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Investigation of Halide Perovskite Precursor Solutions with SAXS

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Abstract

Halide perovskites (HPs) as an absorber material for solar cells has drawn the attention of the scientific community due to their outstanding increase in efficiency up to 26.1% as well as low-cost solution-based processing methods. Despite their popularity, it is not yet fully understood how anions, cations and the solvent influence the early stages of crystallization. For this reason, we used small angle X-ray scattering (SAXS) to investigate the precursor solution of $FAPbI_3$, $MAPbI_3$, $CsPbI_3$, $RbPbI_3$, $KPbI_3$, $NaPbI_3$ and $MAPbBr_3$ in γ-butyrolactone (GBL), dimethylformamide (DMF), dimethyl sulfoxide (DMSO), N-methyl-2-pyrrolidone (NMP) and mixtures thereof. This follows a previous study where we investigated the precursor solution of $MAPbI_3$, $FAPbI_3$ and $MAPbBr_3$ in GBL, DMF and mixtures. We performed SAXS experiments at BESSY II, at PTB's four-crystal monochromator beamline using the ASAXS end station. Previously, we developed a core-shell model with $[PbX_6]$ (X = I, Br) octahedra surrounded by solvent molecules to explain the distance between adjacent scattering objects (d_{exp}). The core can be arranged as a single octahedron or as corner-sharing octahedra, depending on the anion and the solvent. It was shown that a molecular A-cation (MA^+, FA^+) does not affect the precursors' arrangement. In this study, we demonstrate that alkali metals (Na^+, K^+, Rb^+, Cs^+) as A-cation influence d_{exp} due to higher charge density than molecular cations. Thus, we extended the core-shell model assuming that the A-cation and the solvent molecules compete to surround the core. The $[PbX_6]$ octahedra are surrounded by a solvent shell with randomly oriented molecules or by an A-cation shell. The SAXS data analysis (using SASfit) shows higher polydispersity than the previous model, which indicates an increase in the heterogeneity of the solution and aligns well with the proposed extended model.

Keywords

Precursor Solution, SAXS, Halide Perovskites