CPP 44: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V

Time: Thursday 9:30–11:15 Location: ZEU/LICH

Invited Talk CPP 44.1 Thu 9:30 ZEU/LICH

Shedding light on wide bandgap perovskites — •Michael Saliba — Institute for Photovoltaics (ipv), University of Stuttgart, Germany

Low bandgap perovskite solar cells are approaching the Shockley-Queisser limit for single-junction solar cells. Less progress, however, was made for wider bandgap perovskites, which are of interest, e.g., for multijunction photovoltaics. These wide bandgap perovskites are often comprised of fully inorganic components, which are hard to dissolve in conventional solvent systems and require more sophisticated synthesis as well as crystallisation techniques. In this talk, I will discuss strategies to address these challenges by providing a library of hitherto unexplored wider bandgap perovskites using combinatorics.

Unfortunately, the newly formulated liquid precursors often exhibit complex crystallization behaviour struggling to expel the typically used DMSO solvent. To delay the crystallization time, two strategies are proposed to remove the strongly complexating DMSO molecules through a) modified processing of the liquid thin-film and b) a coordination solvent with a high donicity and a low vapor-pressure leading to a marked improvement in the overall film quality. Lastly, interface manipulation, especially on top of the formed perovskite, is becoming a central topic to advance further. Light annealing is introduced to modify the perovskite surface resulting in a reduced surface recombination.

CPP 44.2 Thu 10:00 ZEU/LICH

Perovskite Solar Cells under Orbit-Like Thermal Cycling — •Simon Alexander Wegener[1], Christoph Gernot Lindenmeir[1], Thomas Baier[1], Xiaojing Ci[1], Sigrid Bernstroff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Perovskite solar cells offer strong potential for space power systems due to their high visible-light absorbance, thin active layers, and efficiencies comparable to silicon. These features provide exceptional power-to-weight ratios, and solution processing reduces manufacturing and launch costs relative to multi-junction gallium arsenide cells. Initial demonstrations have confirmed their operability in space. Key challenges remain, particularly the extreme temperature swings in low Earth orbit. Our work examines these stresses using operando grazing-incidence wide-angle X-ray scattering (GIWAXS) to track structural changes in the perovskite during illumination and temperature cycling. Synchrotron radiation enables the necessary temporal resolution to study the multilayer device stack, which combines materials with differing mechanical and thermal properties. Complementary photoluminescence measurements reveal associated changes in optical and electrical behavior. Across -125°C to +100°C, the perovskite shows changes in crystal phase, anisotropic strain, and optoelectronic response. These findings clarify the coupled mechanical and electronic effects driving performance loss and enable strategies to enhance durability of perovskite solar cells for space applications.

CPP 44.3 Thu 10:15 ZEU/LICH

Depth Resolved Structural Analysis on CsPbI3 Nanocrystal Nucleation Seed Induced Pervskite Thin Films — •Altantulga Buyan-Arivjikh[1], Lukas Wolz[1], Ajeet Kumar[2], Yanan An[1], Christopher Everett[1], Guangjiu Pan[1], Jiansheng Zhang[1], Zhuijun Xu[1], Matthias Schwartzkopf[3], Stephan V. Roth[4], Jürgen Hauer[1], Johanna Eichhorn[1], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, 85748 Garching, Germany — [2]Department of Chemical Physics, Lund University, 22100 Lund, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Department of Fibre and Polymer Technology KTH, SE-10044 Stockholm, Sweden

Lead-halide perovskites have attracted significant attention due to their favorable optoelectronic properties, simple processing, and the availability of precursor materials. Their performance is strongly governed by the crystallinity and morphology of the typically polycrystalline thin films. Among strategies to optimize these features, nanocrystal seeding has emerged as a promising route. Here, we show improved crystallographic orientation and reduced defect density in printed FAPbI3 thin films through the introduction of CsPbI3 nanocrystal nucleation seeds. Incidence-angle-varied GIWAXS enabled depth-resolved structural analysis, revealing seed incorporation and corresponding modifications of the energy landscape through the film thickness.

CPP 44.4 Thu 10:30 ZEU/LICH

***In-Situ* KPFM Growth Studies of Pentacene as a Model Hole Transport Material on 2D/3D Heterostructured $Cs_2AgBiBr_6$ for Perovskite Solar Cells** — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Forming low-dimensional perovskite interlayers in perovskite solar cells by applying ammonium salt solutions is a well-known method to improve devices. This has already been approved for the $Cs_2AgBiBr_6$ double perovskite in solar cell geometry by a 2D-modification with BABr or PEABr salts achieving respective low-dimensional phases at the interface. Using pentacene as a model hole conductor, its film growth and contact formation to the different double perovskite phases was investigated via *in-situ* growth studies using Kelvin Probe force microscopy (KPFM). Measuring the morphology and work function at intermittent steps during film deposition allowed to observe their evolution depending on the average pentacene film thickness. Image processing of the resulting KPFM images facilitated to assign different morphological features (from substrate or pentacene) present in the height images to different contributions to the work function and, especially, clearly identified the pentacene grains within other similar morphological features. A much more homogenous growth of pentacene on 2D/3D heterostructured $Cs_2AgBiBr_6$ was observed, forming evenly shaped grains or dendritic islands. This was further accompanied by a more confined work function, speaking for an enhanced contact alignment between the double perovskite and pentacene.

CPP 44.5 Thu 10:45 ZEU/LICH

Gas quenching under ambient condition for efficient and stable perovskite solar cells with surface passivation — •Zhaonan Jin[1], Xiongzhuo Jiang[1], Zerui Li[1], Xiaojing Ci[1], Guangjiu Pan[1], Lixing Li[1], Jinsheng Zhang[1], Xinyu Jiang[2], Sarathlal Koyiloth Vayalil[2,3], Kun Sun[4], Stephan V.Roth[2,5], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg — [3]UPES, India — [4]HZB, Berlin — [5]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

Wide-bandgap perovskite solar cells play a key role in tandem solar cells, which aim to overcome the Shockley-Queisser limit for single-junction solar cells. In this work, we develop and optimize a gas quenching method under ambient conditions for the fabrication of wide-bandgap (1.77 eV) perovskite films. To improve the performance of PSCs, three different organic spacer cations, including aromatic amino molecules (PEAI), aliphatic amino with long alkyl chain molecules (OAI), and short alkyl chain molecules (BAI), are applied and investigated as surface passivation materials. As a result, the 2D perovskite layers form on top of 3D perovskite films. The n-i-p devices with PEAI passivation exhibit a champion PCE of 16.26% along with a high Voc of 1.21 V, exceeding the control device (PCE = 13.42%, Voc = 1.15 V), and maintaining 88% of its initial PCE after 120 minutes of continuous illumination. This work offers a guide for the fabrication of wide-bandgap PSCs under ambient conditions and the choice of organic spacer cations for passivation.

CPP 44.6 Thu 11:00 ZEU/LICH

Solvated PbI2 Clusters Preceding the Crystalization of Lead Halide Perovsites - UV/VIS In Situ Study — •Maximilian Spies[1], Leonard Krapf[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth

The solution-based fabrication of reproducible, high-quality lead iodide perovskite films demands a detailed understanding of the crystallization dynamics. This dynamic is primarily determined by the precursor solution chemistry and processing conditions. We conducted a systematic in-situ study to elucidate the formation mechanism of perovskite films and the role of additives in the pre-crystallization phase. Using

UV absorption spectroscopy during spin coating allows us to track the evolution of iodoplumbate complexes and a solvated pre-crystalline phase (PDS) present in the precursor solution. This PDS phase is proportional to the precursor concentration, even during spin coating. Notably, using different precursor solvents changes the PDS phase evolution substantially. However, when introducing additives we see no difference in this pre-crystalline evolution, suggesting that additives only affect the perovskite film formation at a later stage