CPP 49: Organic Electronics and Photovoltaics IV

Time: Friday 9:30–10:45 Location: H 0107

CPP 49.1 Fri 9:30 H 0107

Interfacial engineering via modifications of the electron blocking layer in PbS quantum dot solar cells — •Huaying Zhong[1], Timo Piecuch[1], Wei Chen[2], and Peter Müller-Buschbaum[1,3] — [1]TUM School of Natural Sciences, Chair for Functional Mateials, 85748 Garching, Germany — [2]SZTU, College of Engineering Physics, Shenzhen 518118, China — [3]TUM, MLZ, 85748 Garching

Colloidal quantum dot solar cells (CQDSC) have received tremendous attention as next generation solar cells. Best performances up to 15% power conversion efficiency (PCE) have been achieved using lead sulfide QDs in a heterojunction cell architecture . PbS CQDs are especially efficient in the infrared region, and thus particular interesting for niche applications like space satellites. Research in the last years mainly has focused on improving the absorber layer and the hole blocking layer, but the potential by improving the electron blocking layer (EBL) has recently aroused increasing interest. In order to reduce interfacial charge carrier recombination and capture large fraction of long wavelength photons at the EBL/active layer interface , the different interfacial energy-level offsets between EBL and absorber layer via tuning the QDs size of EBL are investigated using ultraviolet photoelectron spectroscopy (UPS) and absorption spectroscopy. Furthermore, the corresponding photovoltaic performances are characterized to demonstrate improved interfacial band alignment.

CPP 49.2 Fri 9:45 H 0107

Phase-field simulations of thermal annealing for all-small molecule organic solar cells — •Yasin Christian Ameslon[1], Olivier Ronsin[2], Christina Harreiss[3], Erdmann Spiecker[4], and Jens Harting[5] — [1]HI ERN, Nürnberg, Germany — [2]HI ERN, Nürnberg, Germany — [3]Nürnberg, Germany — [4]IMN, Erlangen, Germany — [5]HI ERN, Germany

Organic solar cells represent an emerging area in the field of photovoltaic devices. The performance relies upon the Bulk Heterojunction (BHJ) morphology whose final structure is impacted by the drying process and additional post treatment. In this study, we investigate the impact of thermal annealing (TA) on the morphology evolution of the well-studied all small molecules DRCN5T:PC71BM mixture. The objective is to determine the physical processes driving the BHJ morphology evolution. Phase field simulations are used to check the impact of the DRCN5T crystallisation related mechanisms (nucleation, growth, crystals stability, impingement, grain boundary coarsening and Ostwald ripening), of the amorphous-amorphous phase separation (AAPS), and of diffusion limitation on the final morphology. The comparison between the simulation results and the experimental data available from literature leads to following conclusions: The BHJ morphology evolution under TA is mainly due to growth of the largest DRCN5T crystals and dissolution of the smallest unstable crystals. Nucleation, impingement, Ostwald ripening, grain boundary coarsening, AAPS are not significantly active during the TA. Finally, the crystal growth could potentially be diffusion limited.

CPP 49.3 Fri 10:00 H 0107

Static and Dynamic Energetic Disorder in Amorphous Organic Semiconductors via Physics-Inspired Machine Learning — •Ke Chen[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]University of Bayreuth

Organic semiconductors (OSCs) are attractive for electronic applications due to their low cost and mechanical flexibility. However, the relatively low charge mobility (σ) of OSCs hinders their adoption in many commercial applications. Designing high-σ OSCs is therefore highly desirable. In thin film applications many OSCs form amorphous structures, where the static and dynamic energetic disorder of site-energies is one of crucial factors determining σ. Multiscale simulations based on density functional calculations and kinetic models can be used to analyze the energetic disorder in OSCs, but this is computationally prohibitive for realistic amorphous simulation cells containing thousands of molecules. In this context, machine learning (ML) can drastically accelerate these analyses by providing fast and accurate surrogates to density functional calculations. In this work, we apply our recently reported [1] physics-inspired ML approach to predict energy levels and orbital locations of OSC molecules in large amorphous systems. This opens the door towards the multiscale modeling of realistic amorphous OSCs.

[1] K. Chen *et al.*, Chem. Sci. **14**, 4913 (2023).

CPP 49.4 Fri 10:15 H 0107

On the role of energy level offset and exciton reformation in non-geminate recombination of organic solar cells — •Nurlan Tokmoldin[1], Dieter Neher[2], and Safa Shoaee[1,3] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany — [2]Soft Matter Physics and Optoelectronics, Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany — [3]Optoelectronics of Disordered Semiconductors, Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam-Golm, Germany

The performance of modern organic bulk-heterojunction solar cells relies on a transition from a localised singlet exciton on an acceptor molecule (S1) to a charge-transfer state (CT), followed by CT dissociation into separated charge (CS) carriers. The latter may afterwards either be extracted or recombine by reforming CT. Losses may occur at every stage of the free carrier generation and during their lifetime and proceed via radiative and non-radiative decay of S1 and CT. The S1 reformation efficiency from CT then comes forward as a key parameter characterizing the distribution of losses via the different channels. We employ a rate equation analysis to determine the singlet reformation efficiency for several low-offset organic solar cells and find a good correlation with the S1-CT offsets extracted from temperature-dependent electroluminescence quantum yield measurements. This supports our earlier observations that the energy offset affects the bimolecular recombination coefficient in OPV blends and indicates that exciton reformation may indeed act a channel for non-geminate recombination.

CPP 49.5 Fri 10:30 H 0107

Unveiling the Thermal Expansion Behaviour of Organic Semiconductor Thin Films — •Meike Kuhn[1,2], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamik und Strukturbildung - Herzig Group, Universität Bayreuth, Universitätsstr. 30, 95447 Bayreuth, Germany — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton, Australia

Semiconducting polymers have emerged as a promising material for next-generation solar cells. However, for the optimization and reliability of such devices, understanding the thermal behaviour of the organic semiconductor layer is crucial. The thermal expansion impacts the molecular packing and crystallinity of polymers, influencing the charge transport properties of a material. Mismatches in the thermal expansion coefficients between the active layer and the other solar cell layers can furthermore lead to mechanical stress and device failure. In this study, we use temperature-dependent in-situ GIWAXS and NEXAFS spectroscopy to systematically investigate the thermal behaviour of the widely used semiconducting polymer PDBD-T-2F (PM6). Specifically, we investigate the influence of the temperature on the molecular packing, crystallinity and orientation. Additionally, we study the thermal behaviour of PM6:Y6 blends, which are widely used for high-efficiency organic solar cells, to examine the impact of temperature on OSC active layers.