# CPP 19: Perovskite and Photovoltaics 2

Time: Wednesday 9:30–11:00 Location: H38

**Invited Talk** CPP 19.1 Wed 9:30 H38

**Elucidating the role of antisolvent polarity on the surface chemistry and optoelectronic properties of lead-halide perovskite nanocrystals** — •Robert Hoye — Department of Materials, Imperial College London, Exhibition Road, London SW7 2AZ, United Kingdom

Lead-halide perovskites (LHPs) have emerged as highly-promising contenders for light-emission applications, particularly in the form of nanocrystals (NCs), owing to their advantages of high photoluminescence quantum yield (PLQY), along with tunable, sharp emission peaks. Achieving high-quality NCs critically depends on the purification process, which often makes use of an antisolvent. Despite its important role, the mechanism by which the antisolvent influences the surface properties of the NCs is not well understood. In this talk, we examine the influence of the polarity of the antisolvent on the properties of the model NC system CsPbBrxI3-x. The antisolvents we compare are (in order of increasing polarity): methyl acetate, acetone and butanol. We find that as the polarity of the antisolvent increases, there is a greater blue-shift in the photoluminescence peak, owing to the removal of iodide. Through detailed nuclear magnetic resonance measurements, we find that this occurs due to more polar antisolvents having a higher propensity to induce a condensation reaction between the oleic acid and oleylamine ligands on the NCs, leading to their removal in the form of amides, which leads to the removal of surface iodides. This work shows that minimising surface damage to LHP NCs requires the selection of low polarity antisolvents.

CPP 19.2 Wed 10:00 H38

**Simulation of the impact of processing conditions on the perovskite film morphology** — •Martin Majewski, Olivier Ronsin, and Jens Harting — Forschungszentrum Jülich GmbH, Helmholtz Institute Erlangen- Nürnberg (IEK-11), Dynamics of Complex Fluids and Interfaces, Cauerstraße 1, 91058 Erlangen, Germany

The solution-processed perovskite layer forms complex structures during drying. This morphology of the dry film heavily influences the efficiency of the final solar cell. The impact of the physical mechanisms on the morphology, like for example nucleation and evaporation rate, in a drying, crystallizing wet film is not really understood yet. Therefore a better understanding of the interplay of these phenomena is needed.

We will present phase field simulations which are capable to describe the main physical processes like: evaporation, diffusion, spontaneous nucleation, crystal growth and advection, to investigate the impact of processing conditions on the final morphology of the perovskite film. Comparisons of the simulation to the theory will be presented. First simulations of drying solutions, including all physical phenomena, will be shown and compared to experiments.

CPP 19.3 Wed 10:15 H38

**Influence of crystallization on the structural and optical properties of lead-free Cs2AgBiBr6 perovskite crystals** — •Melina Armer[1], Julian Höcker[2], Carsten Büchner[1], Sophie Häfele[1], Patrick Dörflinger[1], Maximilian T. Sirtl[3], Kristofer Tvingstedt[1], Thomas Bein[3], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ludwigs Maximilian University München, 80539 München — [3]Ludwigs Maximilian University München, 81377 München

As conventional perovskite solar cells contain lead and therefore suffer from toxicity issues, finding stable lead-free materials for the application in perovskite photovoltaics has become an essential problem to be solved. In this work, lead-free Cs2AgBiBr6 single crystals have been synthesized by slowly evaporating organic solvents and by using the well-known controlled cooling technique. The evaluation of solubility curves showed that slow evaporation enables crystal growth in a wide range of temperatures. We further used the controlled cooling technique as a reference to the slow evaporation method to grow crystals at different temperatures. The quality of the synthesized crystals was characterized by X-ray diffraction (XRD) and energy dispersive X-ray (EDX) measurements. Furthermore, photoluminescence excitation (PLE) and absorption measurements were conducted to investigate the relationship between Urbach energy and the growth method and temperature. As a result, we found that growth temperatures significantly impact the amount of tail-states present in the perovskite crystals.

CPP 19.4 Wed 10:30 H38

**Real-time texture and phase evolution tracking of the annealing process of slot-die coated perovskite by in situ GIWAXS** — •Manuel A. Reus[1], Lennart K. Reb[1], Alexander F. Weinzierl[1], Christian L. Weindl[1], Renjun Guo[1], Tianxiao Xiao[1], Matthias Schwartzkopf[2], Andrei Chumakov[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1,3] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching — [2]DESY, 22607 Hamburg — [3]MLZ, TU München, 85748 Garching

In perovskite solar cell material research the thin-film morphology determines the quality of the absorber material and consequently device performance. To scale up material deposition towards, e.g., roll-to-roll compatible techniques, the influence of the deposition method on morphology needs to be known to control the process. Here, we apply in situ grazing-incidence wide-angle x-ray scattering (GIWAXS) on the annealing process of slot-die coated lead iodide and slot-die coated methylammonium iodide, that react to perovskite under heat. We track the conversion in real-time and extract relevant parameters concerning texture and phase evolution. As a reference, we show GIWAXS data of spin-cast equivalent systems and show the resulting morphology and kinetics differences traced back to the deposition method.

CPP 19.5 Wed 10:45 H38

**Temperature-reduced and rapid growth of hybrid perovskite single crystals** — •Julian Höcker[1,2], Felix Brust[1], Melina Armer[1], and Vladimir Dyakonov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg, Germany — [2]Experimental Physics - Soft Condensed Matter, Ludwig Maximilian University of Munich, 80539 Munich, Germany

Organolead trihalide perovskite single crystals are gaining more and more interest in the field of semiconductor research since they can be used for a variety of technical applications, like photodetectors or solar cells. To date, exclusively solution-processed perovskite crystals have been used for the fabrication of such device prototypes. A supersaturated perovskite solution is caused either by a temperature change, solvent evaporation, chemical reaction, or a combination of the methods. The aim of the various processes is to achieve rapid growth of crystals with controlled structure, size, shape, and yield. In addition, the crystalline components must exhibit high physical and chemical qualities to be applied as semiconducting components. However, these high requirements and numerous criteria cannot always be fully met by standard techniques like inverse temperature crystallisation. In order to grow large-sized OLTP single crystals in a controlled and simple manner from solution in the shortest possible time, we developed a crystallisation process based on primary alcohols. As a result, the blends based on perovskite precursor solution and alcohols lead to a significant reduction in their retrograde solubility and enable a temperature-reduced crystallisation pathway to grow single crystals.