

## CPP 31: Organic Electronics and Photovoltaics II

Time: Wednesday 15:00–17:45

Location: H 0110

CPP 31.1 Wed 15:00 H 0110

**N-type charge transfer complex in DBTTF:HATCN mixtures** — •HONGWON KIM<sup>1</sup>, ANDREAS OPITZ<sup>2</sup>, MARIE SIEGERT<sup>3</sup>, LENNART FROHLOFF<sup>2</sup>, JENS PFLAUM<sup>3</sup>, and WOLFGANG BRÜTTING<sup>1</sup> — <sup>1</sup>Experimental Physics IV, Institute of Physics, University of Augsburg, Germany — <sup>2</sup>Supramolecular System, Institute of Physics, Humboldt University of Berlin, Germany — <sup>3</sup>Experimental Physics VI, University of Würzburg, Germany

Mixtures of the electron donor DBTTF and the acceptor HATCN form a charge transfer complex (CTC), which leads to the appearance of new optical absorption bands below the band gap of the two pristine materials and a significant enhancement of the electrical conductivity. We prepared thin films by co-evaporation through systematic variation of their mixing ratio from pure DBTTF to pure HATCN and measured the temperature-dependent conductivity as well as charge carrier concentration and mobility. Surprisingly, we found n-type behavior for all compositions, except pure DBTTF. This can be understood from the electronic structure of the mixtures through ultraviolet photoelectron spectroscopy (UPS), which conclusively indicate that charge injection and transport occurs via the lowest unoccupied molecular orbital (LUMO) of the CTC. Furthermore, insight into the rich behavior of the electrical conductivity can be gained from morphological studies using Atomic Force Microscopy (AFM).

CPP 31.2 Wed 15:15 H 0110

**Effective Electron-Vibration Coupling Constants by Ab Initio Methods** — •MAXIMILIAN FRANZ-XAVER DORFNER and FRANK ORTMANN — TUM School of Natural Sciences, Technische Universität München, 85748 Garching b. München, Germany

This contribution is concerned with the analysis of different levels of theory for calculating the linear electron-phonon coupling constants. To bridge between density functional theory (DFT) and higher-level many-body approaches, we make use of the quasi-particle picture. Within this framework, we derive an effective quasi-particle linear coupling Hamiltonian, which describes the interaction of quasi-particles with phonons. We use this description to establish an approximate connection between the coupling constants calculated with DFT and higher-level many-body approaches by identifying the Kohn-Sham potential as an approximation to the static part of the self-energy. We determine the conditions under which a pragmatic DFT approach yields, in principle, the same coupling constants as a numerically much more expensive many-body approach. To test the theory, we finally compare the respective coupling constants for a few small molecules. The numerical results are found to be in good agreement with the presented theory.

CPP 31.3 Wed 15:30 H 0110

**Organic photomultipliers working as reservoir** — •KLARA HÄNISCH, HANS KLEEMANN, JOHANNES BENDUHN, and KARL LEO — TU Dresden, Dresden, Deutschland

Reservoir Computing (RC) is a well-known and often-used tool for classification, time prediction or recognition tasks. But software-based computing always has the disadvantage of a high power consumption, latency and the need to digitalize input data. How tempting is therefore the idea of reservoir computing directly implemented in hardware with a low power supply consumption and analogous data handling. Hardware-based RC is a promising concept for direct processing of analog inputs with drastically reduced training effort compared to conventional machine learning techniques. In this work we explore the application of organic photomultipliers as non-linear nodes for hardware-based RC. In particular, we investigate the origin of the nonlinearity, its wavelength-, and frequency-dependent response and discuss possible implication scenarios for reservoir computing. Furthermore, we show that the strength of the nonlinear coupling is connected to the external quantum efficiency of the cell, which opens up the possibility to discriminate selected spectral ranges.

CPP 31.4 Wed 15:45 H 0110

**Understanding the Mechanism of Giant Surface Potential (GSP) in Evaporated Organic Thin Films: A Molecular Dynamics Simulation Approach** — •MUHAMMAD NAWAZ QAISRANI<sup>1</sup>, NAOMI KINARET<sup>1</sup>, FELIX POST<sup>1</sup>, FALK MAY<sup>2</sup>, and DENIS

ANDRIENKO<sup>1</sup> — <sup>1</sup>Max Plank Institute for Polymer Research, Mainz, Germany — <sup>2</sup>Merck Electronics KGaA, Darmstadt, Germany

The emergence of the Giant Surface Potential (GSP) in evaporated organic thin films has gained considerable attention in recent years. However, the molecular mechanism underlying the spontaneous orientation of the net dipole moment that gives rise to GSP remains poorly understood. In this work, we employed coarse-grained molecular dynamics simulations to replicate vacuum deposition experiments and generate the morphology of evaporated thin films consisting of organic semiconductor materials. The simulated morphologies predicted well the orientation of molecular dipoles within the film, yielding the correct sign of the GSP. Notably, our simulation protocol incorporated electrostatic interactions in a coarse-grained model, which was crucial in accurately predicting the sign of experimental GSP. Our findings provide valuable insights into the molecular structure of these thin film materials and their applications in organic electronic devices.

CPP 31.5 Wed 16:00 H 0110

**A novel organic ferroelectric with two parallel sublattices?** — •RAMON JANNASCH<sup>1</sup>, MAXIMILIAN LITTERST<sup>1</sup>, MANJUNATH BALAGOPALAN<sup>2</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, Heidelberg — <sup>2</sup>Department of Chemistry, Norwegian University of Life Science, Oslo

Ferro- and piezoelectric materials find common usage in a range of electronic devices. Although inorganic materials so far dominate the field, they come with significant drawbacks, including energy-intensive production, reliance on toxic and/or rare elements and a lack of mechanical flexibility. Organic ferroelectric may offer a solution to some or even all of these problems.

Here, we investigate the organic material hexamethylenetetramine hydrogen DL-malate through various measurements aimed at assessing its ferroelectric behavior. Combining dielectric relaxation spectroscopy (DRS), capacitance-voltage (CV)-measurements and polarization hysteresis measurements using the double wave method (DWM), we obtain a comprehensive understanding of its ferroelectric properties. The observation of singularities in DRS, a butterfly loop in the CV-measurement, and a saturating switchable polarization during DWM collectively indicate bona fide ferroelectricity. At the same time, we find indications for the presence of two ferroelectric sublattices with different coercive fields but parallel alignment in the ground state.

**15 min. break**

CPP 31.6 Wed 16:30 H 0110

**Charge transfer states do not like cold charges** — •TOBIAS KREBS, CLEMENS GÖHLER, and MARTIJN KEMERINK — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University

The power conversion efficiency of organic solar cells still lags behind their inorganic counterparts. Especially the open circuit voltage (Voc) losses are currently hard to reduce without knowing their exact origins. As different loss mechanisms have distinct temperature and light intensity dependencies, looking at Voc not only at room temperature and 1 sun illumination but also at lower and higher temperatures as well as at lower light intensities to pinpoint the dominant loss channel is imperative. We develop a new analytical rate-equation model based on previous work by Koster et al. [1], which allows us to distinguish different loss channels and incorporates the specific, far-from-equilibrium charge carrier dynamics in organics. For our PM6:Y6 solar cells, the model fits the experimental data over the range of applied temperatures down to 90K and light intensities as low as 1e-6 suns. Our results further suggest that the voltage losses at low light intensities and temperatures are mostly due to charges being stuck in the interfacial charge transfer state. Additionally, we benchmark the model against kinetic Monte Carlo simulations and find good agreement of Voc as well as recombination and escape yields.

[1] \*Quantifying Bimolecular Recombination Losses in Organic Bulk Heterojunction Solar Cells\*, Koster et al. *Advanced Materials* 23, 1670\*1674 (2011).

CPP 31.7 Wed 16:45 H 0110

**Identify the losses occurring in all-polymer solar cells**

— ●SHAHIDUL ALAM<sup>1</sup>, WEJDAN ALTHOBAITI<sup>1</sup>, SAFAKATH KARUTHEATH<sup>1,2</sup>, NING SU<sup>3</sup>, CHRISTOPHER E. PETOUKHOFF<sup>1</sup>, JOSÉ P. JURADO<sup>1</sup>, OLEKSANDR MATIASH<sup>1</sup>, AMR DAHMAN<sup>1</sup>, KHAWLA ALKHEZAIM<sup>1</sup>, VLADIMIR DYAKONOV<sup>4</sup>, ANDREAS SPERLICH<sup>4</sup>, VOJTECH NÁDAZDY<sup>5</sup>, TOBIN J. MARKS<sup>3</sup>, ANTONIO FACCHETTI<sup>3</sup>, and FRÉDÉRIC LAQUAI<sup>1</sup> — <sup>1</sup>KAUST, Kingdom of Saudi Arabia — <sup>2</sup>Tsinghua University, Shenzhen, China — <sup>3</sup>Northwestern University, USA — <sup>4</sup>University of Würzburg, Germany — <sup>5</sup>Slovak Academy of Sciences, Slovak Republic

For unknown reasons, small molecule non-fullerene acceptor-based bulk heterojunction OSCs are ahead of all-polymer solar cells. Here, blends of the donor polymers PCE12 and PM6 with two acceptor polymers, PYN-BDT and PYN-BDTF, are used to study PCE-limiting processes in solar cells. The  $\pi$ -extended naphthalene rings in these compounds make them macromolecular absorbers with large optical cross-sections up to 900 nm. Combining steady-state optical spectroscopy, TRPL, TA, ESR, and TDCF experiments provides a concise and quantitative assessment of losses due to limited photon absorption, geminate and non-geminate recombination (NGR), field-dependent charge generation, and inefficient carrier extraction. Pulsed-laser spectroscopy kinetic parameters reproduce experimentally measured device IV characteristics and show that low FFs are caused by NGR competing with charge extraction or a strong field dependence of charge generation, depending on the acceptor polymer.

CPP 31.8 Wed 17:00 H 0110

**Loss mechanisms in low-bandgap organic solar cells**

— ●GUORUI HE<sup>1</sup>, ATUL SHUKLA<sup>1</sup>, YONGLIN CAO<sup>2,6</sup>, YUFEI GONG<sup>3</sup>, NURLAN TOKMOLDIN<sup>2</sup>, BOWEN SUN<sup>1</sup>, DREW RILEY<sup>4</sup>, MOHAMMAD SHADABROO<sup>2</sup>, JULIAN STEELE<sup>5</sup>, ARDALAN ARMIN<sup>4</sup>, LEI MENG<sup>3</sup>, YONGFANG LI<sup>3</sup>, SAFA SHOAEE<sup>2</sup>, DIETER NEHER<sup>1</sup>, and FELIX LANG<sup>1</sup> — <sup>1</sup>Soft Matter Physics and Optoelectronics, University of Potsdam, Germany — <sup>2</sup>Disordered Semiconductor Optoelectronics, University of Potsdam, Germany — <sup>3</sup>Chinese Academy of Sciences, China — <sup>4</sup>Swansea University, United Kingdom — <sup>5</sup>The University of Queensland, Australia — <sup>6</sup>South China University of Technology, China

We investigate and compare the loss mechanisms of low-bandgap OSCs based on the blend of the donor polymer PTB7-Th with two different NFAs BTPV-4F-eC9 and BTPV-4Cl-eC9, with a bandgap of 1.24 eV and 1.26 eV, respectively. Both NFAs exhibit the same conjugated core, except that in BTPV-4Cl-eC9, the four terminal fluorine atoms are replaced by four chlorines.

To understand how the change of the terminal groups is affecting the device performance, we investigate the various recombination processes of the two systems. The results show that the PTB7-Th:BTPV-4Cl-eC9 blend suffers from stronger bimolecular recombination and geminate recombination. In addition, EMPL reveals a significant voltage loss in both blends. Temperature-dependent SCLC measurements show a rather low electron mobility in PTB7-Th:BTPV-4Cl-eC9 system, which we relate to a larger disorder of the LUMO.

CPP 31.9 Wed 17:15 H 0110

**Enhanced air stability with solid additive EH-P in PBDB-TF-T1:BTP-4F-12 solar cells**

— ●ZERUI LI<sup>1</sup>, SERGEI VAGIN<sup>2</sup>, KUN SUN<sup>1</sup>, XIONGZHUO JIANG<sup>1</sup>, RENJUN GUO<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>3</sup>, STEPHAN V. ROTH<sup>3,4</sup>, BERNHARD RIEGER<sup>2</sup>, and PETER MÜLLER-BUSCHBAUM<sup>1,5</sup> — <sup>1</sup>TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — <sup>2</sup>TUM School of Natural Sciences, Wacker Chair of Macromolecular Chemistry, 85748 Garching, Germany — <sup>3</sup>DESY, 22607 Hamburg, Germany — <sup>4</sup>KTH Royal Institute of Technology, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — <sup>5</sup>MLZ, TUM, 85748 Garching, Germany

Additive plays an important role in organic solar cells. Traditional additives are most liquid, such as DIO, CN, DPE. Nowadays solid additives have called more research interest due to their various advantages in morphology-directing abilities, post treatment, enhanced device performance and stability. We explored an effective solid additive EH-P in green-solvent based organic solar cells (PBDB-TF-T1:BTP-4F-12). Greatly increased device performance and stability were achieved with EH-P doping. In-situ GIWAXS and GISAXS were used to observe the evolution of micro-structure and crystallinity during the degradation process in air under illumination. The stability increase mainly comes from morphology modification rather than photo-oxidation, which was proved with charge mobility measurement and UV-vis spectrum.

CPP 31.10 Wed 17:30 H 0110

**What makes thickness-tolerant organic solar cells?**

— XABIER RODRÍGUEZ-MARTÍNEZ<sup>1</sup>, ●CONSTANTIN TORMANN<sup>2</sup>, MARTA SANZ<sup>3,4</sup>, BERNHARD DÖRLING<sup>3</sup>, MARTÍ GIBERT-ROCA<sup>3</sup>, ALBERT HARILLO-BAÑOS<sup>3</sup>, ENRIQUE PASCUAL-SAN-JOSÉ<sup>3</sup>, JOSÉ PIERS JURADO<sup>3</sup>, LAURA LÓPEZ-MIR<sup>4</sup>, MARTIJN KEMERINK<sup>2</sup>, and MARIANO CAMPOY-QUILES<sup>3</sup> — <sup>1</sup>Institute for Physical Chemistry, Heidelberg University, Germany — <sup>2</sup>Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany — <sup>3</sup>Instituto de Ciencia de Materiales de Barcelona, Bellaterra, Spain — <sup>4</sup>EURECAT, Centre Tecnològic de Catalunya, Barcelona, Spain

Thick-film organic photovoltaics (>200 nm) are desirable to spark commercialization through mass-printing methods. Thickness resilient materials are, however, scarce and not fully understood. In this work, 17 different donor:acceptor blends are screened in terms of photoactive layer (PAL) thickness to build a consistent database of 649 inverted devices. The experimental results can be categorized into two main blend families: one being resilient against increased PAL thickness whereas short-circuit current (JSC), fill factor (FF) and power conversion efficiency (PCE) decrease in the second family. Our kinetic Monte Carlo (kMC) simulations show how the blend morphology alone is able to explain the trends of both blend families without tweaking of recombination parameters (cf. drift-diffusion). The kMC simulations further predict the open-circuit voltage (VOC) to be uncorrelated to the PAL thickness which agrees with the experimentally observed trends for VOC in both blend families.