

CPP 76: Organic Electronics and Photovoltaics: Devices (joint session CPP, HL, TT)

Time: Friday 9:30–12:00

Location: C 130

Invited Talk

CPP 76.1 Fri 9:30 C 130

Strong and switchable magnetic couplings in molecular semiconductor films — ●MICHELE SERRI¹, WEI WU^{1,2}, LUKE FLEET¹, CYRUS HIRJIBEHEDIN², NICHOLAS HARRISON¹, CHRIS KAY², ANDREW FISHER², GABRIEL AEPPLI², and SANDRINE HEUTZ¹ — ¹London Centre for Nanotechnology, Imperial College London, UK — ²London Centre for Nanotechnology, University College London, UK

Polyaromatic molecular thin films are well established as alternative semiconductors, but their magnetic properties have received less attention. This presentation will focus on phthalocyanines (Pc), archetypal molecular semiconductors that can ligate spin-bearing transition metals at their centre. They can be processed as thin films and nanowires [1] from the vapour phase and crystallise as a range of polymorphs. This leads to the formation of spin chains, and may give rise to magnetic exchange whose sign and magnitude depends on the nature of the transition metal and crystal structure [2]. A recent milestone was reached by CoPc, which exhibits antiferromagnetic coupling, with an exchange energy reaching 100 K [3]. This interaction is up to two orders of magnitude larger than in other first-row transition metal Pcs and can be obtained on flexible plastic substrates.

[1] Wang et al. ACS Nano 4 (2010) 3921. [2] Heutz et al. Adv. Mater. 19 (2007) 3618. [3] Serri et al. Nat. Commun. 5 (2014) 3079.

15 min. break

CPP 76.2 Fri 10:15 C 130

Effects of Coulomb repulsion on conductance switching in organic molecules — ●IRINA PETRESKA^{1,2} and GERTRUD ZWICKNAGL¹ — ¹Institut für Mathematische Physik, Technische Universität Braunschweig, 38 106 Braunschweig, Germany — ²Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, 1 000 Skopje, Republic of Macedonia

Charge transfer in phenylene ethynylene oligomers (OPEs), using realistically estimated effective model parameters from first principles is studied by a combined, ab initio and model approach. The aim of our work is to investigate the Coulomb correlation effects on conductance switching in OPEs. In the proposed model, molecular electronic system is restricted to one-level coupled to metallic leads, described by a two-site Hubbard Hamiltonian. Comparison of the current-voltage curves, obtained from rate equations, for the planar and perpendicular conformer, clearly demonstrates enhancement of the switching process due to two-particle correlations.

CPP 76.3 Fri 10:30 C 130

Enhanced performance of polymeric electron injection layers for OLEDs by the use of a solvent-additive. — ●SEBASTIAN STOLZ^{1,5}, MARTIN PETZOLDT^{2,5}, NARESH KOTADIYA^{1,5}, ERIC MANKEL^{3,5}, MANUEL HAMBURGER^{2,5}, ULI LEMMER^{1,4}, NORMAN MECHAU^{1,5}, and GERARDO HERNANDEZ-SOSA^{1,5} — ¹Karlsruhe Institute of Technology, Light Technology Institute — ²University of Heidelberg, Institute of Organic Chemistry — ³Technische Universität Darmstadt, Materials Science Institute, Surface Science Division — ⁴Karlsruhe Institute of Technology, Institute of Microstructure Technology — ⁵InnovationLab GmbH, Heidelberg

In this work, we investigate an amino-functionalized polyfluorene as electron injection layer in OLEDs. We demonstrate that its performance can be considerably increased by adding a functionalized alkane to the polyfluorene solution. X-ray photoelectron spectroscopy shows that the polymer thickness decreases with increasing additive concentration which indicates a better packing of the polymers. At the same time, Ultraviolet photoelectron spectroscopy reveals that the cathode work-function decreases with increasing additive concentration. Finally, we solution process OLEDs that use a PPV derivative commonly known as Super-Yellow as emitting layer and the polyfluorene in combination with silver as cathode layer. OLEDs, that use a mixture of functionalized alkane and polyfluorene, exhibit an about 0.8 eV lower turn-on voltage while the maximum luminance is almost doubled compared to OLEDs without additive. Furthermore, operational lifetimes are improved by a factor of two.

CPP 76.4 Fri 10:45 C 130

Modeling of organic semiconductors: from molecular to de-

vice properties — PASCAL KORDT¹, MUSTAPHA AL HELWI^{2,3}, WOLFGANG KOWALSKY³, FALK MAY⁴, ALEXANDER BADINSKI⁵, CHRISTIAN LENNARTZ⁴, and ●DENIS ANDRIENKO¹ — ¹Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — ²BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — ³IHF Institut, Technische Universität Braunschweig, Brunswick, Germany — ⁴BASF SE, GVE/M-B009, 67056 Ludwigshafen, Germany — ⁵BASF SE, GVM/S-B009, 67056 Ludwigshafen, Germany

We review the progress in modeling of charge transport in disordered organic semiconductors on various length-scales, from atomistic to macroscopic. This includes evaluation of charge transfer rates from first principles, parametrization of coarse-grained lattice and off-lattice models, and solving the master and drift-diffusion equations. Special attention is paid to linking the length-scales and improving the efficiency of the methods. All techniques are illustrated on an amorphous organic semiconductor, DPBIC, a hole conductor and electron blocker used in state of the art organic light emitting diodes (OLEDs). The outlined multiscale scheme can be used to predict OLED properties without fitting parameters, starting from chemical structures of compounds.

CPP 76.5 Fri 11:00 C 130

Combined electrical and optical analysis of the efficiency roll-off in phosphorescent organic light-emitting diodes — SEBASTIAN WEHRMEISTER¹, ●TOBIAS D. SCHMIDT¹, LARS JÄGER¹, THOMAS WEHLUS², ANDREAS F. RAUSCH², THILO C. G. REUSCH², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86153 Augsburg — ²OSRAM OLED GmbH, 93049 Regensburg

We present a method for a comprehensive analysis of the efficiency roll-off with current density in phosphorescent organic light-emitting diodes (OLEDs). By combining electrical and optical excitation in time-resolved spectroscopic experiments we are able to measure the excited states lifetime for different driving conditions. It is thus possible to correlate changes of the triplet lifetime with a decrease of the radiative quantum efficiency of the emitting system due to exciton quenching processes. As compared to the conventional analysis of the measured external quantum efficiency (EQE) in dependence of the applied current density, the lifetime analysis is not affected by changes of the charge carrier balance with current, which can have a significant impact on the interpretation of the results. With this method we show that triplet-polaron quenching is the dominating quenching mechanism for the red phosphorescent emitter Ir(MDQ)₂(acac) doped into an α -NPD matrix up to current densities of 100 mA/cm².

CPP 76.6 Fri 11:15 C 130

Influence of Molecular Orientation on the Coupling of Excitons to Surface Plasmons in Semitransparent Inverted Organic Solar Cells — ●MARK GRUBER, MICHAEL MAYR, BJÖRN GALLHEBER, and WOLFGANG BRÜTTING — Institute for Physics, University of Augsburg, Germany

To prove the principle of coupling between surface plasmons (SPs) and excitons, we investigated semi-transparent organic solar cells, in which SPs are excited at interfaces of thin metal films and a dielectric medium by using a Kretschmann configuration setup. Therefore it is essential, that the dielectric medium has a smaller refractive index than glass, e.g. LiF or air.

To compare the SP coupling to different orientations of the transition dipole moment, two donor materials were used, diindenoperylene (DIP) and dibenzo-tetraphenyl-periflanthen (DBP). Both molecules have the transition dipole moment along the long axis. While DIP crystallizes with nearly upright standing molecules on the underlying PCBM film, DBP grows amorphous with predominantly lying molecules.^{1,2} To locate the angular position of the SP resonance the reflectance of the OPVC is measured angle dependent. A simultaneously measured photo current reveals the impact of SPs in these OPVCs. The use of different donors shows, that coupling from SPs to excitons only leads to a positive effect for upright-standing transition dipole moment orientation.

¹ Wagner et al., Adv. Func. Mater. **20**, 4295, 2010.

² Grob et al., Appl. Phys. Lett. **104**, 213304, 2014.

Invited Talk

CPP 76.7 Fri 11:30 C 130

Excitonic phenomena in molecular semiconductors — ●JENS PFLAUM — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ZAE Bayern, 97074 Würzburg

Excitons constitute the primary electron-hole excitation in organic solid states and offer a broad range of photo-physical phenomena. In this talk we will address two key aspects of excitonic states in molecular semiconductors: i) their sensitivity to structural ordering on various length scales and ii) their implementation as recombination sites yielding access to microscopic current characteristics.

In case of i), we will discuss the impact of molecular packing on the exciton motion [1] and how long-range exciton diffusion enables access to boundary-induced trap states that might lead to suppression

of otherwise prominent singlet exciton decay channels [2]. Regarding ii), the non-invasive optical read-out of molecular recombination dynamics will be demonstrated to provide information on the local current density [3]. As a consequence, by utilizing the triplet emission of suited molecules this approach paves the way towards electrically driven single photon sources operating at room temperature [4]. Financial support within the DFG research programme SPP1355 and FOR1809 is acknowledged.

- [1] A. K. Topczak, et al., Phys. Rev. B 89, 201203(R) (2014).
- [2] B. Gieseck, et al., Phys. Rev. B 90, 205305 (2014).
- [3] B. Stender, et al., Adv. Mater. 25, 2943 (2013).
- [4] M. Nothhaft, et al., Nature Comm. 3, 628 (2012).