

## CPP 18: Organic Electronics and Photovoltaics I

Time: Tuesday 9:30–13:00

Location: H 0110

**Invited Talk**

CPP 18.1 Tue 9:30 H 0110

**Via bottom-up synthesis of nanoobjects and nanocomposites towards brain-inspired electronics** — ●ALEXANDER VAHL — Chair for Multicomponent Materials & Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, Kiel, Germany

The recent rapid developments in artificial intelligence require artificial neural networks with growing complexity, increasingly large training data and steeply rising power consumption bringing contemporary artificial neural networks based on conventional silicon technology to the limits. In contrast, neuron assemblies rely on bottom-up network development in soft matter and continuous stimulus-dependent optimization via dynamic reconfigurations, ultimately achieving an outstanding energy efficiency and robustness. To explore these aspects in brain-inspired electronics, conventional deposition approaches in microtechnology are to be complemented by bottom-up self-organization processes, organic matrices and flexible substrates. This contribution showcases nanoobjects, such as Ag based nanoparticles (NPs) prepared by gas phase synthesis, as interesting building units for brain-inspired electronics on unconventional substrates. Resistive switching is demonstrated for a metal/dielectric nanocomposite with threshold characteristics, directly fabricated onto the apex of conductive AFM cantilevers, as well as for AgAu NPs integrated into sparse, self-organized NP/CNT networks, and also in nanofluids, which are obtained via direct incorporation of Ag NPs into polymer matrices. For highly interconnected NP networks, brain-like avalanches and scale-free switching properties are demonstrated.

CPP 18.2 Tue 10:00 H 0110

**Coordination of tetracyanoquinodimethane-derivatives with tris(pentafluorophenyl)borane provides stronger p-dopants with enhanced stability** — ●ANDREAS OPITZ<sup>1</sup>, AHMED E. MANSOUR<sup>2,1</sup>, ROSS WARREN<sup>1</sup>, DOMINIQUE LUNGWITZ<sup>1</sup>, MICHAEL FORSTER<sup>3</sup>, ULLRICH SCHERF<sup>3</sup>, MORITZ MALISCHEWSKI<sup>4</sup>, and NORBERT KOCH<sup>1,2</sup> — <sup>1</sup>Humboldt-Universität zu Berlin — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — <sup>3</sup>Bergische Universität Wuppertal — <sup>4</sup>Freie Universität Berlin

Strong molecular dopants for organic semiconductors that are stable against diffusion are in demand, to enhance the performance of organic optoelectronic devices. In this study, we demonstrate the coordination of TCNQ-derivatives with four B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub> molecules using a single-step solution mixing process. This results in the formation of bulky dopant complexes, 'F<sub>x</sub>TCN(N)Q-4[B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>]', exhibiting higher oxidation strength than the original materials themselves. [1] Optical and electrical transport measurements with the prototypical P3HT confirm the higher doping efficiency of F<sub>x</sub>TCN(N)Q-4[B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>] compared to F4TCNQ. Additionally, the bulkier structure of F<sub>x</sub>TCN(N)Q-4[B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>] is shown to result in higher stability against drift in P3HT under an applied electric field as compared to F4TCNQ. This simple approach of solution-mixing of readily accessible molecules provides the community with access to enhanced molecular p-dopants.

[1] A.E. Mansour *et al.*, *ACS Appl. Mater. Interfaces* **15** (2023) 46148.

CPP 18.3 Tue 10:15 H 0110

**Curious DC-conductivity in supramolecular organics** — ●HEIKO MAGER<sup>1</sup>, MAXIMILIAN LITTERST<sup>1</sup>, SHYAMKUMAR VADAKKET HARIDAS<sup>2</sup>, MAX VON DELIUS<sup>2</sup>, and MARTIJN KEMERINK<sup>1</sup> — <sup>1</sup>Institute for Molecular Systems Engineering and Advanced Materials, 69120 Heidelberg, University, Heidelberg — <sup>2</sup>Institute of Organic Chemistry, Ulm University, 89081 Ulm

We report the discovery of a surprising DC-conductivity in a group of organic molecules (1) that do not share common properties associated with known organic conductors and semiconductors. The conductivity increases over multiple orders of magnitude when increasing material temperature above room temperature. Increased conductivity at room temperature as well as structural analysis by atomic force microscopy (AFM) and X-ray diffraction (XRD) suggest the supramolecular ordering of the materials under bias application at elevated temperatures plays a crucial role. Long time DC-current measurements allow us to exclude trivial explanations for the observed conductivity, like ionic impurities, electrical double layer formation or degradation. Investigation of multiple molecules with similar structure but key differences in functional groups enables us to find common prerequisites for materials

to exhibit this kind of conductivity. Based on these prerequisites together with references to existing literature we formulate a theoretical framework for a possible conductivity mechanism.

CPP 18.4 Tue 10:30 H 0110

**Langmuir-Blodgett Prepared PMMA Films For All-Solution-Processed Organic Electronics** — ●KIRILL GUBANOV, CHRISTIANE SAUER, FABIAN STRELLER, KATHARINA E. DEHM, RYAN W. CRISP, DUSTIN VIVOD, DIRK ZAHN, and RAINER H. FINK — Department of Chemistry and Pharmacy, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany

A variety of organic materials properties offers opportunities to explore new applications required for the production of sustainable, flexible and low-cost electronic circuitry. Solution-based preparation of high structural quality organic thin films may offer access to such devices. Previously, we reported on successful fabrication of 2-Tridecyl-[1]benzothieno[3,2-b][1]benzothiophene (C13-BTBT) semiconductor crystalline thin films produced via self-assembly at liquid-liquid interface, and microprinted PEDOT:PSS polymer electrodes applied in Organic Field-Effect Transistors (OFETs) for charge-injection or extraction. Here, we report on preparation of Polymethyl methacrylate (PMMA) dielectric films of superior structural quality in the monolayer and multilayer regime by the Langmuir-Blodgett method and their successful application in OFETs. A combined study of NEX-AFS linear dichroism and Molecular-Dynamics simulations revealed a beneficial for charge transport preferential upright standing molecular orientation for vacuum-sublimated C13-BTBT semiconductor monolayer deposited on such PMMA thin films. Combining all preparation steps above, all-solution processed OFETs can be fabricated. Research is funded by the BMBF (contract 05K19WE2) and SolTech initiative.

CPP 18.5 Tue 10:45 H 0110

**Asymmetry of Charge Carrier Properties: Effects on Performance of p- and n-channel Organic Field-Effect Transistors** — ●YURI RADIEV<sup>1</sup>, TOBIAS WOLLANDT<sup>2</sup>, HAGEN KLAUK<sup>2</sup>, and GREGOR WITTE<sup>1</sup> — <sup>1</sup>Philipps-Universität Marburg, Renthof 7, 35037 Marburg, Germany — <sup>2</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany

To leverage the full potential of the electronics based on organic field-effect transistors (OFETs), both p- and n-channel devices of similar performance are required [1]. While p-type organic semiconductors (OSCs) have been long known, environmentally stable OSCs for high-performance n-type OFETs have been synthesized only recently [2]. The analysis of such OFETs revealed that the asymmetry of the charge carrier properties limited the use of n-channel devices: large injection barriers and high susceptibility to trap states significantly reduced the device performance. The contact resistance in particular has been gaining more attention recently, since with high charge carrier mobilities the limiting factor for high-frequency device applications becomes the charge carrier injection at the OSC-electrode interface. In this work we compare various p- and n-channel OFET device structures (based on pentacene, DNTT and PhC<sub>2</sub>-BQQDI, respectively) to demonstrate the effects of the charge carrier properties asymmetry on the device performance and to discuss the ways to alleviate them [3].

[1] Klauk, H., *et al.*, *Nature* **2007**, 445 (7129), 745-748.

[2] Okamoto, T., *et al.*, *Science Advances* **2020**, 6 (18), eaaz0632.

[3] Radiev, Y., *et al.*, *Organic Electronics* **2021**, 89, 106030.

CPP 18.6 Tue 11:00 H 0110

**Doping gradients optimize the thermoelectric power factor of a conjugated polymer** — ●DOROTHEA SCHEUNEMANN<sup>1</sup>, JIAN LIU<sup>2,3</sup>, MARIAVITTORIA CRAIGHERO<sup>3</sup>, VANDNA GUPTA<sup>3</sup>, SRI HARISH KUMAR PALETI<sup>3</sup>, EMMY JÄRSVALL<sup>3</sup>, YOUNGSEOK KIM<sup>3</sup>, KAI XU<sup>4</sup>, JUAN SEBASTIÁN REPARAZ<sup>4</sup>, L. JAN ANTON KOSTER<sup>5</sup>, MARIANO CAMPOY-QUILES<sup>4</sup>, MARTIJN KEMERINK<sup>1</sup>, ANNA MARTINELLI<sup>3</sup>, and CHRISTIAN MÜLLER<sup>3</sup> — <sup>1</sup>Heidelberg University, Germany — <sup>2</sup>Chinese Academy of Sciences, China — <sup>3</sup>Chalmers University of Technology, Sweden — <sup>4</sup>Materials Science Institute of Barcelona, Spain — <sup>5</sup>University of Groningen, The Netherlands

Functionally graded materials (FGMs) that feature continuous changes in doping level have been considered as a tool to improve the overall thermoelectric performance of inorganic semiconductors. For organic

semiconductors this method has been little used so far. However, since the conductivity  $\sigma$  and the thermopower  $\alpha$  vary strongly with the doping level, it can be assumed that a doping gradient also influences the power factor  $\alpha^2\sigma$ . Here, we show that even moderate electric fields can generate lateral doping gradients in polymer films doped with F4TCNQ, with suitable gradients achieving up to 8-fold enhancement in power factor. Kinetic Monte Carlo simulations enabled us to understand under which conditions a doping gradient can result in an increase in power factor. Our findings indicate that the FGM concept is (i) a way to improve the thermoelectric performance of not yet optimally doped organic semiconductors, (ii) facilitates the screening of different polymer:dopant pairs as a thermoelectric material.

### 15 min. break

CPP 18.7 Tue 11:30 H 0110

**Influence and Control of Spontaneous Orientation Polarization in Binary Organic Semiconductor Mixtures** — ●ALEXANDER HOFMANN, ALBIN CAKAJ, PATRICK BUNK, PRAKHAR SAHAY, JOHANNES DWORSCHAK, and WOLFGANG BRÜTTING — Experimental Physics IV, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Spontaneous orientation polarization (SOP) of polar organic molecules is the driving force for the buildup of a giant surface potential (GSP). It has been shown that in organic light emitting diodes (OLEDs) the GSP inside various layers of the device can have positive or negative effects on the overall device performance. Additionally, the introduction of a GSP to former nonpolar layers is possible using the concept of dipolar doping, which has successfully been applied to enhance device performance [1]. To address the effect of polar layers in more detail, the exact properties of dipolar doped layers as well as the underlying physics of SOP in mixtures have to be understood. We investigate prototypical material combinations to gain insight on the orientation mechanisms governing SOP in those mixtures. Understanding the design rules behind dipolar doping will eventually allow the concept to be applied to organic electronic devices other than OLEDs as well.

[1] Noguchi et al., *Adv. Optical Mater.* 2022, 10, 2201278; DOI: 10.1002/adom.202201278

CPP 18.8 Tue 11:45 H 0110

**Charge-carrier photogeneration in single-component organic semiconductors via low excitation power triplet-triplet annihilation** — ●ANDREAS SPERLICH<sup>1</sup>, ANDREI STANKEVYCH<sup>2</sup>, RISHABH SAXENA<sup>2</sup>, JEANNINE GRÜNE<sup>1,3</sup>, STAVROS ATHANASOPOULOS<sup>4</sup>, PRAKHAR SAHAY<sup>5</sup>, WOLFGANG BRÜTTING<sup>5</sup>, VLADIMIR DYAKONOV<sup>1</sup>, HEINZ BÄSSLER<sup>6</sup>, ANNA KÖHLER<sup>2,6</sup>, and ANDREY KADASHCHUK<sup>2</sup> — <sup>1</sup>Experimental Physics 6, University of Würzburg, 97074 Würzburg — <sup>2</sup>Soft Matter Optoelectronics and Bavarian Polymer Institute, University of Bayreuth, 95448 Bayreuth — <sup>3</sup>Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — <sup>4</sup>Departamento de Física, Universidad Carlos III de Madrid, 28911 Madrid, Spain — <sup>5</sup>Institute of Physics, University of Augsburg, 86159 Augsburg — <sup>6</sup>Bayreuth Institute of Macromolecular Research, University of Bayreuth, 95448 Bayreuth

We investigate the carbazole-based material mCBP-CN, a typical host for TADF OLEDs. Our findings challenge established beliefs by demonstrating efficient charge-carrier generation near the absorption edge. Light-induced ESR and luminescence studies at low temperatures unveil slow carrier accumulation and recombination, indicating shallow trapping. Persistent signals in both techniques suggest a common origin. Photocurrent measurements support bimolecular charge generation, emphasizing the role of triplet-triplet annihilation in creating charge pairs. This work highlights unconventional mechanisms in organic semiconductors, relevant beyond OLEDs, but also for long-persistent luminescence, organic photovoltaics, and photocatalysis.

CPP 18.9 Tue 12:00 H 0110

**Comparison of electron affinities in organic semiconductors measured by cyclic voltammetry, conventional inverse photoelectron spectroscopy, and low-energy inverse photoelectron spectroscopy** — ●MIHIRO KUBO<sup>1</sup> and HIROYUKI YOSHIDA<sup>1,2</sup> — <sup>1</sup>Chiba University, Chiba, Japan — <sup>2</sup>Chiba University MCRC, Chiba, Japan

The electron affinity (A) of an organic semiconductor is an essential energy parameter representing the electron transport level. Although A in solid can be determined by inverse photoelectron spectroscopy

(IPES), A is often estimated from the reduction potential ( $E_{red}$ ) measured in solution by cyclic voltammetry. However, because previous IPES data have errors of about 0.3-0.5 eV due to sample damage and low energy resolution, the correlation between  $E_{red}$  and A is uncertain. With the development of low-energy inverse photoelectron spectroscopy (LEIPS)<sup>[1]</sup>, the precision of A better than 0.1 eV became possible. In this work, we establish a new correlation using LEIPS data  $A=(1.24\pm 0.07)*eE_{red}+(5.06\pm 0.15)$  eV<sup>[2]</sup>. In practice, the slope of the correlation is almost similar and A values calculated from this work and previous work differ by less than 0.2 eV over the whole range, although the accuracy of each A should be much higher in LEIPS. Therefore, we further discuss the relationship between the A determined by conventional IPES and LEIPS in terms of energy resolution, sample damage, and vacuum level determination. [1] H. Yoshida, *Chem. Phys. Lett.*, 539-540, 180 (2012); [2] M. Kubo, H. Yoshida, *Org. Electron.*, 108, 106551 (2022).

CPP 18.10 Tue 12:15 H 0110

**Tuning programmable luminescent tags by phosphorescent emitter design** — ●ULIANA TSIKO, HEIDI THOMAS, SEBASTIAN SCHELLHAMMER, and SEBASTIAN REINEKE — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

Purely organic materials with pronounced room temperature phosphorescence (RTP) offer extended emission lifetimes as well as solution processability, mechanical flexibility, and low ecological footprint. These characteristics have led to the development of programmable luminescent tags (PLTs), which allow minimalistic and powerful reusable information storage and labeling [1,2]. To extend the applicability of this technology, emitters with improved RTP efficiency covering a wide spectral range are required.

In our contribution, we present the synthesis as well as the spectroscopic and theoretical analysis of a set of donor-acceptor-donor (D-A-D) materials. Thianthrene as donor unit is combined with nitrogen-containing heterocycles with systematically increasing accepting character. The materials cover a wide range of properties from pronounced fluorescence without RTP to relatively efficient RTP emission but almost no fluorescence. Based on the latter compound, improved PLTs are designed and characterized. Our results provide further insights on structure-property-relationships of RTP emitters strengthening their rational design.

[1] Gmelch et al. *Sci. Adv.* (2019).

[2] Gmelch et al. *Adv. Sci.* (2021).

CPP 18.11 Tue 12:30 H 0110

**On the decisive influence of surface energy on crystal orientation in films of polythiophenes** — ●OLEKSANDR DOLYNCHUK<sup>1</sup>, ROBERT KAHL<sup>1</sup>, FLORIAN MEICHSNER<sup>2</sup>, ALEXANDER MUCH<sup>1</sup>, MUKUNDAN THELAKKAT<sup>2</sup>, and THOMAS THURN-ALBRECHT<sup>1</sup> — <sup>1</sup>Experimental Polymer Physics, Martin Luther University Halle-Wittenberg, Germany — <sup>2</sup>Applied Functional Polymers, University of Bayreuth, Germany

Semiconducting polymers are an appealing class of functional materials with diverse applications in electronics. Understanding and controlling the crystal orientation in semiconducting polymers is critical to optimizing their efficiency and has long been a major challenge. Using substituted polythiophenes as model semiconducting polymers, it is shown that interfacial interactions at the substrate and vacuum interfaces determine the crystal orientation formed in films of polythiophenes during crystallization from the melt. Namely, we gradually increase the surface energies of the edge-on crystals formed at the vacuum interface by attaching various polar groups at the end of the polymer side chains. As a result, a uniform face-on crystal orientation induced by graphene is achieved in films of the polythiophene with the most polar end group as thick as 200 nm. The face-on crystal orientation is formed in the modified polythiophenes crystallized even on the amorphous surfaces, but by a different growth mechanism. Furthermore, we show that the crystal orientation can be switched in the same sample depending on the crystallization conditions if the competition of interfacial interactions at both interfaces is present.

CPP 18.12 Tue 12:45 H 0110

**Systematic search for novel organic ferroelectric materials** — ●MAXIMILIAN LITTERST<sup>1</sup>, MANJUNATH BALAGOPALAN<sup>2</sup>, RAMON JANNASCH<sup>1</sup>, ELIN DYPVIK SØDAHL<sup>2</sup>, OLA NILSEN<sup>2</sup>, CARL HENRIK GØRBITZ<sup>2</sup>, KRISTIAN BERLAND<sup>2</sup> and MARTIJN KEMERINK<sup>1</sup> — <sup>1</sup>IMSEAM, Heidelberg University — <sup>2</sup>Department of Chemistry, Nor-

wegian University of Life Science, Oslo

Piezo- and ferroelectric materials are forming a multi-billion-dollar market due to their wide applications as actuators, ultrasound generators, mechanical sensors and small-scale energy generators. The market is currently dominated by inorganic materials, which show excellent performance but their application, especially in biological environments, is limited by drawbacks like toxicity, rigidity and acoustic impedance mismatch. Organic ferroelectrics could overcome these limitations. However, the currently most used material PVDF has other limitations including a high coercive field.

Building on previous theoretical work to systematically identify new candidates for ferroelectric materials[1], we employed a combination of experimental techniques to search for signatures of ferroelectricity in these materials. Specifically, we used dielectric relaxation spectroscopy, double wave measurements and CV- measurements. Here, we present an overview over the results of this approach, where several of the investigated materials show clear indications of ferroelectric behavior, highlighting the validity of the approach. At the same time, other materials show intriguing, but so far inconclusive behavior.

[1] arXiv:2306.07138 [cond-mat.mtrl-sci]