP 23.2 Tue 9:45 POT 251

Polariton bottleneck dynamics in organic microcavities — ●FELIX LEMKE, HARTMUT FRÖB, and KARL LEO — IAPP, TU Dresden, Germany

Organic molecules are known to be promising candidates for strong coupling experiments due to their large exciton binding energy. Simultaneously, organic materials reveal large inhomogeneously broadened absorption spectra, complicating the investigation. Even so, small organic molecules have advantages in processing, stability (to ambient conditions and high optical excitation) and lifetime.

In this work we will present a method to investigate the microcavity polariton properties utilizing the oligomer Bu4-Ph4-DIP. We perform angle-resolved streak camera measurements and compare the data with a rate-equation model. Simulation and measurement agree very well. From this, we can see directly the influence of the polariton bottleneck, which proves, that our system is in the strong coupling regime. Moreover, we can extract the characteristic time constants and gain an insight into the polariton dynamics.

CPP 23.3 Tue 10:00 POT 251

Charge-exciton quenching in organic transistors — ●WOUTER KOOPMAN^{1,2}, STEFANO TOFFANIN², and MICHELE MUCCINI² — ¹Universität Potsdam, Potsdam, Deutschland — ²CNR-ISMN, Bologna, Italien

Organic Light-Emitting Transistors (OLETs) possess a huge potential for the design of highly integrated multifunctional optoelectronic systems and intense nanoscale light sources, such as the long-searched-for electrically pumped organic laser. In order to fulfill these promises, the efficiency and brightness of the current state-of-the-art devices have to be increased. The dominating quenching process limiting the external quantum efficiency in OLETs is charge-exciton interaction. A comprehensive understanding of this quenching process is therefore of paramount importance. The present talk reports a systematic investigation of charge-exciton interaction in organic transistors employing time-resolved photoluminescence electro-modulation (PLEM) spectroscopy on the picosecond timescale. The results show that the injected charges reduce the exciton radiative recombination in two ways: (i) charges may prevent the generation of excitons and (ii) charges activate a further non-radiative channel for the exciton decay. Moreover, the transient PLEM measurements clearly reveal that not only trapped charges, as it is already reported in literature, but rather the entire injected charge density contributes to the quenching of the exciton population. Finally, lessons for the design of high-efficiency OLET are discussed.

CPP 23.4 Tue 10:15 POT 251

Investigating the doping efficiency of organic semiconductors by thermoelectric measurements — ●BERNHARD NELL¹, MARKUS KRAMMER², KARIN ZOJER², and KOEN VANDEWAL¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — ²Institute of Solid State Physics, Technische Universität Graz, Graz, Austria

We use thermovoltage (Seebeck effect) and temperature-dependent conductivity measurements on doped organic semiconductors to determine the dominating type of charge carriers introduced by the dopant and to gain insight into the position of the transport level with respect to the Fermi level. The investigation of fullerene dopants with a high degree of fluorination in various amorphous host materials allows us to tune the energy level offset between host and dopant and to study their influence on Fermi level position and overall doping efficiency systematically. Combining thermoelectric measurements with Kinetic Monte Carlo simulations gives further insight into the influence of Coulomb interactions on the trapping of mobile charge carriers in doped organic semiconductors. We find that at low doping concentrations a high amount of charge carriers is immobilized in trap states, leading to a reduced doping efficiency. Upon increasing the doping concentration, the trap states are subsequently passivated and an increased doping efficiency can be observed. Furthermore the doping efficiency is increased upon fluorination of the dopant molecules and we find a correlation between the energy level offset and the doping efficiency, at the same molar concentration.

CPP 23.5 Tue 10:30 POT 251

Vibronic coherence in a reference organic photovoltaic blend — ●ANTONIETTA DE SIO¹, EPHRAIM SOMMER¹, JAMES LIM², SUSANA F. HUELGA², MARTIN B. PLENIO², GIULIO CERULLO³, and CHRISTOPH LIENAU¹ — ¹Institut für Physik, Universität Oldenburg, Germany — ²Institut für Theoretische Physik, Universität Ulm, Germany — ³Department of Physics, Politecnico di Milano, Italy

The microscopic mechanisms underlying charge separation in organic solar cells are still highly debated. Although recent theoretical work [1] suggests that vibronic couplings may lie at the origin of efficient charge generation in such systems, clear experimental evidence on the role of vibronic coherence for charge separation is still lacking. Here we use ultrafast two-dimensional electronic spectroscopy with 10-fs time resolution to investigate the initial dynamics of excitons and polaronic species in P3HT and P3HT:PCBM thin films with different acceptor concentration. Our experimental results, supported by theoretical simulations, show that strong vibronic coupling favors exciton delocalization and accelerates charge separation even in presence of disorder, resulting in long-lived coherent oscillatory dynamics of strongly correlated excitons and polaron pair states, mutually coupled to a dominant vibrational mode. These results allow us to gain fundamental new insights into the initial dynamics of charge separation and may open up new perspectives for optimizing devices [2,3].

[1] Tamura et al, *JCP* 137, 22A540, 2012. [2] Falke et al, *Science* 344, 1001, 2014. [3] De Sio et al, *Nat. Commun.* 2016 in press.

CPP 23.6 Tue 10:45 POT 251

Crystalline Packing Motifs in Pentacene-like Organic Semiconductors — ●MICHAEL KLUES and GREGOR WITTE — Fachbereich Physik, Universität Marburg, Germany

While the impact of chemical modifications on the molecular electronic system can be well computed, the influence on solid state properties is hardly predictable. In fact already slight chemical modifications, like the introduction of heteroatoms or small side groups, often lead to dramatically changed crystal structures and thereby rather different charge carrier mobilities or exciton binding energies. Within a comparative study of various pentacene-like organic semiconductors, based on a Hirshfeld analysis [1] we reveal correlations between molecular properties and packing motives. By choosing molecules with nearly identical geometrical dimensions the complexity of intermolecular interactions is considerably reduced and effects of electrostatic potentials, hydrogen bonds and atom sizes can be carved out. Thereby, we attain a simple rule for predicting the occurrence of herringbone packing motifs and point out the relevance of hydrogen bonds for parallel molecular arrangements as found previously for partially fluorinated

HBC. [2] Furthermore we suggest a route to increase intermolecular orbital overlap by integration of large heteroatoms in the periphery of aromatic systems which yields an improved charge carrier mobility in the case of DNTT.

[1] M.A Spackman; D. Jayatilaka, *CrystEngComm*, 11, 19, (2009)

[2] T. Breuer et al., *Phys. Chem. Chem. Phys.*, (2016), DOI: 10.1039/C6CP06126E

Coffee Break

CPP 23.7 Tue 11:30 POT 251

Strongly reduced inhomogeneous broadening of molecular aggregates in hybrid nanostructure system — ●XUAN TRUNG NGUYEN¹, ANTONIETTA DE SIO¹, JAMES LIM², ALEXANDRA MARKOVIC³, JULIA WITT³, GUNTHER WITTSTOCK³, SUSANA HUELGA², MARTIN PLENIO², and CHRISTOPH LIENAU¹ — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — ²Institut für Theoretische Physik and IQST, Universität Ulm, Germany — ³Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The applications of nanostructures based on organic molecular aggregates range from solar cells to all-optical switching. These aggregates are often modeled as disordered systems that exhibit inhomogeneously broadened absorptive line shapes. In such a system, disorder localizes the exciton wavefunction and leads to limited exciton transport efficiency, which is important in devices like solar cells. By using linear and non-linear spectroscopy, we show that the inhomogeneous broadening of a model J-aggregate cyanine dye is strongly reduced in the presence of an ultrathin gold layer and the resulting optical spectra display almost perfect Lorentzian line shapes. Supported by theoretical simulations, we explain the experimental results in terms of increased delocalization of the exciton wavefunction due to electronic coupling to surface plasmon polaritons supported by the aggregate-gold. This coupling can average out the disorder effect and thus increase the exciton transport efficiency.

CPP 23.8 Tue 11:45 POT 251

The Influence of Molecular Packing on Charge-Transfer States at the Pentacene/Perfluoropentacene Interface — ●ANDRE RINN¹, TOBIAS BREUER¹, JULIA WIEGAND², MICHAEL BECK², JENS HÜBNER², MICHAEL OESTREICH², GREGOR WITTE¹, and SANGAM CHATTERJEE³ — ¹Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renhof 5, D-35032 Marburg, Germany — ²Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — ³Institute of Experimental Physics I, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

We study different model systems of intermixed and layered heterostructures of pentacene and perfluoropentacene by means of time resolved photoluminescence spectroscopy to investigate the impact of molecular packing at the interface on the optical properties. We assign the different PL signals visible in the heterostructures to their respective origin and find an increase in the PL intensity of the charge-transfer signal for pi-stacking at the interface. Significantly slower carrier dynamics are measured for the charge-transfer states when compared to bulk exciton emission which are quenched by singlet exciton fission.

CPP 23.9 Tue 12:00 POT 251

Three-dimensional confinement and exciton-polaritons in open organic microcavities — ●SIMON BETZOLD¹, MARCO DUSEL¹, JÜRGEN OHMER², UTZ FISCHER², CHRISTOF P. DIETRICH¹, and SVEN HÖFLING^{1,3} — ¹Technische Physik, Universität Würzburg — ²Institut für Biochemie, Universität Würzburg — ³SUPA, School of Physics and Astronomy, University of St Andrews

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies making them stable at room temperature, rendering polariton experiments at ambient air conditions possible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Since organic materials are very sensitive to the deposition of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation possible. Open cavities are tunable systems and comprise a bottom semiconductor distributed Bragg reflector (DBR) with the active material (the organic semiconductor) on top and a concave top DBR separated by a micrometer sized air gap. This configuration allows a

3D photonic confinement and brings unprecedentedly high quality factors into reach. Here, we show the versatility of open cavities by performing reflectivity and photoluminescence measurements in Fourier imaging configuration and exemplarily investigate the strong exciton-photon coupling between a fluorescent protein and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex systems like photonic lattices and active regions including 2D monolayer materials or hybrid organic-inorganic bilayers.

CPP 23.10 Tue 12:15 POT 251

Improving lasing properties of a hybrid OLED/microcavity structure — ●STEFAN MEISTER, ROBERT BRÜCKNER, MARKAS SUDZIUS, HARTMUT FRÖB, and KARL LEO — IAPP, TU Dresden, Germany

Organic materials have many advantages which can be utilized in different kinds of devices such as light-emitting diodes, solar cells, or even lasers. Some examples are the spectrally separated broad absorption and emission spectra, the possibility to build very thin and flexible devices, and the fact of having an intrinsic four-energy-level-system.

The goal of realizing an electrically driven organic solid state laser is so far well beyond reach. As a first step, we incorporate an OLED into a microcavity (MC) consisting of two Distributed Bragg Reflectors (DBR). These devices are investigated electrically and with a micro-photoluminescence setup to determine the optical functionality. The optical measurements further allow to compare it to standard organic MCs. These insights are analyzed and addressed with the help of photolithography to improve the quality of the metal layers. Further, different very thin (60nm - 0.15mm) encapsulation methods are tested to allow measurements under ambient conditions.

CPP 23.11 Tue 12:30 POT 251

High temperature stable single carrier hole only devices — ●SHAHIDUL ALAM^{1,2}, PETER FISCHER³, ULRICH S. SCHUBERT^{1,2}, and HARALD HOPPE^{1,2} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena) Friedrich-Schiller-Universität Jena Philosophenweg 7a 07743 Jena, Germany — ²Institute of Organic and Macromolecular Chemistry Friedrich-Schiller-Universität Jena Humboldtstr. 10 07743 Jena, Germany — ³Institut für Werkstofftechnik, TU Ilmenau, Gustav-Kirchhoff-Str. 6, 98693 Ilmenau, Germany

Thin hole transport layers (HTL) are crucial elements in organic semiconductor based devices. Metal oxides are an encouraging material class for this purpose. Metal oxides can be used to modify either of the two contacts in a device for improved wettability as well as chemical and electronic compatibility of the contacts with the organic layer. Several materials like NiO, V2O5, WO3 and MoO3 have demonstrated encouraging prospective for performing as efficient charge transport layers. Among them molybdenum oxide (MoO3) attracted extensive interest due to its superior performance. In order to evaluate charge transport properties of annealed semiconductor films, devices are required to be stable at high annealing temperature. Whereas PEDOT:PSS has generally proper charge injection and extraction properties, these may drastically change upon heating above certain temperature. In this work, we show that a MoO3 interlayer can efficiently substitute PEDOT:PSS as hole transport layer within single carrier hole only devices (SCHD), because of its better stability at high annealing temperature.

CPP 23.12 Tue 12:45 POT 251

Tuning the conductivity in organic-based charge-transfer materials: A combined NEXAFS and electrical transport study — ●ANTONIA MORHERR¹, SEBASTIAN WITT¹, ALISA CHERNENKAYA², KATJA MEDJANIK², GERD SCHÖNHENSE², HARALD O. JESCHKE³, ROSER VALENTI³, and CORNELIUS KRELLNER¹ — ¹Physikalisches Institut, Goethe Universität, 60438 Frankfurt am Main — ²Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz — ³Institut für theoretische Physik, Goethe Universität, 60438 Frankfurt am Main

Single crystals of the novel charge transfer complexes phenanthrene and picene/TCNQ-F_x (x=0,2,4) were grown by physical vapor transport [1] and investigated by electrical transport measurements, near-edge X-ray absorption spectroscopy (NEXAFS) and density functional theory calculations. The electrical conductivity and the mobility of the samples increase with increasing acceptor strength. The activation energy of the complexes was studied by temperature dependent measurements and compared to the electrical band structure investigated by NEXAFS [2]. The results were compared to the DFT calculations for the electrical band structure and simulated NEXAFS spectra.

[1] A. Morherr et al., *Physica B* 496, 98-105 (2016)

[2] A. Chernenkaya et al., J. Chem. Phys. 145, 034702 (2016)

CPP 23.13 Tue 13:00 POT 251

Three-dimensional photonic confinement of imprinted pillars in an organic Tamm-plasmon structure — ●MARCO DUSEL¹, SIMON BETZOLD¹, CHRISTOF P. DIETRICH¹ und SVEN HÖFLING^{1,2} — ¹Technische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg — ²SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK

The fluorescence of organic solids at room temperature is governed by the radiative decay of Frenkel excitons that are characterized by

large exciton binding energies and short Bohr radii compared to inorganic semiconductors. Due to their very large oscillator strength, organic materials further strongly interact with light, in particular in microcavities.

So far, photonic confinement within the cavity plane has mainly been achieved by tailoring the dielectric part of the cavity. Here, we present a novel technology that enables 3D photonic confinement within the active organic layer of a Tamm-plasmon structure (metal-clad cavity) by laterally imprinting pillars. The fabricated pillars have diameters ranging from 7 to 20 μm and heights between 2 and 4 μm . The developed technology enables far more complicated photonic potentials including coupled pillars, chains and lattices.