

## CPP 43: Organic Electronics and Photovoltaics III (joint session CPP/HL)

Time: Thursday 9:30–12:30

Location: GÖR 226

CPP 43.1 Thu 9:30 GÖR 226

**Determining exciton diffusion lengths in organic non-fullerene acceptors with Kinetic Monte Carlo Simulation** — ●WENCHAO YANG, SAFAKATH KARUTHEATH, CATHERINE CASTRO, JULIEN GORENFLOT, and FREDERIC LAQUAI — KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Optimal exciton diffusion length ( $L_D$ ) is a key parameter for reducing losses during exciton to charge carrier conversion in organic solar cells (OSC). However, different research groups report contradicting numbers for the same non-fullerene acceptors (NFA) using different lifetimes to calculate  $L_D$ . In this work, in order to verify the measured  $L_D$ 's in NFAs (ITIC, IT4F, ITM and IT2Cl) using transient absorption (TA) spectroscopy, we employed the Kinetic Monte Carlo (KMC) method to simulate the exciton dynamics and calculate the corresponding  $L_D$ . With the assumption of Förster resonant energy transfer type exciton hopping rate in a cubic lattice, the TA decay kinetics under different fluences are reproduced by the KMC simulation, and the only free parameter: the energetic disorder  $\sigma$  is extracted. The use of the lifetime  $\tau$  measured by time-resolved photoluminescence in neat NFA enables to reproduce the transients using more realistic  $\sigma$  values. The  $L_D$ 's in the NFAs are further calculated with the  $\tau$ 's and found to be consistent with the experimental values. This work provides microscopic descriptions of exciton diffusion and more insight into the determination of  $L_D$  in organic semiconductors.

CPP 43.2 Thu 9:45 GÖR 226

**A thorough analysis of conformational locking and related electrical properties in fluorinated thieno-quinoxalines** — ●MD MOIDUL ISLAM<sup>1,2</sup>, ARTHUR MARKUS ANTON<sup>1,2,5</sup>, SHAHIDUL ALAM<sup>6</sup>, RICO MEITZNER<sup>1,2</sup>, CHRISTOS L. CHOCHOS<sup>3,4</sup>, ULRICH S. SCHUBERT<sup>1,2</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany — <sup>2</sup>Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — <sup>3</sup>Institute of Chemical Biology, National Hellenic Research Foundation, Athens 11635, Greece — <sup>4</sup>Advent Technologies SA, Patra, Greece — <sup>5</sup>Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Leipzig, Germany — <sup>6</sup>King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Kingdom of Saudi Arabia

Thieno-quinoxaline derivatives with low band gaps are promising donor materials for organic solar cells. Therefore, investigations have been conducted on thieno-quinoxaline polymers with systematically varied fluorination sites. Cyclic voltammetry revealed that fluorination lowers both the HOMO as well as LUMO energy levels, whereas the size of photochromic units is affected through the particular kind of fluorination demonstrated by UV-Vis absorption spectra. Furthermore, excitation-emission mapping exposed excitation-independent and excitation-selective PL pathways.

CPP 43.3 Thu 10:00 GÖR 226

**Orientation and Order of Molecular Subunits and Excited State Dynamics in a P3HT Bottlebrush Copolymer** — ●ARTHUR MARKUS ANTON<sup>1,2</sup>, FRIEDRICH KREMER<sup>1</sup>, JENNY CLARK<sup>2</sup>, and FRANK CICHOS<sup>1</sup> — <sup>1</sup>Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig, Germany — <sup>2</sup>The University of Sheffield, Department of Physics and Astronomy, Hounsfield Rd, Sheffield S37RH, United Kingdom

Orientation and order at different length scales are believed to play a crucial role for the performance of organic semiconductor devices. Taking advantage of the material properties of *bottlebrush copolymers* and gain control of structure formation, a poly-(3-hexylthiophene) grafted copolymer has been studied [1]. In order to investigate the structure on the molecular scale the technique of *Infrared Transition Moment Orientational Analysis* (IR-TMOA) has been employed [2,3]. The absorbance of structure-related bands is evaluated depending on the inclination of the sample film ( $\theta$ ) and polarization of the IR light ( $\varphi$ ). This combination then allows to determine the tensor of absorption separately for the respective molecular moieties and to deduce their orientation ( $\Theta, \Phi$ ) relative to a sample-fixed coordinate system. In addition

*transient absorption* measurements have been conducted. The dynamics of exciton and polaron formation and decay has been investigated and the derived results on the basis of the bottlebrush copolymer are compared with results from linear P3HT. [1] Heinrich and Thelakkat, *J. Mater. Chem. C* **4** (2016) 5370 [2] Anton et al, *J. Am. Chem. Soc.* **137** (2015), 6434 [3] Anton et al, *Macromolecules* **49** (2016) 1798

CPP 43.4 Thu 10:15 GÖR 226

**Utilizing High Gain and Spectral Narrowing for Near-Infrared Organic Photodetectors** — ●LOUIS CONRAD WINKLER<sup>1</sup>, JONAS KUBLITSKI<sup>2</sup>, JOHANNES BENDUHN<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>TU Dresden, Germany — <sup>2</sup>Federal University of Technology Paraná UTFPR, Curitiba, Brazil

There is a multitude of applications for infrared photodetectors that demand high-volume fabrication, including blood oxygen determination, continued monitoring of food quality, control of industrial processes, and many more. Organic photodetectors (OPDs) have great potential to enrich today's photodetector market with their low-cost fabrication, flexible devices and tunable response. However, most studied organic semiconducting materials have neglectable absorption above 1000 nm. This contribution presents a donor-acceptor blend with a low-energy and broad charge-transfer (CT) feature. To overcome the inherent increase of charge carrier recombination of such low-energy systems, we introduce two photocurrent multiplication (PM) mechanisms. By embedding this OPD into an optical micro-cavity, a spectral response (SR) of 15 AW-1 at 1095 nm is achieved. Furthermore, a very narrow response of only 18 nm makes this architecture ideal for spectroscopic resolved measurements that could be easily integrated into CMOS readout circuitry due to the optimization for operation under reverse bias.

CPP 43.5 Thu 10:30 GÖR 226

**Realizing a high-performance, fully thermal-evaporated, blue narrowband organic photodetector** — ●TIANYI ZHANG, JOHANNES BENDUHN, and KARL LEO — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, Dresden, Germany

Organic photodetector (OPD) boasts of its tunable absorption window, mechanical flexibility, transparency, non-toxicity, facile processing, and cheaper cost. Recent development of high-performing polymers and small molecules further reveals its potential in numerous communication and biomedical applications. To realize visible light communication, commercially available inorganic photodetector usually incorporates additional optical filters, which further increases the complexity and cost of the sensing system. Therein, we demonstrate a blue absorbing organic photodetector with ultrahigh specific detectivity ( $D^*$ ) approaching  $10^{14}$  Jones. By employing a wide bandgap hole transporting layer BF-DPB with Rubrene:C<sub>60</sub> active layer, the absorption peaks at 450nm with an external quantum efficiency (EQE) of 50% at zero bias. The parasitic absorption renders the narrowband characteristic of the blends to span merely over the blue wavelength region. Upon BF-DPB incorporation, ultrafast responses are also observed at sub-microseconds. We conclude that the judicious choice of transporting layer is critical for achieving application-tailored properties, namely high speed or high  $D^*$ . To date, those values are among the best-reported blue OPDs.

CPP 43.6 Thu 10:45 GÖR 226

**Investigation of high performance organic photodetectors based on single component photoactive layer** — ●JAKOB WOLANSKY<sup>1</sup>, CEDRIC HOFFMANN<sup>2</sup>, FELIX TALNACK<sup>3</sup>, MICHEL PANHANS<sup>4</sup>, DONATO SPOLTORÉ<sup>5</sup>, STEFAN C.B. MANNSFELD<sup>3</sup>, FRANK ORTMANN<sup>4</sup>, NATALIE BANERJI<sup>2</sup>, JOHANNES BENDUHN<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>IAPP, TU Dresden — <sup>2</sup>University of Bern — <sup>3</sup>Cfaed, TU Dresden — <sup>4</sup>TU Munich — <sup>5</sup>University of Parma

In organic semiconductor applications such as organic photovoltaics and photodetectors, an intermolecular interface with an energetic gradient between electron donating and accepting materials is usually required for efficiently generating charges. This driving force facilitates the dissociation of the photogenerated excitons. At the same time, this energy offset reduces the maximum possible open-circuit voltage, and the additional interface can act as a recombination site and increases

the dark current. Therefore, single-component devices are extensively researched to overcome these drawbacks.

Here, we report on single-component devices that perform very well as organic photodetectors. By utilizing different device processing parameters and employing different interface layers, we optimized the device characteristics such as external quantum efficiency, dark current, and specific detectivities of more than  $1e13$  Jones. Investigations of the morphology, combined with ultrafast transient absorption measurements, give insight into the charge generation mechanism in our material system.

CPP 43.7 Thu 11:00 GÖR 226

**Reduced defect density in crystalline halide perovskite films via methylamine treatment for the application in photodetectors** — ●EMILIA ROSA SCHÜTZ<sup>1</sup>, AZHAR FAKHARUDDIN<sup>1</sup>, YENAL YALCINKAYA<sup>2,3</sup>, EFRAIN OCHOA-MARTINEZ<sup>4</sup>, SHANTI BIJANI<sup>5</sup>, ABD. RASHID BIN MOHD YUSOFF<sup>6</sup>, MARIA VASILOPOULOU<sup>7</sup>, TOBIAS SEEWALD<sup>1</sup>, ULLRICH STEINER<sup>4</sup>, STEFAN WEBER<sup>2,3</sup>, and LUKAS SCHMIDT-MENDE<sup>1</sup> — <sup>1</sup>University of Konstanz, Konstanz, Germany — <sup>2</sup>Max Planck Institute for Polymer Research, Mainz, Germany — <sup>3</sup>Johannes Gutenberg University Mainz, Mainz, Germany — <sup>4</sup>Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland — <sup>5</sup>Unidad de Nanotecnología, Centro de Supercomputador y Bioinnovación SCBI, Universidad de Málaga, Málaga, Spain — <sup>6</sup>Pohang University of Science and Technology, Pohang, Republic of Korea — <sup>7</sup>National Center for Scientific Research Demokritos, Attica, Greece

The quality of a perovskite layer strongly depends on the processing conditions. Consequently, the fabrication process is often complex, and reproducibility is a challenge. Our methylamine gas-based method is able to recrystallize perovskite layers of any given quality in a controlled way, leading to millimeter-sized domains. Crystallinity significantly increases upon methylamine treatment, and crystal growth follows a preferred orientation. Photoluminescence- and space-charge limited current measurements imply that the trap density decreases after recrystallization. When applied in photodetectors, the improved film quality of the recrystallized films leads to increased detectivities and shorter response times.

### 15 min. break

CPP 43.8 Thu 11:30 GÖR 226

**Reducing Dark Current in Highly Ordered Rubrene:C<sub>60</sub> Heterojunctions for Organic Photodetectors** — ●ANNA-LENA HOFMANN<sup>1</sup>, JAKOB WOLANSKY<sup>1</sup>, LUCY WINKLER<sup>1</sup>, MAX HERZOG<sup>1</sup>, FELIX TALNACK<sup>2</sup>, EVA BITTRICH<sup>3</sup>, JOHANNES BENDUHN<sup>1</sup>, and KARL LEO<sup>1</sup> — <sup>1</sup>IAPP, TU Dresden, Dresden, Germany — <sup>2</sup>Cfaed, Dresden, Germany — <sup>3</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Vacuum-deposited rubrene can form highly ordered phases, demonstrating an exceptionally high charge carrier mobility for holes ( $> 10 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) even in thin films. Depending on the post-treatment of our films, we can control different crystalline phases. For fast-response OPDs, the triclinic phase is very promising since it exhibits high hole mobility in the vertical direction. However, the high surface roughness is a key reason why these devices fall short in specific detectivity. In this work, we employ different strategies to reduce the impact of Ohmic shunts within the device to minimize the noise current of our devices. We characterize the morphology of our films and investigate the performance parameters of fully working devices. Finally, these characteristics are compared to rubrene's other two crystalline phases.

CPP 43.9 Thu 11:45 GÖR 226

**Utilizing charge-transfer states for narrowband and highly sensitive photodetection** — ●JOHANNES BENDUHN, LOUIS CONRAD WINKLER, AWAIS SAWAR, JONAS KUBLITSKI, and KARL LEO — IAPP, TU Dresden, Germany

Near-infrared (NIR) spectroscopic material sensing has the potential to revolutionize many aspects of life, ranging from food control to ma-

terial determination. However, currently available products are either too bulky or too expensive to be used in mobile customer applications. In this regard, organic photodetectors (ODPs) can open new perspectives due their cheap and versatile processing techniques. Nevertheless, the external quantum efficiency (EQE) as well as the specific detectivity of those devices in the NIR wavelength range are still lacking behind. In this contribution, we explore photomultiplication (PM) in fully vacuum deposited OPDs. Broadband devices achieve a maximum EQE of almost 2000% at -10 V. Employing very sensitive measurement techniques as well as optical modelling of our devices, we are able to proof that the photomultiplication can take place even if weakly absorbing charge-transfer states are responsible for the photon harvesting. Employing a suitable donor-acceptor system as well as an optimized device architecture for photomultiplication and constructive interference in the NIR wavelength range, we achieve narrowband OPDs with the spectral response of more than  $10 \text{ A W}^{-1}$  at a wavelength of 1100 nm with full width at half maximum even below 20 nm. These results demonstrate the versatility of OPDs and their potential for spectroscopic material sensing.

CPP 43.10 Thu 12:00 GÖR 226

**Design of Integrated All-Organic Oxygen Sensors** — ●TONI BÄRSCHNEIDER and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), Technische Universität Dresden

Organic electronic devices, such as light-emitting diodes (OLEDs) and photodetectors (OPDs), are ideal for sensor applications because of their versatility and flexibility. Additionally, they can be easily fabricated on any substrate, making integrated sensor applications possible. This allows for easy miniaturization and cheap fabrication. Organic room temperature phosphorescence (RTP) materials are well suited for optical oxygen sensing because of their strong oxygen dependency.

In this work, we developed a monolithic all-organic oxygen sensor composed of a RTP sensing layer, an ultraviolet OLED as an excitation source, and a narrow bandwidth OPD for detection. The RTP sensing layer simultaneously shows fluorescence and phosphorescence at room temperature, which enables self-referencing to avoid photodegradation-caused distortion. Due to the long phosphorescence lifetime, sensing within the ultra-trace range is possible.

The presented sensors overcome drawbacks of current optical oxygen sensors, such as complexity, expensive read-out electronics, and a lack of possible miniaturization.

CPP 43.11 Thu 12:15 GÖR 226

**Atomistic insights on the electrode material CuDEPP** — ●CHRISTOPH JUNG<sup>1,2</sup> and TIMO JACOB<sup>1,2</sup> — <sup>1</sup>Universität Ulm, Institut für Elektrochemie, Ulm, Germany — <sup>2</sup>HIU, Ulm, Germany

Devices for electrical energy storage need to provide high energy yields as well as output power while at the same time guaranteeing safety, low costs and long operation times. The porphyrin CuDEPP [5,15-bis(ethynyl)-10,20-diphenylporphyrinato]copper(II) is a promising electrode material for various battery systems both as anode or cathode. CuDEPP combines the positive properties of lithium ion batteries (high energy density) with those of a supercapacitor (fast electron release and absorption). While its functionality has been demonstrated experimentally, there had been no atomistic information as to why CuDEPP expresses these interesting properties or how the incorporation of ions affects its structure. Starting with the smallest possible unit (i.e. a single molecule) we successively increased the spatial dimensionality of the structure by studying: a) di- and trimers, b) molecular stacking in a 1D chain, c) extending these chains to planar CuDEPP sheets and finally c) a three-dimensional extended polymer structure. Combining the individual results of the molecule, the chain, the plane and the extended polymer lead to a comprehensive and consecutive understanding of the CuDEPP system. Afterwards the insertion (or intercalation) of different ions (including Li, Mg and Na) has been studied. Based on the optimal ion intercalation structure, discharge voltage curves have been calculated and compared to experimental measurements.