CPP 1: Organic Electronics and Photovoltaics 1

Time: Monday 9:30–13:00 Location: H38

Invited Talk CPP 1.1 Mon 9:30 H38

Ternary blend approach for boosting performance and stability of organic solar cells — •Tayebeh Ameri — University of Edinburgh, School of Engineering, Edinburgh, UK

Organic solar cells (OSCs) have now reached power conversion efficiencies over 18% on laboratory-scale devices, an important milestone towards their commercialization. The evolution in organic photovoltaic technology along with introducing non-fullerene acceptor materials and ternary blend approach caused this significant boost in the performance of solar cells.

However, for longer than a decade, when researchers were focused on boosting the power conversion efficiency of solar cells, the importance of lifetime and stability issues was overlooked by the organic photovoltaic community. Recently, more studies have been conducted and reported on the lifetime and stability of OSCs, employing different strategies to either understand the degradation mechanisms or enhance the lifetime of solar cells.

In this presentation, we overview how the ternary blend approach was developed to boost the power conversion efficiency. Moreover, we discuss how this approach can also address the stability issues related to the mostly used electron transport layer of zinc oxide and significantly increase the photostability of organic solar cells. And finally, we explain how zinc oxide must be manufactured and pretreated to avoid UV light activation, and in parallel, increase the thermal stability of the devices.

CPP 1.2 Mon 10:00 H38

Structure control during in situ printing of donor-acceptor blend films — Kerstin S. Wienhold[1], Manuel A. Reus[1], Dan Yang[1], Baojun Lin[2], Heng Zhao[2], Wei Ma[2], and •Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049 China — [3]Heinz Maier-Leibnitz Zentrum (MLZ), TU München, 85748 Garching, Germany

Among the next generation solar cells, in particular organic photovoltaics are gaining impact as a promising alternative to conventional silicon-based solar cells. However, despite big achievements in the last years, it remains an unresolved challenge to fabricate large-area organic solar cells without sacrificing efficiencies. The reason behind is that basic understanding is still very limited due to the complexity of the systems. Moreover, presently a substantial number of researchers use spin-coating for film fabrication, which is not compatible with the needs of a large scale production. Thus, using up-scalable fabrication methods such as printing are of immanent interest. In the present work, we use GISAXS and GIWAXS in situ during printing of donor:acceptor blends to gain fundamental understanding about the underlying film formation processes. Different examples of polymer donors and small molecule acceptors are presented and the resulting morphologies are correlated with solar cell device performance.

CPP 1.3 Mon 10:15 H38

Revealing the Thermally Induced Degradation of PM6:Y6 based Bulk Heterojunction Organic Solar Cell — •Shahidul Alam, Hua Tang, Maryam Alqurashi, Wejdan Althobaiti, Si Chen, Haya Aldosari, Jafar I. Khan, and Frédéric Laquai — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center (KSC), Physical Sciences and Engineering Division (PSE), Material Science and Engineering Program (MSE), Thuwal 23955-6900, Kingdom of Saudi Arabia

Thermally-induced degradation in bulk-heterojunction OSCs is an obvious barrier to the fabrication of stable devices. Thus, practical approaches and strategies need to be identified their inherent thermal instability. In this work, the thermally induced degradation of the most commonly used system PM6:Y6 is investigated by varying temperatures and different exposure conditions. The degradation pathways have been identified by applying several opto-electrical and spectroscopic characterizations methods. Due to the reduced charge carrier mobility and extraction probability, the thermally degraded device exhibits significant losses in the VOC and FF. Furthermore, the field dependence of charge generation, charge extraction, photo-generated charge density, and charge recombination dynamics in solar cells were studied by the TDCF optical-pump electronic-probe technique. By using all the analyses, we can explain the significant recombination process that dominates device performance and thermal stability. Finally, device simulation by SETFOS of the JV characteristics was used to confirm experimentally determined thermally induced degradation.

CPP 1.4 Mon 10:30 H38

Developing the next generation of photovoltaics with high efficiencies — •Elisabeth Erbes[1,2], Matthias Schwartzkopf[1], Constantin Harder[1,3], Susann Frenzke[1], Benedikt Sochor[1], Naireeta Biswas[1,2], Stephan V. Roth[1,4], and Simone Techert[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Institute for X-ray Physics, Goettingen University, Goettingen, Germany — [3]Technical University of Munich, Munich, Germany — [4]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology, Stockholm, Sweden

A crucial challenge in bio-inspired energy research is to develop a rationale for the synthesis and use of sustainable, bio-based materials. Cellulose fibers have excellent mechanical strength, are thermally stable, are very lightweight and have a very low surface roughness in thin films. On the other hand, the use of small molecules in OSC is well known to increase the power conversion efficiency. The idea is to combine the use of cellulose and small molecules to create a sustainable organic solar cell with high efficiencies. The current study aims to investigate systematically the OSC matrix PM6:Y6 doped with optical-light absorbing, electron transfer (ET) dyes. The structural and morphological integrity of the dyes were studied with grazing incidence small angle and wide angle X-ray scattering techniques (in situ GISAXS and static GIWAXS) and photo-sensitization experiments. This analysis showed us the intercalation dynamics, distribution and function of pyrene-based photo-dopants within the PM6:Y6 matrix and whether these dopants alter the overall polymer structures.

CPP 1.5 Mon 10:45 H38

Ultrafast charge carriers separation at organic donor-acceptor interfaces - Influence of molecular vibrations — •Maximilian F. X. Dorfner[1], Sebastian Hutsch[1], Raffaele Borrelli[2], Maxim F. Gelin[3], and Frank Ortmann[1] — [1]Department of Chemistry, Technische Universität München, 85748 Garching b. München (Germany) — [2]DISAFA, University of Torino, Largo Paolo Braccini 2, I-10095 Grugliasco (TO), Italy — [3]School of Sciences, Hangzhou Dianzi University, Hangzhou 310018, China

In this work the charge transfer dynamics of photogenerated excitons at a donor-acceptor interface of an organic solar cell blend is examined. This is done by means of a fully quantum mechanical treatment of an effective Holstein model including the relevant electronic orbitals coupled to over one hundred vibrational modes, parametrized by density functional theory calculations. To solve this coupled electron-phonon system we make use of the numerically quasi-exact matrix-product-state ansatz. We find that, depending on the driving energy, different mechanisms are predominantly responsible for the charge separation at the interface. For near zero driving the ultrafast electron transfer is prevalently due to kinetic processes, while at larger driving the separation of carriers can be traced back to dissipative phonon emission connected with the dominant molecular vibrations. This charge transfer picture is consistent with a novel semi-classical hopping approach, with which we compare. These results show that dissipation of energy to the phonon is essential for charge separation for systems with a moderate driving force.

CPP 1.6 Mon 11:00 H38

Revealing the formation kinetics of the active layer for non-fullerene organic solar cells — •Xinyu Jiang[1], Suo Tu[1], Manuel A. Reus[1], Julija Reitenbach[1], Christian L. Weindl[1], Matthias Schwartzkopf[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]DESY, Notkestraße 85, 22607 Hamburg

Bulk heterojunction (BHJ) organic solar cells have gained significant improvements in the past few years, however, traditional laboratory deposition methods like spin coating are limited to small-scale production. In addition, it is difficult to observe the structure formation process of the active layer during deposition, which is crucial for gaining a fundamental understanding. Encouragingly, the emergence of printing techniques and the development of in-situ observation technology open new windows for lager-area device manufacturing and inspection of the formation process of the printed active layer, respectively. In this work, we fabricate an active layer, which contains a donor polymer (PDTBT2T-FTBDT) and a non-fullerene acceptor (BTP-4F) with a slot-die coating. The structure formation of the polymer domains kinetics is followed in-situ during the printing process with GIWAXS and UV-Vis spectroscopy measurements, respectively. Thus, structure evolution is coupled with optical properties during the printing process, thereby providing an understanding of the drying of non-fullerene organic BHJ thin films.

15 min. break

CPP 1.7 Mon 11:30 H38

Re-evaluation of Published Figures of Merit and Introduction of Novel figure of merit for Transparent Conducting Electrodes used in Photovoltaics — •Aman Anand[1,2], Md Moidul Islam[1,2], Rico Meitzner[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstraße 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

Transparent conductive electrodes (TCEs) are one of the important components of photovoltaic technologies. Since they are transparent and conductive, they allow light to enter the device and the photocurrent generated to be drawn into the outer electric circuit. In theory, TCEs should have the highest light transmission and conductivity. Both traits, however, must be balanced. The selection of the best TCE depends on the photovoltaic material system and is evaluated using so-called figures-of-merit (FOM). A novel and exact FOM is presented here that explicitly analyzes the impact on photovoltaic performance. This novel and exact FOM has several important properties, including i) proportionality to the solar device's potential power output, ii) normalization to the theoretically ultimately attainable photovoltaic performance, and, thus, iii) significant direction for the development of advanced TCEs. This work reassesses and compares a variety of realized state-of-the-art semitransparent electrodes.

CPP 1.8 Mon 11:45 H38

Cycling stability of cellulose-based electronics — •Stephan V. Roth[1,2], Calvin J. Brett[1,2], Ola K. Forslund[1], Elisabetta Nocerino[1], Lucas P. Kreuzer[3], Lionel Porcar[4], Norifumi L. Yamada[5], Martin Mansson[1], Peter Müller-Buschbaum[3], and L. Daniel Söderberg[1] — [1]KTH Royal Institute of Technology, SE-10044 Stockholm — [2]DESY, D-22607 Hamburg — [3]TU München, Physik-Department, Lehrst. f. Funktionelle Materialien, D-85748 Garching — [4]ILL, F-38042 Grenoble — [5]KEK, Tokai (JPN)

In organic electronics, hybrid materials combining high-strength biomaterials and conducting organic polymers allow for disentangling mechanical flexibility and functionality. Yet, degradation in such complex organic electronics applications is still less addressed. We thus combine sprayed cellulose nanofibrils (CNF) templates due to their hierarchical, nanoporous morphology and a conductive polymer blend poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) to correlate the impact of cyclic relative humidity changes with device performance and nanostructure evolution. The conductivity of the CNF/PEDOT:PSS hybrid shows reversible changes: The PEDOT:PSS blend undergoes cyclic wetting/dewetting on the CNF backbone accompanied by swelling and deswelling of PEDOT:PSS moieties in the pores. The cycling stability of the device performance is ensured by reversible rearrangement of the CNF backbone. With CNF acting as structural reinforcing template, interestingly, no macroscopic swelling is observed, proving the applicability in e.g. supercapacitors.

CPP 1.9 Mon 12:00 H38

Dual-Gate Organic Electrochemical Transistors and Circuits — •Hsin Tseng, Anton Weissbach, Karl Leo, and Hans Kleemann — Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Dresden, Germany

Organic mixed ionic-electronic conductors (OMIECs) are currently in the spotlight of research for diverse applications. Among all, organic electrochemical transistors (OECTs) stand out as organic synaptic devices for integrated bioelectronics leading to neuromorphic computing applications, thanks to their low operating voltage, biocompatibility, and the ionic and electronic interactions in OMIECs. Modifying OMIECs by molecular design enables accumulation-mode OECTs, resulting in broad IC applications. However, the side chain molecular design of the polymer is unfavorable for IC design and manufacturing processes. Here, we show an OECT with photo-patternable solid electrolyte advancing towards integrated circuits. We discuss how alterable device parameters can be employed to adjust the OECT performance. In particular, we demonstrate how the biasing conditions govern the time constant of OECTs. In addition, we discuss how a dual-gate OECT architecture can be employed to tune the threshold voltage of OECTs and control the ionic and electronic charge transport in the electrolyte and OMIECs without any complicated molecular design. The electrical analysis of solid-state electrolyte OECTs provides new insights stimulating higher investigations on ionic and electronic interactions and coupled transport properties in OMIECs and paves the foundation for the integration of OECTs for advanced applications.

CPP 1.10 Mon 12:15 H38

Design of Monolithic 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 application because of their versatility and flexibility. Additionally, they can be easily fabricated on any substrate, making monolithic sensor application possible. This allows for an easy miniaturization and a cheap fabrication. Organic room temperature phosphorescence (RTP) materials are well suited for optical oxygen sensors because of their strong oxygen dependency.

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

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

CPP 1.11 Mon 12:30 H38

Towards all solution-processed OFETs using microcontact printed electrodes — •Kirill Gubanov[1], Manuel Johnson[1], Melda Akay[1], Kim Thomann[1], Dan Shen[1,2], Xing Cheng[2], and Rainer H. Fink[1] — [1]Physikalische Chemie II, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]South University of Science and Technology, Shenzhen, China

Printed electronics is expected to facilitate low-cost solvent prepared devices for potential applications in RFID, flexible displays, OLEDs and transistors. Furthermore, microcontact printing may be used in a large-scale production using roll-to-roll printing with direct access to structures on the micrometer level. The preparation of the microstructured conductive electrodes using PEDOT:PSS ink for applications in OFETs was successful in various aspects: the electrodes were fabricated with very good structural definition and high reproducibility on solvent-prepared 2D-extended single-crystalline C8-BTBT films. A defined mechanical load of the PDMS stamps pre-treated with O2 plasma yielded good structural quality and competitive electrical performance. In particular, the implementation of the MWCNTs in the PEDOT:PSS ink has a direct impact on the charge carriers transport efficiency, leading to the contact resistance decrease. In addition to electrical characterization made with KPFM and IV-curves, the morphology and structure analysis was performed using VLM, AFM and 3D Microscopy, providing with an insight into the structural quality of the contacts and relate their structures to the overall device performances. The research is funded by the BMBF (contract 05K19WE2).

CPP 1.12 Mon 12:45 H38

Effect of trap states on the performance of organic photodetectors — •Jakob Wolansky[1], Sebastian Hutsch[2], Felix Talnack[1], Michel Panhans[2], Jonas Kublitski[1], Stefan Mannsfeld[1], Frank Ortmann[2], Johannes Benduhn[1], and Karl Leo[1] — [1]Technische Universität Dresden, Dresden, Germany —

[2]Technische Universität München, Garching b. München, Germany

Due to the broad range of modern applications, the demand for photodetectors is drastically increasing, and in particular, organic photodetectors (OPDs) can meet the diverse requirements. However, the specific detectivity of OPDs is significantly below the thermal limit and is currently restricted by the high noise spectral density. Kublitski *et al.*[1] recently showed that the shot noise and hence the dark current (J_D) dominates the noise spectral density at negative bias. Further, the authors suspect that mid-gap trap states cause the high J_D.

Here, we study devices with a well-performing absorber layer without an electron acceptor and, therefore, we do not expect any charge-transfer states to form. Nevertheless, we can observe sub-bandgap absorption in ultra-sensitive external quantum efficiency measurements. By utilizing different device processing parameters and employing different interface layers, we identify the origin of these sub-bandgap excitations. Interestingly, we observe a clear correlation between the device performance and the presence and quantity of trap states. The relation between molecular structure and device performance gives a new direction for reducing J_D further in OPDs and improving their specific detectivity. [1] Kublitski, J. *et al.* Nat Commun 12, 551 (2021)