CPP 2: Electrical, Dielectrical and Optical Properties of Thin Films I

Time: Monday 9:30–11:00 Location: C 230

CPP 2.1 Mon 9:30 C 230

Singlet fission in pentacene blends with tunable charge-transfer interactions — •Katharina Broch[1], Johannes Dieterle[1], Federico Branchi[2], Nicholas Hestand[3], Yoann Olivier[4], Hiroyuki Tamura[5], Chad Cruz[6], Valerie Nichols[6], Alexander Hinderhofer[1], David Beljonne[4], Francis Spano[3], Giulio Cerullo[2], Christopher Bardeen[6], and Frank Schreiber[1] — [1]Universität Tübingen, Tübingen, Germany — [2]Politecnico di Milano, Milano, Italy — [3]Temple University, Philadelphia, Pennsylvania, USA — [4]University of Mons, Mons, Belgium — [5]Tokyo University, Tokyo, Japan — [6]University of California at Riverside, Riverside, USA

Singlet fission (SF), which transforms an excited singlet state into two triplet states, is receiving increasing attention due to its potential to boost organic solar cell efficiencies [1]. While the key role of intermolecular charge transfer in SF has been demonstrated [2], the impact of reduced intermolecular interactions on SF time scales is not yet fully understood. To gain deeper insight, a continuous modification of the interaction strength between the two extremes of isolated chromophores and single crystals would be valuable, but remains challenging. We demonstrate the possibility to modify charge transfer interactions of pentacene, a prototypical SF material [3], in blends with weakly interacting spacer molecules and discuss the impact on SF time constants in these mixed films.

[1] M. Smith and J. Michl, Chem. Rev. 110 (2010), [2] B. Basel et al., Nat. Comm. 8 (2017), [3] M. Wilson et al., JACS 133 (2010).

CPP 2.2 Mon 9:45 C 230

Investigation of Charge Carrier and Electric Field Distribution in OLEDs by Means of Photoluminescent Molecular Probes — •Thomas Ferschke[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

Recently, it has been shown that current densities can be determined on nanometer length scales by means of photoluminescence (PL) studies on single guest dye molecules.[1] Here we transfer this concept to common Alq_3/α-NPD OLEDs by utilizing Tetraphenyldibenzoperiflanthene (DBP) entities as molecular probes. DBP is intentionally embedded as dopant (0.1 v-%) at defined depth within the Alq_3 emissive layer. Upon charge injection a reduction in dopant PL is observed which can be attributed to non-radiative electron - exciton interaction. The macroscopic current density scales related to the PL quenching with the distance from the injecting electrode in qualitative agreement with a SCLC model. The validity of this model and thus, variations in vertical charge carrier distribution are studied as a function of current density. Even at reverse bias condition PL quenching of DBP guest molecules in proximity of 5 nm to the Alq_3/α-NPD interface is observed. This can be attributed to strong localized electric fields at the interface caused by interfacial charges of Alq_3.[2] In addition to quenching measurements a comparative study on the integral interface charging is performed by means of impedance spectroscopy.

[1] Nothaft *et al.*, *ChemPhysChem*, **2011**, 12, 2590–2595

[2] Noguchi *et al.*, *J. Appl. Phys.*, **2012**, 111(11):114508

CPP 2.3 Mon 10:00 C 230

Advanced synthesis of transparent and conductive poly(3,4-ethylenedioxy thiophene) films via vapor-based routes — •Florian Meierhofer[1,2], Laurie Neumann[1,3], Wolfgang Kowalsky[1,3], Hans-Hermann Johannes[1,3], and Tobias Voss[1,2] — [1]Laboratory for Emerging Nanometrology (LENA), TU Braunschweig, Germany — [2]Institute of Semiconductor Technology (IHT), TU Braunschweig, Germany — [3]Institute of High-Frequency Technology (IHF), TU Braunschweig, Germany

Conducting polymers (CP) combine the electrical properties of semiconductors and metals with mechanical flexibility and stretch of insulating polymers, and therefore offer a huge potential for light emitting diodes (LEDs) and photovoltaics (PV). During the past two decades, PEDOT:PSS has become one of the most attractive CPs and is often applied in spin-coated 2D-layers. The coating of more complicated 3D-surfaces, e.g. nanowires/-trenches, however, typically results in an incomplete surface coverage. This issue can be overcome by applying the polymerization directly from the vapor phase. In this work, we use vapor-phase polymerization (VPP) and oxidative chemical vapor deposition (oCVD) for the fabrication of layers of PEDOT and other thiophene derivatives. Aiming for high transparency and electrical conductivity, we systematically screen oxidizing agents and polymerization temperatures. First results for the vapor-synthesized PEDOT demonstrate a transparency of about 90% and 5 S/cm electrical conductivity, which is even superior to PEDOT:PSS as the commercial benchmark.

CPP 2.4 Mon 10:15 C 230

Investigation of the n-type polymer P(NDI2OD-T2) for thermoelectric applications — •Regina Michaela Kluge, Nitin Saxena, and Peter Müller-Buschbaum — TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching

Thermoelectric generators pose a promising approach in renewable energies as they are able to convert waste heat into electricity. In order to build high efficiency devices, suitable thermoelectric materials are needed. Among them, conjugated polymers possess the encouraging ability of easy and various types of scalable solvent processes like roll-to-roll printing. Although they are still less efficient than their inorganic counterparts, their easy synthesis, flexibility and eco-friendliness make them a valuable alternative. However, in order to build a thermoelectric device, both n- and p-type materials are needed. Whereas p-type polymers are frequently studied, n-type polymers have often been neglected in the past which may originate from their sensitivity towards oxygen and moisture. We investigate the air-stable, high-mobility n-type polymer P(NDI2OD-T2) in terms of its optical properties such as its absorbance. Moreover, thermoelectric properties such as the Seebeck coefficient and the electrical conductivity are probed, which allows to determine the power factors of these films.

CPP 2.5 Mon 10:30 C 230

Investigating optical excitations in push-pull molecular J-aggregates by TDDFT first-principles simulations — •Michele Guerrini[1,2], Arrigo Calzolari[2], and Stefano Corni[2,3] — [1]Dept. of Physics, Information and Mathematics , University of Modena and Reggio Emilia, Italy — [2]CNR Nano Modena, Italy — [3]Dept. of Chemical Sciences, University of Padova, Italy

J-aggregates are a class of molecular crystals which show interesting optical properties such as an intense and narrow red-shifted absorption peak (aka J-band) with respect to the monomer units they are composed of. In this work we investigated the electronical optical properties of a J-aggregate molecular crystal made of ordered arrangements of organic push-pull chromophores. By using a TDDFT first-principles approach, we assessed the role of molecular packings in the formation of the enhanced and red-shifted J-band and the major effects of confinement in the optical absorption when moving from bulk to low-dimensional crystal structures. In particular, we simulated the optical absorption of different configurations (i.e. monomer, dimers, extended polymer chain and monolayer sheet) obtained from the bulk crystal. By analyzing the induced charge density associated to the J-band, we concluded that this characteristic peak is mostly associated to a longitudinal excitation that is delocalized along linear chains within the bulk crystal and its red-shift is explained in terms of couplings between transition densities along these chains, as well as changes in single particle excitations, that lowers the total excitation energy.

CPP 2.6 Mon 10:45 C 230

Study on conductive silver nanowire networks in 3D printed polymers — •Lewis Akinsinde[1], Tomke Glier[1], Ferdinand Otto[1], Calvin J. Brett[2,3], Milena Lippmann[3], Stephan V. Roth[3,4], and Michael A. Rübhausen[1] — [1]Institut für Nanostruktur und Festkörperphysik, Universität Hamburg — [2]Department of Fluid Physics, Royal Institute of Technology (KTH), Stockholm, Sweden — [3]Photon Science, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]Royal Institute of Technology (KTH), Stockholm, Sweden

Nowadays, increasing attention has been devoted to transparent conductive films because of their various applications in Solar cells and OLEDs. 3D printing is an alternative promising fabrication process. The embedding of silver nanowires in a UV sensitive polymer matrix enables 3D printable conductive objects. Hence silver nanowires were synthesized via the polyol method resulting in an average diameter of approximately 130 nm and a length up to 100 μm. With optimization through dry etching sheet electrical resistance could be reduced to ca. 1.5 Ω/square. This is highly competitive with existing candidates such as indium tin oxide (ITO). As a next step layer systems consisting of UV cured 1,6-Hexanediol diacrylate (HDDA) and silver nanowires were prepared. The structure and morphology of the silver nanowire incorporated thin films were investigated by scanning electron microscopy (SEM), atomic force microscopy (AFM), conductivity measurements and spectroscopic measurements. Inner film morphology was studied using grazing incidence small-angle X-ray scattering (GISAXS)