

CPP 73: Organic Electronics and Photovoltaics II

Time: Wednesday 16:15–18:30

Location: ZEU 260

CPP 73.1 Wed 16:15 ZEU 260

Investigation of Sub-Molecular Parts in Blends for Organic Solar Cells — ●ARTHUR MARKUS ANTON^{1,2}, SHAHIDUL ALAM³, RICO MEITZNER³, MARTIN HAGER³, JOHANNES AHNER³, ULRICH S. SCHUBERT³, WICHARD J. D. BEENKEN⁵, DANIEL AYUK MBI EGBE⁶, FRIEDRICH KREMER², and HARALD HOPPE^{3,4} — ¹The University of Sheffield, Department of Physics & Astronomy, Sheffield, UK — ²Leipzig University, Peter Debye Institute for Soft Matter Physics, Leipzig, Germany — ³Center for Energy and Environmental Chemistry, Jena, Germany — ⁴Friedrich Schiller University Jena, Institute for Organic Chemistry and Macromolecular Chemistry, Jena, Germany — ⁵Technische Universität Ilmenau, Institute of Physics, Ilmenau, Germany — ⁶Johannes Kepler University Linz, Institute of Polymeric Materials and Testing, Linz, Austria

It is believed that orientation and order of molecular units play an essential role for the performance of organic semiconductors. On the basis of infrared transition moment orientational analysis (IR-TMOA) [1] it is demonstrated how the orientation and order of sub-molecular parts in PBDB-T:ITIC and AnE-PVstat:ITIC polymer:acceptor blends can be analyzed. On the one hand, PBDB-T:ITIC is well suited for bulk heterojunction solar cells; on the other hand, AnE-PVstat:ITIC fall short, although photoluminescence indicates efficient quenching of donor emission [2]. A reason for this seemingly contradiction can be provided on the basis of molecular orientation. [1] A. M. Anton et. al., *J. Am. Chem. Soc.* 137 (2015) 6034 [2] S. Alam et. al., *Chem. Pap.* 72 (2018), 1769

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Simulation of active layer formation and stability in solution-processed organic solar cells — ●OLIVIER RONSIN and JENS HARTING — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Forschungszentrum Jülich, Fürther Straße 248, 90429 Nürnberg, Germany

Solution-processed organic bulk-heterojunction active layers form sophisticated structures during the drying of the wet-deposited solution, because of complex physical processes such as crystallization and/or liquid-liquid phase separation. This structure highly impacts the photovoltaic performance and is usually far from equilibrium and hence unstable. In order to reach significant improvements, a better understanding of the physics driving the active layer formation and stability is strongly needed.

We propose a phase-field simulation framework to determine the dry film structure. To this end, evaporation, crystal nucleation and growth, liquid-liquid phase separation are taken into account. We show the impact of the thermodynamic (especially miscibility) and kinetic (evaporation, diffusion and crystal growth rate) parameters on the time-dependent morphology of the wet film during drying up to the dry state. We also investigate the structural evolution of the dry film.

15 min. break

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Morphological investigations on fullerene-free bulk heterojunction blends for photovoltaic applications — ●SEBASTIAN GROTT¹, LORENZ BIESSMANN¹, NITIN SAXENA¹, WEI CAO¹, SIGRID BERNSTORFF², and PETER MÜLLER-BUSCHBAUM¹ — ¹TU München, Physik-Department, LS funktionelle Materialien, 85748 Garching — ²Elettra-Sincrotrone Trieste, 34149 Basovizza, Italy

In the last decades, the focus of research has been drawn towards the field of organic electronics due to their advantageous properties, such as versatility, flexibility, low-cost manufacturing processes, as well as their tuneable characteristics, such as solubility and absorption. These properties open up a wide range of applications, especially, in the field of photovoltaics. Hence, organic photovoltaics represent a promising alternative for the conventional inorganic photovoltaics. Even though the power conversion efficiency is lower than the ones of conventional devices, values of over 10% have been reported and thus receive industrial attention for commercialization. We study the inner morphology of a low band gap, fullerene-free bulk heterojunction blend, namely PBDB-T and ITIC of different compositions with grazing-incidence small-angle X-ray scattering (GISAXS). The obtained structural infor-

mation are correlated with current density voltage characteristics and the absorbance of the active layer in order to improve the efficiency.

CPP 73.4 Wed 17:15 ZEU 260

Triplet Exciton Losses in Polymer:Non Fullerene Acceptor Blends — ●STEFANIE DIETZ, HANNAH LINDL, JANNIS KLOTZ, MARIA KOTOVA, ANDREAS SPERLICH, and VLADIMIR DYAKONOV — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Organic bulk heterojunction solar cells utilizing non fullerene acceptors (NFA) received a lot of attention in the past few years as their power conversion efficiency exceeds 16%. This is achieved by a closer matching of donor and acceptor energy levels, but has unfortunately led to a new loss pathway via the now energetically lower lying triplet exciton. We build high performance bulk heterojunction solar cells using the polymer PM6 (a fluorine substituted PBDB-T, PBDB-T-2F) and the NFA Y6 (a fluorine-substituted BTP, BTP-4F). To probe potential losses due to triplet formation we use inherently spin-sensitive methods based on electrical and photoluminescence detected magnetic resonance (EDMR, PLDMR). By comparing pristine materials, blends and ultimately solar cells under realistic operating conditions conclusions can be drawn about potential radiative and non-radiative losses and the involvement of triplet excited states in these organic solar cells.

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Charge separation in non-fullerene acceptor solar cells — ●FRÉDÉRIC LAQUAI — King Abdullah University of Science and Technology (KAUST), KAUST Solar Center, Thuwal, Saudi Arabia

In organic solar cells, the energetic landscape at the donor-acceptor interface provides the driving force for charge separation. The precise mechanism of and the prerequisites for efficient charge separation have been investigated intensively in fullerene-based systems. However, with the recent development of novel high-efficiency non-fullerene acceptors (NFAs), several of the findings previously obtained on fullerene-based systems are currently being revisited for NFA-based systems. In this contribution, I present our latest insight into the photophysical processes in NFA-based systems obtained by a combination of steady-state and transient (ultrafast) spectroscopy techniques. More precisely, I report on the driving force required for charge separation in a series of polymer and small molecular donor / NFA blends, including some of the current state-of-the-art material systems. Interestingly, we found that it is the ionization energy (IE) offset, which dominates the charge separation efficiency in many NFA-based systems, while the electron affinity (EA) offset seems to be of minor importance. The reasons for this striking observation and the implications for future donor / acceptor material design strategies are discussed.

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Effect of Solvent Additives on the Morphology and Device Performance of Printed Non-fullerene Acceptor Based Organic Solar Cells — ●KERSTIN S. WIENHOLD¹, VOLKER KÖRSTGENS¹, SEBASTIAN GROTT¹, XINYU JIANG¹, MATTHIAS SCHWARTZKOPF², STEPHAN V. ROTH^{2,3}, and PETER MÜLLER-BUSCHBAUM^{1,4} — ¹TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — ²DESY, 22607 Hamburg — ³KTH, Department of Fibre and Polymer Technology, SE-100 44 Stockholm, Sweden — ⁴Heinz Maier-Leibnitz-Zentrum, Lichtenbergstr. 1, 85748 Garching, Germany

Printing of active layers of high efficiency organic solar cells with a meniscus-guided slot-die coater enables up-scaling of the solar cell production. However, an optimization of this thin film deposition is necessary as insights gained from spin-coating cannot simply be transferred to printed photovoltaics. In this work, active layers of the conjugated polymer PBDB-T-SF and the non fullerene small molecule acceptor IT 4F are slot die coated with different concentrations of 1,8 diiodoctane (DIO) and the effect on the inner nano structure and surface morphology of the material is studied with grazing incidence small angle X-ray scattering (GISAXS), grazing incidence wide angle X ray scattering (GIWAXS), scanning electron microscopy (SEM) and atomic force microscopy (AFM). The optical properties are studied with photoluminescence (PL), UV/Vis absorption spectroscopy and external quantum efficiency (EQE) measurements and correlated to the corre-

sponding power conversion efficiencies.

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Barrierless free charge generation in the high-performance PM6:Y6 bulk heterojunction non-fullerene solar cell — ●LORENA PERDIGÓN-TORO¹, HUOTIAN ZHANG², ANASTASIA MARKINA³, FENG GAO², DENIS ANDRIENKO³, SAFA SHOAEI¹, and DIETER NEHER¹ — ¹Institute of Physics and Astronomy, University of Potsdam, Germany — ²Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden — ³Max Planck Institute for Polymer Research, Mainz, Germany

Organic solar cells are currently experiencing a second golden age thanks to the development of novel non-fullerene acceptors (NFAs). Surprisingly, some of these blends exhibit high efficiencies despite a low energy offset at the heterojunction. In this work, we investigate photocurrent generation in the high-performance blend of the donor polymer PM6 with the NFA Y6 as a function of internal field and excitation energy by means of time-delayed collection field (TDCF). Results show that generation is essentially barrierless with near-unity efficiency, regardless of excitation energy. Complementary temperature-dependent external quantum efficiency and open-circuit voltage measurements reveal that efficient generation is maintained over a wide temperature range, down to 100 K, despite the small driving force for charge generation. Studies on a blend with a low concentration of the NFA, measurements of the energetic disorder, and theoretical modelling suggest that charge generation is assisted by the electrostatic interfacial field which for Y6 is large enough to compensate the Coulomb dissociation barrier.

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Impact of Thermal Treatment and Humidity on Work Function of PEDOT:PSS Thin Films — ●AMAN ANAND^{1,2,3}, JOSE PRINCE MADALAIMUTHU^{1,2,3}, RICO MEITZNER^{1,2,3}, SHAHIDUL ALAM^{1,2,3}, ULRICH S. SCHUBERT^{1,2,3}, and HARALD HOPPE^{1,2,3} — ¹Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Jena, Germany — ²Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany — ³Jena Center for Soft Matter (JCSM), Friedrich Schiller University, Jena, Germany

Poly (3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) is the most common and commercially, successful conductive polyelectrolyte in the field of optoelectronics. Its properties such as high transparency in the visible range, electrical conductivity, and work function enable multiple applications in the field of electronics. Properly tuning the work functions within semiconductor devices is very crucial in terms of performance and may be strongly influenced by unmonitored processing conditions. For example, PEDOT:PSS is highly hygroscopic in nature, which may impact on its functionality. In the present work, we have investigated the impact of the thermal treatments and relative humidity during film casting or storage on the work function of PEDOT:PSS films. We find clear trends between the processing conditions and absolute work function as obtained with a carefully calibrated Kelvin Probe setup. As a conclusion, we can suggest suitable processing parameters for a wide range of formulations and targeted electronic properties.