

CPP 10: Organic Electronics and Photovoltaics, Electrical and Optical Properties (joint session CPP/KFM)

Time: Thursday 13:30–16:15

Location: H3

Invited Talk

CPP 10.1 Thu 13:30 H3
Nanophotonic structures by inkjet printing — YIDENEKACHEW J. DONIE¹, QIAOSHUANG ZHANG¹, GUILLAUME GOMARD^{1,2,3}, and •ULI LEMMER^{1,2} — ¹Light Technology Institute, Karlsruhe Institute of Technology (KIT), Germany — ²Institute of Microstructure Technology (KIT), Karlsruhe Institute of Technology, Germany — ³present address: Carl Zeiss AG, Eggenstein-Leopoldshafen, Germany

Inkjet printing (IJP) is a versatile method for additive manufacturing of electronic and optoelectronic devices with a typical spatial resolution on the order of 30 microns. For realizing photonic nanostructures using this approach, the deposited materials have to be controlled on a subwavelength length scale. Here, we demonstrate that this can be realized, both, in vertical and in lateral direction. Using the spontaneous phase-separation of two polymers from a common ink, we realize quasi-periodic and disordered assemblies of light scatterers. The phase separated nanostructures feature sizes that can be tuned from a few microns down to the sub-100 nm level. Applications are in the field of photonic sensors and organic optoelectronic devices. An even more precise control is necessary for realizing one-dimensional photonic crystals (dielectric mirrors) by IJP. Such an approach enables digitally controlled dielectric mirror pixels for various opto-electronic applications.

CPP 10.2 Thu 14:00 H3
On the role of interfaces in controlling the molecular orientation in thin films of polythiophenes — •OLEKSANDR DOLYNCHUK¹, PHILIP SCHMODE², MATTHIAS FISCHER¹, MUKUNDAN THELAKKAT², and THOMAS THURN-ALBRECHT¹ — ¹Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — ²Applied Functional Polymers, University of Bayreuth, Germany

Directed crystallization on a substrate is a superior method for inducing crystal orientation in many ordered materials. Although a preferred face-one molecular orientation was evidenced in monolayers of poly(3-hexylthiophene) (P3HT) on graphite, a full face-one orientation in thicker P3HT films has not been realized so far. By using surface-sensitive GIWAXS, here we show that thin films of P3HT crystallized on graphene exhibit a double-layered face-on and edge-on crystal orientation with the latter formed on the top surface [1]. We assume that it is a result of two competing interfacial orientations initiated at the interfaces to graphene and vacuum. By increasing the side-chain polarity in poly[3-(6-bromohexyl)]thiophene, the influence of the interface to vacuum can be reduced, resulting in full face-on orientation in films with a thickness of up to 26 nm [1]. Our findings evidence that directed crystallization can be used to control the orientation of semicrystalline conjugated polymers in thin films if interactions with both interfaces are properly taken into account.

[1] Dolynchuk et al. *Macromolecules* 2021, 54, 5429-5439.

CPP 10.3 Thu 14:15 H3
Molecular Charge Transfer Effects on Perylene Diimide Acceptor and DNTT / DIP Donor Systems — •NADINE RUSSEGER, 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 and in the excited state.

In this work, we present a comprehensive investigation on co-crystal formation and charge transfer effects in weakly interacting organic semiconductor mixtures. We choose dinaphthothienothiophene (DNTT) and diindenoperylene (DIP) as donor and several perylene-diimide derivatives with different side chains in the imide position as acceptor molecules (PDIF-CN₂, PDIC3 and PDIC8-CN₂).

For a full structural overview of the resulting 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 and photoluminescence. For the various equimolar mixed systems of DNTT as well as DIP and the different perylene-diimide derivatives different charge transfer effects were determined [1].

The results allow us to correlate the structural morphology and the

charge transfer effects depending on the side chains and to evaluate the energy levels of the CT complexes in the different mixed systems.

[1] V. Belova et al., *J. Phys. Chem. C*, **2020**, 124, 11639-22651.

CPP 10.4 Thu 14:30 H3
Dynamics in polymer-fullerene blends for photovoltaic applications and the influence of performance enhancing measures — •DOMINIK M. SCHWAIGER¹, WIEBKE LOHSTROH², and PETER MÜLLER-BUSCHBAUM^{1,2} — ¹Technische Universität München, Physik-Department, Lehrstuhl für Funktionelle Materialien James-Frank-Straße 1, 85748 Garching, Germany — ²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

In organic photovoltaics, donor - acceptor bulk heterojunctions are often used as active layer due to their superior performance compared to e.g. planar structured devices. In this optically active polymer layer, photons are absorbed, excitons are created, subsequently dissipated at a material interface and hence free charges are provided. A promising low-bandgap electron donor material is the conjugated polymer PTB7. Besides a large number of studies on structure and electrical properties, the level of knowledge about dynamics in this system is very limited. We investigated films of PTB7, the fullerene derivate PCBM and different blends of these two, prepared out of chlorobenzene solutions. Quasielastic neutron scattering experiments were done at the cold neutron time of flight spectrometer TOFTOF (MLZ, Garching) to determine hydrogen dynamics on a pico- to nanosecond timescale. In addition, two well established techniques for performance enhancement in organic photovoltaics, namely the addition of DIO to the casting solution and a methanol posttreatment of the active layer, are applied and their influence on the polymer dynamics is investigated.

CPP 10.5 Thu 14:45 H3
Thermally Evaporated Donor Molecules Well-Suited for Low-Voltage Loss Organic Solar Cells — •PASCAL KAIENBURG¹, HELEN BRISTOW², ANNA JUNGBLUTH¹, IRFAN HABIB¹, DAVID BELJONNE³, and MORITZ RIEDE¹ — ¹Clarendon Laboratory, Department of Physics, University of Oxford, UK — ²Department of Chemistry, University of Oxford, UK — ³Laboratory for Chemistry of Novel Materials, University of Mons, Belgium

Novel molecules are key drivers in the development of efficient organic solar cells (OSCs). Device fabrication via solution-casting, mostly of polymer-blends, and thermal evaporation of small molecule blends in vacuum have proven successful. The advent of non-fullerene acceptors (NFAs) in solution processing pushed OSC efficiency by 50%, outpacing the development of vacuum-deposited OSCs.

We take an important first step towards efficient NFA-based evaporated OSCs by demonstrating that donors commonly used in vacuum deposition benefit from being combined with NFAs. We do so by evaporating donors onto solution-cast NFAs and performing in-depth analysis of voltage losses via sensitive EQE and electroluminescence on the resulting bilayer devices. We find that voltage losses of donor/NFA systems are reduced by up to 400mV compared to corresponding donor/C60 systems, without compromising photocurrent.

Together with evaporated OSCs' advantages such as industrial scalability as proven by OLEDs, our findings highlight the technology's potential and stress the need for evaporable non-fullerene acceptors, which - once available - will significantly increase OSC efficiency.

15 min. break

CPP 10.6 Thu 15:15 H3
Cellulose-silver nanoparticle composites for optical applications — CALVIN J. BRETT^{1,2}, BJÖRN FRICKE¹, ALEXANDROS E. ALEXAKIS², TIM LAARMANN^{1,3}, VOLKER KÖRSTGENS⁴, PETER MÜLLER-BUSCHBAUM^{4,5}, DANIEL SÖDERBERG², and •STEPHAN V. ROTH^{1,2} — ¹Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — ²KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — ³The Hamburg Centre for Ultrafast Imaging CUI, 22761 Hamburg, Germany — ⁴Lehrstuhl f. Funktionelle Materialien, Physik-Department, Technische Universität München, 85748 Garching, Germany — ⁵Heinz Maier-Leibnitz Zentrum (MLZ), Technische

Universität Muenchen, 85748 Garching, Germany

Cellulose nanofibrils (CNF) provide biocompatibility and are emerging candidates for functional composites and for templating organic optoelectronics. Here we present a facile fabrication of biocompatible hybrid thin films with tunable optical responses by establishing a thin film composite of silver nitrate precursor and CNF films. Subsequent thermal annealing induces the transformation of the silver nitrate into metallic silver nanoparticles and their CNF-template assisted growth. Correlating nanoparticle morphology and optical spectroscopy, our results show the ability to tailor the electronic band gap of the silver nanoparticles and thus of the hybrid material by adjusting the time scale of the thermal transformation.

[1] Brett et al., ACS Appl. Mater. Interfaces 13, 27696 (2021)

CPP 10.7 Thu 15:30 H3

Tunability of the Circular Dichroism through Photoluminescent Moiré Patterns — ●OLHA AFTENIEVA¹ and TOBIAS A.F. KÖNIG^{1,2} — ¹Leibniz Institute for Polymer Research Dresden e.V. Hohe Straße 6, 01069 Dresden, Germany — ²Center for Advancing Electronics Dresden (cfaed) Technische Universität Dresden 01062 Dresden, Germany

In nanophotonics, there is a current demand for ultrathin, flexible nanostructures that are simultaneously easily tunable, demonstrate a high contrast, and have a strong response in photoluminescent polarization. In this work, the template-assisted self-assembly of water-dispersed colloidal core-shell quantum dots into 1D light-emitting sub-micrometer gratings on a flexible substrate is demonstrated. Combining such structures with a light-absorbing metallic counterpart by simple stacking at various angles results in a tunable Moiré pattern with strong lateral contrast. Furthermore, a combination with an identical emitter-based grating leads to a chiroptical effect with a remarkably high degree of polarization of 0.72. Such a structure demonstrates direct circular polarized photoluminescence, for the first time, without a need for an additional chiral template as an intermediary. The suggested approach allows for reproducible, large-area manufacturing at reasonable costs and is of potential use for chiroptical sensors, photonic circuit applications, or preventing counterfeit.

CPP 10.8 Thu 15:45 H3

Ultrafast Energy Conversion in Organic Photovoltaic Materials: First-principles modelling of the prototypical P3HT-PCBM blend heterojunction — ●ELISA PALACINO-GONZÁLEZ and

THOMAS LA COUR JANSEN — University of Groningen, Faculty of Science and Engineering, Nijenborgh 4, 9747 AG Groningen

One of the reasons behind the low energy conversion efficiency of organic photovoltaic cells has been ascribed to electronic-vibrational dynamics affecting the ultrafast charge separation material upon light absorption. The absence of a comprehensive theoretical description of this process has restrained further advancements in this direction. Here the first step towards this is presented by introducing a first-principles modelling of the key prototype P3HT-PCBM heterojunction system with a realistic description of the blend environment. MD simulations with the GROMOS 53A6 force field are performed to determine structural and dynamical properties of the blend. Representative strongly coupled subsystems of donor-acceptor pairs with a few P3HT-PCBM moieties are selected from the MD structures, with the bright donor state localised on the P3HT molecule and the charge transfer state with a hole on P3HT and the electron on PCBM. Using an electronic basis, the Hamiltonian includes localised excitons and charge transfer states. Excitation energies fluctuating along the MD trajectory are determined using TDDFT and an electrostatic mapping scheme, which are used to define the spectral densities of the system-bath coupling. The resultant molecular Hamiltonian will be used in the quantum dynamical and spectral simulations in the following step.

CPP 10.9 Thu 16:00 H3

Understanding directional charge transfer in a bacterial reaction center: effect of molecular vibrations — ●MARIO MARQUES¹ and LINN LEPPERT^{2,1} — ¹Institute of Physics, University of Bayreuth, Bayreuth 95440, Germany — ²MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

The primary energy conversion reactions of photosynthesis in purple bacteria occur in the reaction center (RC), a complex structure in which photo-active pigments arranged along two pseudo-symmetric branches mediate excitation and charge transfer. Our previous first-principles calculations of optical excitations in the RC of *Rhodospira rubra* indicated that charge transfer occurs along both pigment branches, in contradiction with well-established experimental observations that show charge transfer along only one branch. In this work, we use (time-dependent) density functional theory to investigate the influence of molecular vibrations on the excited states of the main RC pigments of purple bacteria, to unravel their role in the directional charge transfer.