

CPP 43: Organic Electronics and Photovoltaics V (joint session CPP/HL/O/DS)

Time: Thursday 15:00–18:45

Location: H34

Invited Talk

CPP 43.1 Thu 15:00 H34

Quantum coherence controls the charge separation in a prototypical artificial light harvesting system — ●C. LIENAU¹, S. M. FALKE¹, C. A. ROZZI², N. SPALLANZANI², A. RUBIO², E. MOLINARI², D. BRIDA³, M. MAIURI³, G. CERULLO³, H. SCHRAMM⁴, and J. CHRISTOFFERS⁴ — ¹Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — ²Istituto Nanoscienze - CNR, Centro S3, Modena, Italy — ³IFN-CNR, Dipartimento di Fisica, Politecnico di Milano, Italy — ⁴Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

The efficient conversion of light into electricity or chemical fuels is a fundamental challenge. In artificial photosynthetic and photovoltaic devices this conversion is generally thought to happen on ultrafast time scales in the fs to ps range and to involve an incoherent electron transfer process. In some natural biological systems, however, there is now growing evidence that the coherent motion of electronic wavepackets is an essential primary step, raising questions about the role of quantum coherence in artificial devices. Here we investigate the primary charge transfer process in a supramolecular triad, a prototypical artificial reaction center. Combining high time-resolution femtosecond spectroscopy and time-dependent density functional theory, we provide compelling evidence that the driving mechanism of the photoinduced current generation cycle is a correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We highlight the fundamental role of the interface between chromophore and charge acceptor in triggering the coherent wavelike electron-hole splitting.

CPP 43.2 Thu 15:30 H34

Simulations of Electron Transfer in a Fullerene Hexapyropheophorbide-a Complex — ●THOMAS PLEHN, JÖRG MEGOW, and VOLKHARD MAY — Humboldt-Universität zu Berlin, Germany

Electron transfer (ET) is studied between electronically excited chromophores and a C60 fullerene forming a highly flexible complex, which is dissolved in a solvent. Such investigations are of particular interest with regard to future artificial photosynthetic reaction centers and respective applications in future components of photovoltaic devices. The whole discussion is based on extended MD-simulations. To obtain reliable ET results three differently advanced theories are used. The first treatment uses the classical Marcus theory. Respective Marcus parameters are obtained from literature [1]. A generalized ansatz can be derived by the Landau-Zener theory [2]. Secondly, a semi-classical surface-hopping method [3] is chosen. For this approach the conformation-dependent free-energy surfaces and Marcus parameters are calculated directly from the MD-trajectory. The third approach uses the dispersed-polaron/spin-boson model [3]. This method enables the approximation of a quantum-mechanical harmonic oscillator bath and thus the treatment of nuclear tunneling. A comparative discussion of the outcome of these three methods also in relation to experiment [1] is given finally.

[1] Regehy M. et al., J. Phys. Chem. B 2007, 111, 998

[2] Hlilczar M. et al., J. Photochem. Photobiol. A 2003, 158, 83

[3] Warshel A. et al., Q. Rev. Biophys. 2001, 34, 4, 563

CPP 43.3 Thu 15:45 H34

Highly conductive PEDOT:PSS for flexible structured ITO-free solar cells — ●CLAUDIA M. PALUMBINY¹, CHRISTOPH HELLER¹, ROBERT MEIER¹, GONZALO SANTORO², STEPHAN V. ROTH², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik Department, LS Funktionelle Materialien, James-Franck-Str.1, 85747 Garching, Germany — ²HASYLAB at DESY, Notkestr. 85, 22603 Hamburg, Germany

PEDOT:PSS is widely used as selective intermediate electrode in flexible electronics. The mechanical stability of the electrodes yet play a crucial role and is limited by the instability of the ITO/FTO electrode and the low conductivity of PEDOT:PSS. We investigate a recently developed post treatment method enhancing the conductivity of PEDOT:PSS reaching the order of ITO. For a deeper understanding of the nanomorphology is investigated with surface imaging techniques (AFM, SEM) and the inner morphology and crystallinity is addressed with GISAXS and GIWAXS. The morphological changes are consequently related to the electronically changes. Furthermore, we intro-

duce a novel structuring routine for PEDOT:PSS, plasticizer assisted soft embossing [1]. Being able to control the interface between the transparent electrode and the active material, the device efficiency of OPVs under oblique light can be increased. Combining highly conductive PEDOT:PSS with controlled structuring, these results reveal new paths for flexible structured ITO-free solar cells of enhanced efficiency.

[1] R. Meier, C. Birkenstock, C.M. Palumbiny and P. Müller-Buschbaum, Phys. Chem. Chem. Phys., 14, 15088-15098 (2012)

CPP 43.4 Thu 16:00 H34

Electropolymerized polythiophenes as contact layers in organic solar cells — ●SIDHANT BOM and VEIT WAGNER — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electropolymerized thiophene offers additional advantages to solution processable thiophenes because the doping concentration can be controlled with electrical parameters. The in-situ electrochemical doping provides a handle for the optimization of organic solar cells, either as a bulk polymer in the active layer or as an electron blocking layer. Here in this study, thiophenes are grown electrochemically with a standard three electrode system on Indium Tin Oxide (ITO) contacts. Characterization by UV-Vis measurements reflects the tunable final oxidation state of the thiophene layer. Thin layers are used in diode configuration using metal contacts like Au, Ag, Al and Cu. Static IV measurement allows the characterization of the contact according to Schottky model. Impedance measurements are used to determine the doping level of the layer. The doping level is found to be systematically depending on the applied negative bias during growth at the working ITO electrode with respect to the counter electrode. Applying a negative bias for a short interval at the end of the growth results in highly doped layers which are suitable for contact layers in solar cells.

CPP 43.5 Thu 16:15 H34

Efficient solution processed p-type doping for OLEDs — ●CHRISTIAN TÖPEL, THORSTEN UMBACH, ANDRÉ JOPPICH, JEANETTE BÖCKMANN, ANNE KÖHNEN, and KLAUS MEERHOLZ — University of Cologne, Chemistry Department

Organic light emitting diodes (OLEDs) have drawn much attention in science and industry. Application such as new generation lighting and display devices contribute strongly. However, drawbacks are inefficient charge carrier injection into and low conductivity of the organic materials. A promising solution for this problem is molecular doping which is commonly used in vacuum processed OLEDs, yielding in highly efficient luminescent devices (pin concept). In this case, the molecular doping leads to partial redoxchemical doping. As vacuum deposition is very cost intensive and does not allow high volume processing, researchers focus more and more on solution processing. Here, we present efficient molecular p-type doping using various crosslinkable small-molecule hole transporting materials combined with a range of molecular dopants. Unipolar devices feature an increase in current density by several orders of magnitude compared to the undoped devices at the same voltage. We will also introduce these layers into all-solution-processed multiple-layer OLEDs. These devices are compared with their vacuum-processed counterparts to show the influence of the deposition method and doping ratio on OLED lifetime and device performance.

CPP 43.6 Thu 16:30 H34

Degradation induced decrease of the radiative quantum efficiency in organic light-emitting diodes — ●TOBIAS D. SCHMIDT¹, DANIEL S. SETZ², MICHAEL FLÄMMICH³, BERT J. SCHOLZ¹, ARNDT JAEGER², CAROLA DIEZ², DIRK MICHAELIS³, NORBERT DANZ³, and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²OSRAM Opto Semiconductors GmbH, Leibnizstrasse 4, 93055 Regensburg, Germany — ³Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

The efficiency decrease during electrical operation of organic light-emitting diodes is a crucial issue for both applied and fundamental research. In order to investigate degradation processes, we have performed an efficiency analysis for phosphorescent state-of-the-art devices in the pristine state and after an accelerated aging process at high current density resulting in a luminance drop to less than 60 % of

the initial value. This loss in efficiency can be explained by a decrease of the radiative quantum efficiency of the light-emitting guest/host system from 70 % to 40 %, while other factors determining the efficiency are not affected.

15 min. break

CPP 43.7 Thu 17:00 H34

Enhanced light outcoupling from corrugated top-emitting OLEDs — ●C. FUCHS¹, T. SCHWAB¹, A. ZAKHIDOV^{1,2}, K. LEO¹, M. C. GATHER¹, and R. SCHOLZ¹ — ¹Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden — ²Fraunhofer COMEDD, Maria-Reiche-Str. 2, 01109 Dresden

We analyse the emission spectra of phosphorescent top-emitting OLEDs grown on corrugated substrates. The corrugation is produced using photolithography. Thereby photoresist, spin-coated on a glass substrate is illuminated by an incoherent UV source across a contact mask with periodic structures in the sub- μm range. The optical microcavity of the OLED grown on top is defined by a thick metallic bottom contact, organic layers following the p-i-n concept, a thin metallic top contact, and an organic capping layer maximizing the outcoupling efficiency. Depending on the periodicity of the substrate, Bragg scattered wave guide modes may interfere constructively or destructively with the cavity mode inside the air light cone, hence enhancing or decreasing light emission with respect to a planar microcavity. Thus, the emission pattern deviates strongly from a Lambertian shape, but the angle-integrated external quantum efficiency can be enhanced by up to a factor of about 1.2 with respect to a fully optimized planar reference. Besides a quantitative assignment of sharp features in the emission spectra, an analysis of Bragg scattering for different periodicities can be used for designing a particular angular emission pattern, e.g. very strong forward characteristics.

CPP 43.8 Thu 17:15 H34

Characterization of Gravure Printed Polymer Light-Emitting Electrochemical Cells — ●GERARDO HERNANDEZ-SOSA, RALPH ECKSTEIN, SERPIL TEKOGU, FLORIAN MATHIES, ULI LEMMER, and NORMAN MECHAU — Lichttechnisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Deutschland

In this work we present the fabrication, characterization and ink formulation of gravure printed polymer light-emitting electrochemical cells (LECs). These light emitting devices are fabricated by sandwiching a blend of a semiconducting polymer with a solid polymer electrolyte (SPE) between two electrodes, regardless of their work function. When applying a voltage to the device, the ionic species in the active film will help to form p or n doped layers at the corresponding electrode. Following the injection of carriers, the light emission will come from the semiconductor through the formation and successive recombination of excitons in the intrinsic layer between the p and n doped regions. We correlate the LEC ink formulation to the film quality and device performance. The properties of the formulation are characterized by viscosity and contact angle measurements while the properties of the film are studied by impedance spectroscopy and atomic force microscopy.

CPP 43.9 Thu 17:30 H34

Strongly Fluorescent Copper Complexes for Application in OLEDs Using the Singlet-Harvesting Effect — ●RAFAL CZERWIENIEC and HARTMUT YERSIN — Institut für Physikalische und Theoretische Chemie, Universität Regensburg, D-93040, Germany.

A series of strongly luminescent Cu(I) complexes is presented. The emissions cover a broad spectral range from the blue to the orange. The ambient temperature quantum yields are as high as 90 % and the decay times lie in the order of several microseconds. From a detailed analysis of the photophysical behavior, the ambient temperature emission is assigned to a thermally activated delayed fluorescence (TADF). This is in contrast to the situation at low temperatures, e.g. below 100 K, at which the emission stems from the lowest triplet state decaying as long-lived phosphorescence (order of several hundred microseconds). The observed photophysical properties are related to small energy separations between the S_1 (singlet) and T_1 (triplet) excited states. The results demonstrate the high potential for application of these materials as OLED emitters by exploiting the recently reported singlet harvesting mechanism.

Literature:

1. R. Czerwiec, J. Yu, H. Yersin, *Inorg. Chem.*, 2011, 50, 8293-8301.
2. H. Yersin, A. F. Rausch, R. Czerwiec, T. Hofbeck, T. Fischer, *Coord. Chem. Rev.*, 2011, 255, 2622-2652.

CPP 43.10 Thu 17:45 H34

Insight into the photophysics of photocatalytically active polymeric carbon nitride: an optical quasi-monomer — ●CHRISTOPH MERSCHIANN¹, TOBIAS TYBORSKI^{1,2}, STEVEN ORTHMANN^{1,3}, FLORENT YANG¹, KLAUS SCHWARZBURG¹, MICHAEL LUBLOW^{1,4}, and THOMAS SCHEDEL-NIEDRIG¹ — ¹Helmholtz-Zentrum-Berlin für Materialien und Energie — ²Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, Berlin — ³Technische Universität Berlin — ⁴Leibnitz-Institut für Katalyse, Rostock

A comprehensive investigation of the luminescent properties of photocatalytically active carbon nitride polymers, based on tri-*s*-triazine units, has been conducted for the first time. Steady-state temperature- and excitation-power-dependent as well as time-resolved measurements with near-UV excitation ($\lambda = 325 \text{ nm}$ & 405 nm) yield strong photoluminescence, covering the visible spectrum. The spectral, thermal and temporal features of the photoluminescence can be satisfactorily described by the excitation and radiative recombination of molecular excitons, localized at single tri-*s*-triazine units. The discussed model is in accordance with the recently reported absorption features of carbon nitride polymers. Thus, from the point of view of optical spectroscopy, the material effectively behaves as a monomer rather than a classical semiconductor.

CPP 43.11 Thu 18:00 H34

Polymer semiconductors for electro chemical measurements in biosensing applications — ●MARTIN SCHMID — Helmholtz Zentrum München, Munich, Germany

There is an increasing need in medical diagnosis for reliable fast and simple biosensing devices. Sensors based on organic semiconducting polymers, which are suitable for large-area, low-cost, flexible, and eventually single-use throwaway electronics, provide a unique opportunity in that sense. We report on organic field-effect transistors (OFETs) with regioregular poly(3-hexylthiophene) (P3HT) operable at low-voltages in liquid solutions, suitable for in vitro biosensing applications. Measurements in electrolytes have shown that the performance of the transistors did not deteriorate and they can be directly used as ion-sensitive transducers. Here we show the detection of pH alterations in a wide linear range. With the intention to use the sensors as biosensing devices in biomedical applications, the experiments were performed under physiological conditions and temperature.

CPP 43.12 Thu 18:15 H34

Magneto-resistive Field-Effect Transistors based on Spiro-TAD/Spiro-PFPy Donor/Acceptor-Blends — ●THOMAS REICHERT, CAROLIN ISENBERG, TOBAT SARAGI, and JOSEF SALBECK — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132, Kassel, Germany.

One promising opportunity for the realization of next generation magneto-optoelectronic devices is the use of the electron spin as an additional control parameter. In organic semiconductors the spin states of quasiparticles can be adjusted with low magnetic fields, which leads to large (up to 20% at 10mT) magneto-resistive effects at room temperature. We show that the sign of magneto-resistance (MR) in organic field-effect transistors (OFETs) can be tuned from positive to negative by simply applying illumination. In darkness an external magnetic-field increases the resistance (positive MR) while a magnetic-field induced resistance decrease (negative MR) can be achieved under illumination. The key aspect of this promising effect is the application of co-evaporated Spiro-TAD/Spiro-PFPy blends as the charge transport layers in OFETs. Due to the hole (electron) stabilizing properties of Spiro-TAD (Spiro-PFPy) a mixed donor/acceptor blend is formed, which leads to the observed photo-induced MR sign change. This effect can pave the way to future multifunctional spintronic devices.

CPP 43.13 Thu 18:30 H34

In-wire device: combination of organic semiconductors with electrodes in an individual nanowire — ●CHENGLIANG WANG, HUAPING ZHAO, LIAOYONG WEN, YAN MI, and YONG LEI — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & IMN MacroNano*

(ZIK), Technische Universitaet Ilmenau, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany

One-dimensional wires constituted with kinds of segments attracted much attention due to their potential application in nanogaps obtained from on-wire lithography, plasmonic disk arrays, optimized Raman *hot spots* and heterojunction structures¹. Here, we will talk about the in-wire device, which combined the organic semiconductor and the electrodes in an individual nanowire, based on anodic alumina oxide (AAO) template²⁻³. This kind of nanodevice could be applied in organic diodes, transistors or memories, which attracted extensive at-

tention due to the flexibility, the ease to be functionalized, the colorful and the low cost⁴.

Reference:

- [1] S. J. Hurst, E. K. Payne, L. Qin, C. A. Mirkin, *Angew. Chem. Int. Ed.* 2006, 45, 2672.
- [2] Y. Lei, S. Yang, M. Wu, G. Wilde, *Chem. Soc. Rev.* 2011, 40, 1247.
- [3] Y. Lei, W. Cai, G. Wilde, *Progress in Materials Science* 2007, 52, 465.
- [4] C. Wang, H. Dong, W. Hu, Y. Liu, D. Zhu, *Chem. Rev.* 2012, 112, 2208.