CPP 48: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI

Time: Thursday 11:30–12:45 Location: ZEU/LICH

CPP 48.1 Thu 11:30 ZEU/LICH

Simulating Light Induced Phase Separation in Mixed Halide Perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekatarina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By varying the halide composition in mixed organic-inorganic perovskites such as $MAPbBr_{1.8}I_{1.2}$ (MA-methylammonium), one can precisely tune the band gap. This is a desirable property for solar cell design, as it allows for the production of high efficiency solar cells. However, illumination with visible light drives these materials to phase-separate into Br-rich and I-rich domains, thereby degrading the tuned bandgap. To better understand and potentially control this behavior, we employ phenomenological approaches such as Cahn-Hilliard and Monte Carlo models. While Cahn-Hilliard methods were initially explored, they proved challenging in reproducing experimentally observed dynamics. On the other hand, Monte Carlo methods have shown themselves to enable a systematic exploration of how factors such as halide ratio, charge-carrier density, temperature, and illumination intensity influence light-induced phase separation. Overall, we found that Monte Carlo simulations, with appropriately chosen parameters, can successfully reproduce key features observed in experimental diffraction measurements.

CPP 48.2 Thu 11:45 ZEU/LICH

Reorientation-driven degradation in oriented perovskite films: shifting facet engineering to thermodynamic stability — •Xiaojing Ci[1], Xiongzhuo Jiang[1], Guangjiu Pan[1], Kun Sun[1], Altantulga Buyan-Arivjikh[1], Zerui Li[1], Lixing Li[1], Thomas Baier[1], Matthias Schwartzkopf[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg

Hybrid perovskite solar cells suffer from underexplored links between crystallographic orientation and thermal stability. We fabricate highly oriented mixed Sn-Pb perovskite films via an additive-free two-step method. Accelerated aging studies under high temperature reveal that high orientation paradoxically compromises stability and PSCs built from highly oriented perovskite films retain only 73% of their initial PCE versus 89% in less-oriented devices. Operando GIWAXS of the PSCs shows that thermal stress induces significant reorientation and lattice distortion in the oriented crystallites. Structural analyses confirm progressive crystallographic transitions, including grain reconfiguration, shifts toward isotropy, and systematic diffraction migrations. Critically, we demonstrate that metastability is an intrinsic consequence of high crystallographic order, which is why the very high alignment strategies that enhance performance induce thermodynamic vulnerability. This necessitates redesigning crystal engineering priorities where suppressing instability requires engineering thermodynamic equilibrium states over maximizing alignment for stable perovskite photovoltaics.

CPP 48.3 Thu 12:00 ZEU/LICH

Understanding the molecular origins of giant surface potential: a case study of TPBi — •Mauricio Sevilla[1], Naomi Kinaret[1], Muhammad Nawaz Qaisrani[1,2], Albin Cakaj[4], Alexander Hofmann[4], Falk May[3], Wolfgang Brütting[1], and Denis Andrienko[4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Technische Universität Ilmenau, Ilmenau, Germany — [3]Merck Electronics KGaA, Darmstadt, Germany — [4]University of Augsburg, Augsburg, Germany

In the context of organic light-emitting diodes, the molecular orientation in thin layers of organic materials plays a crucial role in charge injection, light outcoupling, and the formation of internal electrostatic fields due to the alignment of molecular dipoles. This latter phenomenon is referred to as the giant surface potential (GSP). Predicting GSP soleley from the chemical structure is challenging, as it is highly sensitive to processing conditions such as temperature and deposition rate during the physical vapor deposition process. Using both all-atom and coarse-grained simulations, we develop and test a framework capable of predicting the molecular ordering of organic materials under varying substrate temperatures and deposition rates. The framework's accuracy is validated by comparing the predicted GSP and birefringence of thin films to experimentally measured values, for a series of TPBi isomers.

CPP 48.4 Thu 12:15 ZEU/LICH

Additives to enhance efficiency and stability of PPDT2FBT:PC60BM organic solar cells — •Hassan Ismail[1,2], Jose Prince Madalaimuthu[1,2], Ulrich 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

The development of organic solar cells (OSCs) requires simultaneous optimization of photovoltaic performance and long-term thermal stability, often mediated by processing solvents and additives. This study investigates the role of small amphiphilic molecules (AMs) as surfactants in stabilizing the bulk heterojunction morphology of PPDT2FBT:PCBM-based OSCs. Our research goal is to understand how the chemical nature of AMs and their interface engineering within the device affect stability and efficiency. We demonstrate that the AM's polar headgroup chemistry is a critical determinant for operational stability, and by strategically applying interface engineering across all major interfaces, we identify optimal scenarios for enhancing both efficiency and device durability. Interface engineering not only improves charge transport and mitigates degradation but also supports large-area fabrication and practical device reliability, addressing prominent challenges for commercialization. These findings guide future molecular design and interface engineering strategies, contributing to the realization of more robust and reliable organic solar cells.

CPP 48.5 Thu 12:30 ZEU/LICH

Controlling singlet fission in diketopyrrolopyrole diner through solvent choices — •Sruthy Asa Rajan[1,2], Isaac M. Etchells[3], Jegadesan Subbiah[2], Sergey Bagnich[1], Paul E. Shaw[3], David Jones[2], and Anna Köhler[1] — [1]Universität Bayreuth — [2]University of Melbourne — [3]University of queensland

The efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which is arises from thermalisation loss. Singlet fission (SF) offers a promising pathway to surpass this efficiency limit. However, a key challenge lies in identifying SF molecules with triplet energy levels that align with the silicon band gap, enabling the efficient formation of correlated triplet pairs, 1(TT), and their separation. PDPP is a molecule with a comparable triplet energy to the silicon bandgap. But monomer molecules are not SF active in solution. We prepared PDPP-dimers with a pyrene bridge. We investigate the influence of solvent properties on the optical behaviour of these N-alkylated pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-alkylated pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the optical properties of the evolution of different species. At an intermediate temperature, we observed an intermediate emission, which then, on further decreasing the temperature (less than 100K), is replaced by 1(TT) emission. We also measured TA on different solvents which showed different pathway. In protic polar solvent, our molecule showed intermolecular SF whereas in aprotic polar solvent it showed intermolecular