CPP 100: Focus: In-situ probes toward better understanding of hybrid halide perovskites (PhD symposium) I (joint session CPP/AKjDPG)

Metal-halide perovskites have attracted tremendous attention as absorber material in solar cells due to their rapid increase in power conversion efficiency. However, results within the field suffer from a range of variation and a lack of reproducibility. Thus detailed understanding of the highly dynamic material need correlation with the measurement conditions. To this end in-situ, operando and multimodal measurements are being developed. In this symposium, we want to bring together this in-situ expertise from various techniques which help to unravel material responses in hybrid perovskites. Organized by: Shambhavi Pratap (TU München), Hannah Funk (Helmholtz-Zentrum Berlin für Materialien und Energie) and Klara Suchan (Lund University, Sweden).

Time: Thursday 17:15–18:30 Location: ZEU 222

Invited Talk CPP 100.1 Thu 17:15 ZEU 222

Real-time Investigation of Crystallization Pathways of Organo-Metal-Halide Perovskites Solar — •Michael F Toney — SLAC National Accelerator Laboratory, Menlo Park, Ca, USA

Perovskite solar cells (PSCs) have gained tremendous attention as materials for photovoltaics due to their high efficiencies and their compatibility with low-cost low-temperature fabrication methods (such as solution processing). Perovskite film formation is complex, involving the formation of intermediates and/or metastable phases that strongly affect the final perovskite film microstructure. Therefore, understanding the mechanism of perovskite formation and the crystallization pathways is key for facile control of perovskite formation. We are using time-resolved x-ray scattering to investigate the perovskite formation of MAPbI3-based perovskites and mixed cation (Cs, FA)PbI3 perovskites in-situ during spin coating and the subsequent post-deposition treatments. Our work highlights the importance of real-time investigation of perovskite film formation which can aid in establishing processing-microstructure-functionality relationships and help to provide a fundamental understanding of the mechanisms of perovskite formation.

CPP 100.2 Thu 17:45 ZEU 222

Understanding the crystallization of solution processed, alloyed perovskites by multimodal characterization — •Shambhavi Pratap[1,2], Nobumichi Tamura[2], Zhenghao Yuan[3], Alastair MacDowell[2], Nicola Barchi[4], Jonathan Slack[2], Carolin Sutter-Fella[4], and Peter Müller-Buschbaum[1] — [1]Lehrstuhl für Funktionelle Materialien, TU München, 85748 Garching, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA — [3]Eberly College of Science, The Pennsylvania State University, State College,16801, USA — [4]Chemical Sciences Division, Lawrence Berkeley National Laboratory, 94720 Berkeley, USA

The crystallization behavior of solution processed hybrid plumbohalide perovskites is an ideal study to understand the formation of chemical alloys. Precursors corresponding to two different perovskites are mixed to serve as the precursor for an alloyed species. During crystallization, distinct crystalline species are isolated and characterized, as the equilibrium between the complex precursor intermediates and perovskites is transformed to the crystalline product by annealing the structure. The evolution of chemical structures is temporally resolved and the transient structures are studied for their optoelectronic transformation by photoluminescence.

CPP 100.3 Thu 18:00 ZEU 222

Small-Footprint Optical Monitoring to Study Perovskite Thin Film Formation — Aboma Merdasa[1,2], Rahim Munir[1], Carolin Rehermann[1], Katrin Hirselandt[1], Janardan Dagar[1], Klara Suchan[2], and •Eva Unger[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Lund University, Sweden

Record performance of Metal-Halide Perovskite (MHP) based solar cells have been achieved for small area devices based on spin-coating. Developing this device technology towards larger area prototypes will require the utilisation of scalable process technology. Processing strategies developed for spin-coating have been developed by incremental modifications of MHP ink and process conditions. Translating these processing strategies to scalable process technology requires a fundamental understanding of the formation mechanism. We recently developed a small-footprint spectroscopy setup based on fibre-optics enabling the monitoring of thin film formation processes. The setup can be easily integrated in process equipment such as spin-coater or slot-die coaters. UV-Vis measurements in reflectance mode enable us to describe the thinning of precursor solution during initial stages of MHP deposition as well as the onset of MHP crystallisation. As examples, the role of the anti-solvent drip in thin film formation, inhomogeneous crystallisation of MHP materials from mixed bromide/iodide precursors, crystallisation of reduced dimensional 2D/3D materials and effect of spin-coating and annealing time on MHP device performance will be discussed.

CPP 100.4 Thu 18:15 ZEU 222

Investigating MAPbI_{3} Thin Film Formation during Spin Coating by Simultaneous in Situ Absorption and Photoluminescence Spectroscopy — Mihirsinh Chauhan[1,2], Yu Zhon[1], Konstantin Schötz[1], Brijesh Tripathi[2], Anna Köhler[1], Sven Huettner[1], and •Fabian Panzer[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]Pandit Deendayal Petroleum University, Gandhinagar, India

Until today, the two-step processing method represents an attractive route for the thin film formation of halide perovskites. However, a fundamental understanding about the film formation dynamics in case of spin coating methylammonium iodide (MAI) on PbI_{2} has not been established yet. Here we apply in-situ optical spectroscopy during the two-step film formation of the model halide perovskite MAPbI_{3} via spin coating. We identify and analyze in detail the optical features that occur in photoluminescence and corresponding absorption spectra during processing. We find that the film formation takes place in five consecutive steps, including the formation of a MAPbI3 capping layer via an interface crystallization and the occurrence of an intense dissolution-recrystallization process. Consideration of confinement and self-absorption effects in the PL spectra, together with consideration of the corresponding absorption spectra allows to quantify the growth rate of the initial interface crystallization to be 13 nm/s for our processing conditions. We find the main dissolution recrystallization process to happen with a rate of 445 nm/s, emphasizing its importance to the overall processing.