

## CPP 36: Organic Electronics and Photovoltaics II (joint session CPP/HL)

Time: Wednesday 15:00–17:30

Location: GÖR 226

CPP 36.1 Wed 15:00 GÖR 226

**Charge-carrier dynamics across seven orders of magnitude in double-cable polymer-based single-component organic solar cells** — ●YAKUN HE<sup>1,2</sup>, BINGZHE WANG<sup>1</sup>, LARRY LUEER<sup>1</sup>, DIRK GULDI<sup>1</sup>, NING LI<sup>1</sup>, and CHRISTOPH BRABEC<sup>1</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — <sup>2</sup>KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Single-component organic solar cells (SCOSCs) with intrinsically high stability have witnessed efficiencies from 2-3% to 6-11%. For boosting higher efficiencies of SCOSCs, essential information of charge-carrier dynamics as a function of microstructure is highly demanded, requesting systematical investigation on photophysics. In this work, for the first time, the charge-carrier dynamics of a representative double-cable polymer, which achieves efficiencies of over 6% as an active layer in SCOSCs, is investigated across seven orders of magnitude in time scale, from fs-ps TAS and ps-ns TRPL for probing charge generation to ns-us TAS for charge recombination. Specific emphasis is placed on understanding the impact of thermal post-treatment on the charge dissociation, transport, and recombination dynamics. By increasing the thermal annealing temperature, geminate recombination is reduced accompanied by more efficient charge dissociation and suppressed bimolecular recombination. Annealing the photoactive layer at 230 °C results in the highest photovoltaic performance correlating well with the findings from transient studies. This work intends to present a complete picture of the charge-carrier dynamics in SCOSCs.

CPP 36.2 Wed 15:15 GÖR 226

**What determines the Recombination Order in Organic Solar Cells?** — ●KATHRIN BROCKER, JANA SEILER, DOROTHEA SCHEUNEMANN, CLEMENS GÖHLER, and MARTIJN KEMERINK — Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University

Organic Solar Cells provide an interesting and low-cost alternative to conventional inorganic photovoltaics. Upon illumination, excitons are created that separate into free electrons and holes at the donor-acceptor-interface and can be extracted to deliver electricity. The opposing loss mechanism is the recombination of charge carriers, which happens in the bulk both prior to and after charge separation. To understand these processes, the recombination order is crucially important. Experimentally, orders around or above 2 are typically found. Surprisingly, kinetic Monte Carlo (kMC) simulations that otherwise accurately reproduce experimental observations, yield values closer to 1. Here, we investigate the factors that might lead to higher recombination orders. Apart from the influence of morphology and contacts, special focus is laid on the effect of charge carrier delocalisation, which is shown to facilitate charge carrier separation and increase the fraction of bimolecular recombination. Simulation results are compared to experimental data obtained via the Steady State Bias Assisted Charge Extraction (BACE) method on P3HT:PCBM and PM6:Y6 solar cells.

CPP 36.3 Wed 15:30 GÖR 226

**Modeling of the photoluminescence of geminate pairs using a hopping based Monte Carlo simulation** — ●MAIK SCHWUCHOW, ANGELA THRÄNHARDT, CARSTEN DEIBEL, and SIBYLLE GEMMING — TU Chemnitz, Institut für Physik, 09126 Chemnitz, Deutschland

The investigation of the transport and recombination characteristics of optically excited charge carriers in organic materials is an on-going research topic. Studying the underlying effects is crucial for understanding and improving practical applications, e.g. organic solar cells (OSCs). A main step in the process of free charge carrier generation in OSCs is the formation of geminate pairs, so called charge transfer complexes, consisting of spatially separated, Coulomb-bound charges. The radiative recombination of geminate pairs yields a photoluminescence (PL) decay  $\propto t^{-3/2}$  ( $t$  is time) on long time scales which arises due to a combination of thermally activated diffusion and attractive Coulomb interaction. While a continuous drift-diffusion model is able to theoretically explain this experimentally observed decay, weak molecular interaction and disorder are known to cause charge carrier localization. Therefore, a hopping model, based on tunneling between localized states, is usually more appropriate to describe charge transport in organic materials. We simulate the diffusion and recombination of

hopping charge carriers using the Monte Carlo method and investigate the influence of different parameters, e.g. temperature and energetic disorder, on the PL data and the asymptotic slope.

CPP 36.4 Wed 15:45 GÖR 226

**Time-consistent hopping, transient localization, and polarons - new insights and approaches for carrier transport in organic crystals** — SEBASTIAN HUTSCH, MICHEL PANHANS, and ●FRANK ORTMANN — Technische Universität München, Germany

Charge transport in organic semiconductors is affected by the complex interplay of electronic degrees of freedom and molecular vibrations. This is further complicated due to the rich vibrational spectrum of these materials with mode energies covering two orders of magnitude. If the electronic coupling between molecules is small, hopping approaches are a popular choice to model charge transport for which we have recently derived a time-consistent hopping theory. [1]

Similarly, for high-mobility materials a recent improvement has been realized based on a mode-specific treatment of molecular vibrations. This leads to an unprecedented level of accuracy for the prediction of the carrier mobility for a large number of systems. [2] I will finally discuss physically motivated predictors with a very good correlation to the mobility and low computational costs.

[1] S. Hutsch, M. Panhans and F. Ortmann, Phys. Rev. B. 104, 054306 (2021).

[2] S. Hutsch, M. Panhans and F. Ortmann, npj Comput. Mater. 8, 228 (2022).

CPP 36.5 Wed 16:00 GÖR 226

**Analysis of industrial viability for single-component organic solar cells** — ●YAKUN HE<sup>1,2</sup>, NING LI<sup>1</sup>, THOMAS HEUMÜLLER<sup>1</sup>, JONAS WORTMANN<sup>1</sup>, and CHRISTOPH BRABEC<sup>1</sup> — <sup>1</sup>Friedrich-Alexander-Universität Erlangen-Nürnberg, Martensstrasse 7, 91058 Erlangen, Germany — <sup>2</sup>KAUST Solar Center, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Despite approaching 20% efficiency, organic solar cells still lag behind for industrial application. The industrial figure of merit (i-FOM) of OSCs is analyzed, including PCE, photostability, and synthetic complexity (SC) index. Single-component organic solar cells (SCOSCs) employing materials with donor and acceptor moieties chemically bonded within one molecule or polymer exhibit intrinsically high morphological stability. SCOSCs exhibit overall much higher i-FOM values than the corresponding bulk heterojunction OSCs, and the highest value reaches 0.3, which is even higher than the famous PM6:Y6, even though the PCE (8%) is only half of PM6:Y6. Synthetic complexity of SCOSCs is slightly higher than that of the corresponding BHJ OSCs due to extra synthetic step for connecting donor and acceptor moieties. This feature however overcomes the large-scale phase separation and stability issue. SCOSCs based on dyad 1 exhibit surprisingly high photostability under concentrated light (7.5 suns and 30 suns), corresponding to almost unchanged device stability up to 10,000 hours under 1-sun illumination. For realizing industrial application, SCOSCs have to achieve higher efficiencies, while BHJ should be developed with less complicated synthesis.

**15 min. break**

CPP 36.6 Wed 16:30 GÖR 226

**Temperature-induced morphology changes at the organic-metal interface: effects on the structure, electronic and thermoelectric performance** — ●BENEDIKT SOCHOR<sup>1</sup>, YUSUF BULUT<sup>1,2</sup>, MARIE BETKER<sup>1,3</sup>, ANNA LENA OECHSLE<sup>2</sup>, SIMON SCHRAAD<sup>1,4</sup>, CHRISTOPHER R. EVERETT<sup>2</sup>, CONSTANTIN HARDER<sup>1,2</sup>, TZU-YEN HUANG<sup>5,6</sup>, ANTON LE BRUN<sup>5</sup>, TIM LAARMANN<sup>1,4</sup>, PETER MÜLLER-BUSCHBAUM<sup>2,7</sup>, and STEPHAN V. ROTH<sup>1,3</sup> — <sup>1</sup>Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — <sup>2</sup>TUM School of Natural Sciences, Chair for Functional Materials, James-Franck-Str. 1, 85748 Garching, Germany — <sup>3</sup>KTH Royal Institute of Technology, Teknikringen 56-58, 100 44 Stockholm, Sweden — <sup>4</sup>University Hamburg, Department of Physics, Notkestr. 85, 22607 Hamburg, Germany — <sup>5</sup>ANSTO, New Illawarra Road, Lucas Heights, NSW 2234, Australia — <sup>6</sup>NSRRRC, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu 30076, Taiwan — <sup>7</sup>MLZ, TUM, Lichtenbergstr. 1,

85748 Garching, Germany

Flexible organic electronics are one of the most sought-after devices in the field of photovoltaics, sensors, or smart wearables. Here, the structure of the organic-metal interface and its modification potential are of utmost interest for future large-scale production. This study focuses on two semiconducting Poly(3-hexylthiophene-2,5-diyl) diblock variants, whose sprayed and doped thin films show excellent potential as thermoelectric generators. Using AFM, ellipsometry, *in situ* GISAXS/GIWAXS, and NR measurements, the structural changes of the polymer-gold interfaces were tracked during thermal annealing.

CPP 36.7 Wed 16:45 GÖR 226

**Compatible solution-processed interface materials for improving the efficiency of organic solar cells** — ●ZHUO XU<sup>1,2</sup>, JOSE PRINCE MADALAIMUTHU<sup>1,2</sup>, JOSEF BERND SLOWIK<sup>1,2</sup>, RICO MEITZNER<sup>1,2</sup>, AMAN ANAND<sup>1,2</sup>, SHAHIDUL ALAM<sup>1,2,4</sup>, HÉCTOR CORTE<sup>5</sup>, STEFFI STUMPF<sup>1,3</sup>, ULRICH S. SCHUBERT<sup>1,2,3</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena, Jena, Germany. — <sup>2</sup>Center for Energy and Environmental Chemistry Jena, Friedrich Schiller University Jena, Jena, Germany. — <sup>3</sup>Jena Center for Soft Matter, Friedrich Schiller University Jena, Jena, Germany. — <sup>4</sup>King Abdullah University of Science and Technology, KAUST Solar Center, Physical Sciences and Engineering Division, Material Science and Engineering Program, Thuwal, Kingdom of Saudi Arabia. — <sup>5</sup>Nanosurf AG, Liestal, Switzerland.

The electron transport layer (ETL) is a key component for better performance and stability in OSCs. Herein, conjugated PDINO, sol-gel derivatized under stoichiometric TiO<sub>x</sub>, and the same combination as the ETL was used to fabricate solution-processed PBDTTT-C-T:PC71BM-based OSCs. A hybrid of organic-inorganic ETL revealed less bimolecular and trap-assisted recombination than a single ETL of either material. Furthermore, the efficiency of devices using blend ETLs showed better performance in comparison to single ETLs in both fullerene and non-fullerene systems. This blending strategy has demonstrated beneficial consequences in device stability and efficiency, which will play a key role for future commercialization of OSCs.

CPP 36.8 Wed 17:00 GÖR 226

**Influence of dye-doping on the nanostructure of the highly efficient PM6:Y6 solar cells** — ●ELISABETH ERBES<sup>1,2</sup>, CON- STANTIN HARDER<sup>1,3</sup>, BENEDIKT SOCHOR<sup>1</sup>, SUSANN FRENZKE<sup>1</sup>, NAI- REETA BISWAS<sup>1,2</sup>, JAN RUBEK<sup>1</sup>, MATTHIAS SCHWARTZKOPF<sup>1</sup>, VOLKER KÖRSTGENS<sup>3</sup>, PETER MÜLLER-BUSCHBAUM<sup>3,5</sup>, STEPHAN V. ROTH<sup>1,4</sup> und SIMONE TECHERT<sup>1,2</sup> — <sup>1</sup>DESY, Hamburg, DE — <sup>2</sup>Institute for X-ray Physics, Goettingen University, Goettingen, DE — <sup>3</sup>TUM School

of Natural Sciences, Chair for Functional Materials, Garching, Germany — <sup>4</sup>KTH Royal Institute of Technology, Stockholm, SWE. — <sup>5</sup>MLZ, TUM, Garching, DE

Organic solar cells based on the donor polymer PM6 and the acceptor Y6 give power conversion efficiencies (PCE) of 13-16% without any additives. The current study aims to investigate systematically the effect of doping PM6:Y6 with optical-light absorbing, electron transfer (ET) dyes. These pyrene-based dyes (PyxDMA) have inter- and intramolecular charge transfer properties and a very high quantum yield. Also the absorption in the UV regime extends the absorption range of the PM6:Y6 system. The structural and morphological integrity of the dopants within the active layer were studied with grazing incidence X-ray scattering experiments. The analysis showed the intercalation and distribution of the dyes within the PM6:Y6 matrix. The sprayed solar cell architecture Cu/PM6:Y6:PyxDMA/PEDOT:PSS/Au/ITO/Glass was used to measure the PCEs. Correlating these efficiencies with the molecular and nanostructural results allows explaining the changing PCE due to different doping levels of PyxDMA.

CPP 36.9 Wed 17:15 GÖR 226

**Hydrogenated nanodiamonds as efficient electron extraction layers in organic solar cells** — ●AURELIEN SOKENG DJOUMESSI<sup>1,2</sup>, ANASTASIA SICHWARDT<sup>1,2</sup>, DARIA MILIAIEVA<sup>3</sup>, JAN ČERMÁK<sup>3</sup>, MAXIMILIAN SCHAAL<sup>4</sup>, FELIX OTTO<sup>4</sup>, ŠTĚPÁN STEHLÍK<sup>3</sup>, VOJTECH NÁDAŽDY<sup>6</sup>, TORSTEN FRITZ<sup>4</sup>, BOHUSLAV REZEK<sup>5</sup>, ULRICH S. SCHUBERT<sup>1,2</sup>, and HARALD HOPPE<sup>1,2</sup> — <sup>1</sup>Laboratory of Organic and Macromolecular Chemistry, Friedrich Schiller University Jena (IOMC), Jena, Germany — <sup>2</sup>Center for Energy and Environmental Chemistry (CEEC), Friedrich Schiller University Jena, Jena, Germany — <sup>3</sup>Institute of Physics, Czech Academy of Sciences, Prague 6, Czech Republic — <sup>4</sup>Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — <sup>5</sup>Faculty of Electrical Engineering, Czech Technical University, Prague, Czech Republic — <sup>6</sup>Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovak Republic

Surface tunability is one property of nanodiamonds (NDs), which enables attachment of a range of functional groups on their surfaces. This may have a significant impact on NDs' electrical and optical characteristics and be helpful for charge extraction in solar cell devices. Herein, the surface chemistries of HPHT NDs modified by hydrogenation in a hydrogen atmosphere exhibit sp<sup>2</sup>-phases, which may help in improving the material's electrical conductivity and electron extraction when employed as an electron transport layer in PBDB-T:ITIC-based solar cells. The device performance was 7%, which differs only marginally from the outcomes of the state-of-the-art ETLs (ZnO, SnO<sub>2</sub>).