

CPP 2: Molecular Electronics - organized by Derck Schlettwein (Justus Liebig University Giessen, Giessen)

Time: Monday 9:00–16:30

Location: CPPa

CPP 2.1 Mon 9:00 CPPa

Organic light-emitting diodes for high-brightness operation: self-heating and switched-back regions — ●ANTON KIRCH¹, AXEL FISCHER¹, MATTHIAS LIERO², JÜRGEN FUHRMANN², ANNEGRET GLITZKY², and SEBASTIAN REINEKE¹ — ¹Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Germany — ²Weierstrass Institute Berlin, Germany

Nonlinear effects typically involve switching phenomena that can lead to abrupt catastrophic device failure. For example, organic light-emitting diodes (OLEDs) suffer from strong electrothermal feedback that arises upon Joule self-heating. The interaction between temperature-dependent conductivity and power dissipation results in a positive feedback loop that finally destroys the device by thermal runaway. The situation becomes more severe for large-area OLEDs where the operation regime can locally differ. Former modeling studies, using a network of thermistors, led to the proposal that a so-called *switched-back* region arises. In this area, the current density, as well as the brightness, decreases although the total device current still increases when running an IV scan.

Here, we experimentally prove the existence of a switched-back region. We demonstrate that its appearance agrees with the simulation that solely uses electrothermal modeling. Our study aims to improve the long-term stability of high brightness OLED lighting tiles e.g. as applied in the automotive sector.

CPP 2.2 Mon 9:20 CPPa

Numerical Modeling of Transient Electroluminescence based on Thermally Activated Delayed Fluorescence — ●JEANNINE GRÜNE, NIKOLAI BUNZMANN, SEBASTIAN WEISSENSEEL, VLADIMIR DYAKONOV, and ANDREAS SPERLICH — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic light emitting diodes (OLEDs) based on thermally activated delayed fluorescence (TADF) show increased efficiencies due to effective upconversion from the non-emissive triplet states to the emissive singlet state via reverse intersystem crossing (RISC). A promising approach in this field are donor:acceptor configurations, whereby an intermolecular exciton is formed at the interface of two molecules, also called exciplex. A proven material combination is among others 4,4',4''-Tris[(3-methylphenyl)phenylamino]triphenylamine (m-MTDATA), as donor and Tris(2,4,6-trimethyl-3-(pyridin-3-yl)phenyl)borane (3TPYMB), as acceptor. The characteristic behaviour especially in transient measurements differs from what is commonly observed in state of the art intramolecular emitters. In order to gain insight into the ongoing processes in exciplex based OLEDs, we performed numerical fits on transient electroluminescence (trEL) measurements at different temperatures. The kinetic model adapted for EL measurements on TADF systems includes second order terms to consider the existing annihilation processes such as triplet-triplet annihilation. Using this procedure, we can quantify the impact of efficiency-enhancing and efficiency-reducing processes as well as the time-dependent excited state populations.

CPP 2.3 Mon 9:40 CPPa

Two-dimensional electronic spectroscopy of phthalocyanine on rare gas clusters — ●ULRICH BANGERT, LUKAS BRUDER, MARCEL BINZ, FRIEDEMANN LANDMESSER, ELENA LEISSLER, DANIEL UHL, and FRANK STIENKEMEIER — Institute of Physics, University of Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg, Germany

With the recent advances of two-dimensional electronic spectroscopy (2DES) towards the gas phase, versatile samples like rare gas cluster beams become accessible [1]. Doping rare gas clusters with multiple molecules yields well defined many body systems. These systems are comparable to highly dilute thin film, however feature weak interaction with the substrate and are cooled down to ≤ 10 K. In previous experiments, such systems provided valuable details about singlet fission and super radiance in acene molecules [2,3]. We now apply for the first time 2DES to this approach and study free-base phthalocyanine in different environments: embedded in superfluid helium nanodroplets, deposited on the surface of neon clusters and as a thermal vapor. We find distinct differences in the photodynamics of the molecular assemblies.

[1] L. Bruder et al., J. Phys. B: At. Mol. Opt. Phys. 52 183501 (2019).

[2] S. Izadnia et al., J. Phys. Chem. Lett. 8, 2068 (2017).

[3] M. Müller et al., Phys. Rev. B 92 (12), 121408 (2015).

CPP 2.4 Mon 10:00 CPPa

Clarifying the orientation mechanism of homoleptic Iridium-carbene complexes — ●MARKUS SCHMID¹, KRISTOFFER HARMS², THOMAS MORGENSTERN¹, ALEXANDER HOFMANN¹, HANS-HERMANN JOHANNES², WOLFGANG KOWALSKY², and WOLFGANG BRÜTTING¹ — ¹Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — ²Institute for high frequency technology, TU Braunschweig, 38106 Braunschweig, Germany

Horizontal orientation of the emitting species is one of the most promising techniques to increase the efficiency of state of the art organic light emitting diodes. Especially metal-organic compounds have attracted great attention. While the alignment has been observed and explained for many heteroleptic Iridium complexes, there has been less progress for their homoleptic counterparts. Only few homoleptic compounds have been reported to show a beneficial morphology in guest-host systems. In this study, we investigated multiple derivatives and isomers of the sky-blue dye tris(N-dibenzofuranyl-N'-methylimidazole)iridium(III) (Ir(dbfmi)₃) doped in the hosts Bis[2-(diphenylphosphino)phenyl]ether oxide (DPEPO) and 3,6-bis(diphenylphosphoryl)-9-phenylcarbazole (PO9). By a combination of optical techniques to probe the transition dipole orientation and electrical measurements to access the permanent dipole moment, we revealed that this homoleptic complex is significantly aligned in both matrices. From our insights into the film morphology we postulate that an anisotropic interaction is responsible for the orientation and even identified the region of the molecule that causes this behavior.

CPP 2.5 Mon 10:20 CPPa

Understanding Ultrafast Proton Transfer in Molecular Crystals — ●HYEIN HWANG^{1,2}, VANDANA TIWARI³, SIMON /F. BITTMANN¹, HONG-GUANG DUAN⁴, FRIEDJOF TELLKAMP¹, AJAY JHA⁵, and R. J. DWAYNE MILLER⁶ — ¹Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — ²Department of Chemistry, University of Hamburg, Germany — ³European XFEL, Hamburg, Germany — ⁴Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — ⁵RFI, Harwell Oxford, United Kingdom — ⁶Department of Chemistry, University of Toronto, Ontario, Canada

Ultrafast proton transfer reaction is a topic of great interest particularly due to their association with the understanding of primary and elementary reaction pathways in functional electrochemical and biological systems. Although this reaction has been extensively investigated in solution for the role of interaction between the solute and the solvent-bath, but the dynamics in single molecular crystals remains elusive. Here, we study ultrafast intramolecular proton transfer reaction in hydroxyanthraquinones in crystalline form, where molecular system forms lattice. We use ultrafast transient absorption studies complemented with quantum chemistry calculations to reveal the role of spatial arrangement of the reactants within the lattice in reaction dynamics. Our work highlight the importance of intermolecular interactions guiding ultrafast dynamics in crystals.

20 min. meet the speakers - break

Invited Talk

CPP 2.6 Mon 11:00 CPPa

Singlet fission in blends of organic semiconductors — ●KATHARINA BROCH¹, CLEMENS ZEISER¹, LUCA MORETTI², CHAD CRUZ³, GIULIO CERULLO², ROEL TEMPELAAR⁴, and CHRISTOPHER BARDEEN³ — ¹Institute for Applied Physics, University of Tübingen, Germany — ²Department of Physics, Polytechnic University of Milan, Italy — ³Department of Chemistry, University of California at Riverside, USA — ⁴Department of Chemistry, Northwestern University, USA

Singlet fission (SF), the photophysical process converting an singlet state into two triplets, is a promising approach to boost solar cell efficiencies [1], and is, due to a triplet-pair state intermediate, also

interesting from the viewpoint of fundamental research. SF rates are controlled by the interplay of intermolecular interactions, energetics and electron-phonon coupling and a controlled modification of these parameters is key to a fundamental understanding of this complex process. Blends of organic semiconductors present an interesting alternative to established methods of chemical functionalization [2,3] and their potential for the study and control of SF pathways will be discussed using two examples of acene blends [3,4].

[1] M. B. Smith, J. Michl, *Annu. Rev. Phys. Chem.* **64** (2013); [2] D. Lubert-Perquel et al., *Nat. Commun.* **9** (2018); [3] K. Broch et al., *Nat. Commun.* **9** (2018); [4] C. Zeiser et al., *Angew. Chem. Int. Ed.* **59** (2020)

CPP 2.7 Mon 11:40 CPPa

Influence of alkyl chain variation on co-crystal formation and molecular charge transfer — ●NADINE RUSSEGER, OLEG VLADIMIROV, ALEXANDER HINDERHOFER, and FRANK SCHREIBER — Institut für Angewandte Physik, Universität Tübingen, Germany

A very important and fundamental process for organic semiconductors is the charge transfer effect between electron donor and electron acceptor molecules in the ground state and in the excited state.

In this work, the charge transfer effect of weakly interacting organic semiconductor mixtures is comprehensively investigated depending on the influence of alkyl chain variation with different acceptor molecules. We choose dinaphtho[2,3-b:2',3'-f]thieno[3,2-b]thiophene (DNFT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different alkyl chain length in the imide position as acceptor molecules (PDIF-CN₂, PDI-C3, PDI-C5, and PDI-C8-CN₂).

For a full structural overview of the resulting molecularly mixed co-crystals, the bulk-heterojunction films were evaluated by surface X-ray scattering. The optical and electronic properties of the intermolecular interactions were characterized by optical absorption, photoluminescence as well as *in-situ* differential reflectance spectroscopy. For the various equimolar mixed systems of DNFT as well as DIP and different perylene-diimide derivatives charge transfer effects were estimated [1].

The results allow us to correlate the structural morphology and the charge transfer effects depending on the chain length and their configuration of the different mixed systems.

[1] V. Belova et al., *J. Am. Chem. Soc.*, **2017**, *139*, 8474-8486.

CPP 2.8 Mon 12:00 CPPa

Anisotropic Charge Transfer Formation at Crystalline Pentacene/Perfluoropentacene Interfaces — ●SEBASTIAN HAMMER¹, CLEMENS ZEISER², KATHARINA BROCH², and JENS PFLAUM^{1,3} — ¹Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — ²Institute for Applied Physics, University of Tübingen, 72076 Tübingen — ³ZAE Bayern, 97074 Würzburg

Strongly bound charge transfer (CT) states critically influence the performance of devices based on donor/acceptor (D/A) heterojunctions such as light emitting diodes or photovoltaic cells. Whereas the excited states in the archetypical CT system Pentacene:Perfluoropentacene (P:PFP) have been vastly studied in thin films [1][2], the role of molecular orientation on CT formation and energetics has not been evaluated to the same extent, so far. Utilizing heteroepitaxial growth of PFP on P (001) single crystals surfaces we were able to prepare long-range ordered D/A heterojunctions in an edge-on molecular configuration as confirmed by XRD. Optical analyses by temperature dependent cw-fluorescence spectroscopy and *in-situ* differential reflectance spectroscopy on the PFP/P interfaces revealed no indication for CT formation in case of edge-on molecular orientation, in contrast to the face-to-face geometry. By means of bilayer as well as heterojunction diode structures we demonstrate that by controlling the molecular orientation at the PFP/P interface, thus, utilizing the anisotropic CT characteristics, the overall performance can be significantly improved.

[1] K. Broch et al., *Phys. Rev. B* **83**, 245307 (2011)

[2] T. Breuer, G. Witte, *J. Chem. Phys.* **21**, 138 (2013)

CPP 2.9 Mon 12:20 CPPa

Ab initio modelling of local interfaces in doped organic semiconductors — ●ANA MARIA VALENCIA, GUERRINI MICHELE, and CATERINA COCCHI — Humboldt-Universität zu Berlin

Despite the intensive efforts in the last decade, a clear and comprehensive understanding of the microscopic properties of doped organic semiconductors is still missing. Due to the complexity of these systems, which notoriously exhibit high level of disorder, also the results from quantum-mechanical ab initio methods are somehow constrained by the choice of the model structures. For a reliable prediction of elec-

tronic and optical properties, it is essential to rationalize the role of local interfaces between interacting donor and acceptor species. We address this problem from hybrid density-functional theory and many-body perturbation theory, investigating the structural, electronic, and optical properties of oligothiophenes doped by F4TCNQ. We consider different structures from isolated dimers and trimers, to periodic stacks and crystalline arrangements. Our results show that, depending on the amount and the nature of the local donor/acceptor interfaces, the choice of the simulated structure critically impacts the resulting electronic structure and degree of charge transfer. On the other hand, the optical spectra appear less sensitive to these characteristics, although a detailed inspection of the electron and hole densities discloses different excitation character depending on the relative donor/acceptor concentration [1] as well as on the donor length [2].

[1] Valencia, Guerrini, Cocchi, submitted (2019).

[2] Valencia & Cocchi, *JPCC* **123**, 9617 (2019).

CPP 2.10 Mon 12:40 CPPa

Impact of electron-phonon-interaction on transport in organic molecular crystals: Naphthalene as a case study — ●KONRAD MERKEL, MICHEL PANHANS, SEBASTIAN HUTSCH, and FRANK ORTMANN — Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden

Understanding charge carrier transport in organic semiconductors is a key requirement for developing advanced electronic and opto-electronic devices such as OLEDs, OFETs and organic solar cells. However the general transport mechanism remains unclear. It is widely believed that electron-phonon-interaction plays an important role, due to the large fluctuations in the electronic coupling associated to the van-der-Waals-bonds between adjacent molecules. The interaction leads to a subtle interplay of scattering and phonon-assisted transport. Within the Kubo formalism, we derive a simulation technique, where we model the low-frequency phonon modes as local and non-local disorder in a tight-binding scheme and where all material parameters are calculated from density functional theory. We study the impact of such modes in naphthalene and compare our results to studies from literature.

60 min. meet the speakers - break

Invited Talk

CPP 2.11 Mon 14:00 CPPa

Small, but highly effective: Functional molecules in polymer devices — ●ULRIKE KRAFT — Max Planck Institute for Polymer Research, Mainz, Germany

The incorporation of small functional molecules such as dopants, plasticisers or molecular switches into polymer films can strongly affect their properties and even induce additional functionalities. Here, two examples will be discussed in which small functional molecules significantly influence the (electronic) properties of polymer devices:

Firstly, intrinsically stretchable interconnects and electrodes are printed from conductive inks consisting of PEDOT:PSS and ionic additives. In this approach, the ionic additives act as dopants and plasticisers and film properties can be tuned by orders of magnitude.

Secondly, the bias stress stability of polymer transistor is significantly improved by the addition of specific functional molecules. While on-state bias stress stability is widely studied, the off-state bias stress is mostly overlooked, even though equally important. We close this gap, focus on the off-state bias stress stability and show that threshold voltage shifts can be remarkably reduced.

CPP 2.12 Mon 14:40 CPPa

Single step production of a self-organized, low work function cathode interlayer from polymer blend solution — ●DOMINIQUE LUNGWITZ¹, KELI FABIANA SEIDEL², ANDREAS OPITZ¹, THOMAS KRÜGER³, JAN BEHREND³, SETH R. MARDER⁴, and NORBERT KOCH^{1,5} — ¹Institut für Physik und IRIS Adlershof, Humboldt Universität zu Berlin, Germany — ²Physics Department, Universidade Tecnológica Federal do Paraná, Brasil — ³Berlin Joint EPR Lab and Institut für Experimentalphysik, Freie Universität Berlin, Germany — ⁴School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics (COPE), Georgia Institute of Technology Atlanta, USA — ⁵Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Using cathode interlayers for reducing the work function of electrodes in organic electronic devices is a widely studied method. Here, we report a simple procedure to obtain a self-organized interlayer on ITO electrodes from a blend solution of P(NDI2OD-T2) and PEI. Reduced

contact resistance and increased polymer conductivity are observed due to vertical phase separation. Fermi level pinning of P(NDI2OD-T2) at PEI covered ITO electrodes leads to the lowest possible electron injection barrier. Furthermore, an increased charge carrier density was measured. Finally, we relate the increase in polymer conductivity to a reduction of interfacial electron trapping and a morphology change. The results show clearly the importance of differentiation between work function reduction upon interfacial layers and conductivity increase upon changes of structural conformation.

CPP 2.13 Mon 15:00 CPPa

Morphological investigations on fullerene-free bulk heterojunction blends for photovoltaic applications — ●SEBASTIAN GROTT¹, LORENZ BIESSMANN¹, NITIN SAXENA¹, WEI CAO¹, SIGRID BERNSTORFF², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS funktionelle Materialien, 85748 Garching — ²Eletra-Sincrotrone Trieste, 34149 Basovizza, Italy

In the last decades, the focus of research has been drawn towards the field of organic electronics due to their advantageous properties, such as versatility, flexibility, low-cost manufacturing processes, as well as their tuneable characteristics, such as solubility and absorption. These properties open up a wide range of applications, especially, in the field of photovoltaics. Hence, organic photovoltaics represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 10% have been reported and thus receive industrial attention for commercialization. We study the inner morphology of a low band gap, fullerene-free bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural information are correlated with current density voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

CPP 2.14 Mon 15:20 CPPa

Fast Processing of Charge Transport Layers in Organic Solar Cells — ●HARALD HOPPE^{1,2}, SHAHIDUL ALAM^{1,2}, AMAN ANAND^{1,2}, AURELIEN SOKENG DJOURMESSI^{1,2}, JOSE PRINCE MADALAIMUTHU^{1,2}, PETER FISCHER⁴, and ULRICH S. SCHUBERT^{1,2,3} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University, Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University, Jena, Germany — ³Jena Center for Soft Matter (JCSM), Friedrich Schiller University, Jena, Germany — ⁴Faculty of Mechanical Engi-

neering, Ilmenau University of Technology, Ilmenau, Germany

Charge transport layers (CTLs) are very important in organic solar cells to allow for an efficient and selective extraction of photogenerated charge carriers. Upon their optimization important photovoltaic parameters such as fill factors are being directly affected, for example since the series resistance and parallel resistance are often improved in combination with each other, when the contact becomes more selective. Unfortunately, CTLs often require an additional and rather intensive annealing process, which will add to the energy investment to such solar cells. In addition, such annealing processes may often either require too high temperatures to be compatible with flexible substrates or may be too time-consuming for fast web speeds. As one solution, we demonstrate the successful application of flash sintering for the annealing of CTLs.

CPP 2.15 Mon 15:40 CPPa

Polarized blue photoluminescence of mesoscopically ordered electrospun non-conjugated polyacrylonitrile nanofibers — XIAOJIAN LIAO¹, ●FRANK-JULIAN KAHLE², BIN LIU^{3,4}, HEINZ BÄSSLER², XINGHONG ZHANG³, SEEMA AGARWAL¹, ANNA KÖHLER², and ANDREAS GREINER¹ — ¹Macromolecular Chemistry II, U Bayreuth, Germany — ²Softmatter Optoelectronics, U Bayreuth, Germany — ³MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Zhejiang University, P. R. China — ⁴School of Energy and Power Engineering, North University of China, China

We demonstrate the fabrication of electrospun fibers from the non-conjugated polymer polyacrylonitrile (PAN) that can be aligned by a simple heat-stretching process. Upon excitation at 340 nm ribbons made from the nanofibres show polarized deep blue luminescence with an anisotropy of 0.37 and a quantum yield of about 0.31. Furthermore, they exhibit room temperature green phosphorescences with a lifetime of about 200 ms as well as a delayed deep blue fluorescence resulting from triplet-triplet annihilation (non-coherent photon upconversion). Wide and small angle X-ray scattering experiments show that the stretched electrospun nanofibers are highly aligned with nearly perfect uniaxial orientation within the fabricated ribbons. This results in mechanical robustness and flexibility, with a high specific tensile strength (534 ± 28) $MPa \cdot cm^3/g$ and toughness (79 ± 7) J/g . The combination of efficient polarized deep blue luminescence, room temperature phosphorescence, TTA, mechanical robustness and flexibility of these fibers opens up new avenues for applications.

30 min. meet the speakers - break