

*X-ray absorption spectroscopy applied to solar absorbers*Michael F Toney¹¹SLAC National Laboratory, Menlo Park, United States

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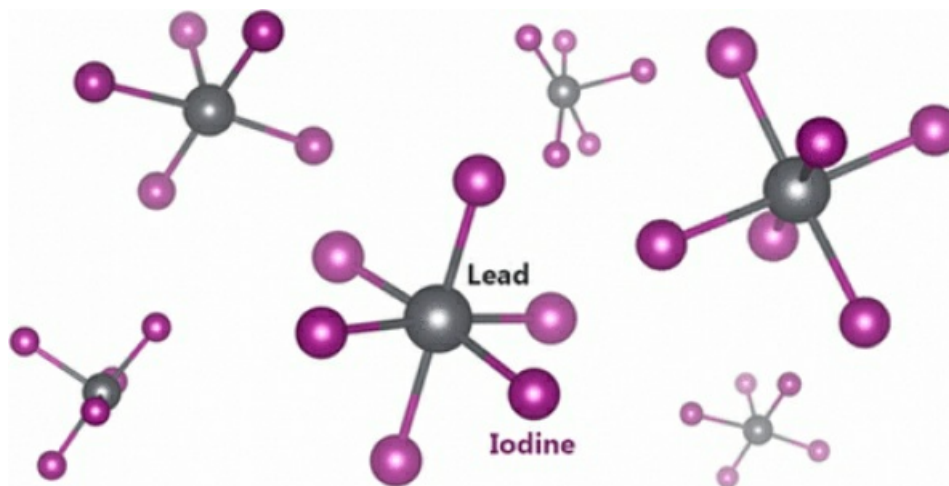
Lead halide perovskite solar cells have attracted substantial academic and commercial interest due to their ability to achieve relatively high power conversion efficiencies (>20%) using readily scalable solution-based fabrication protocols [1,2]. The precursor solution chemistry (precursor molar ratio, solvent, additives, etc.) has been shown to strongly affect the final thin film morphology (roughness, coverage, grain size). Specifically, it has been demonstrated that a molar excess of the organic precursor, methyl ammonium iodide (MAI), is required to produce a continuous, compact, dense film whereas a solution containing stoichiometric amounts of lead iodide and MAI produces a highly discontinuous morphology consisting of needlelike one dimensional features. As the final film morphology dramatically affects photovoltaic performance, it is imperative to understand the relationship between solution chemistry and film morphology.

We have used x-ray absorption spectroscopy (XAS) to characterize the lead coordination environment in solution as a function of precursor stoichiometry as well as using the processing additive hydriodic acid (HI) [3]. By analyzing the extended x-ray absorption fine structure (EXAFS), we are able to determine that in a stoichiometric precursor solution lead ions are coordinated by both solvent molecules and iodide ions but as a molar excess of MAI is added solvent molecules are displaced by additional iodide ions, thus increasing the iodide coordination number. Similarly, the addition of HI to a stoichiometric solution of PbI₂ and MAI results in the displacement of solvent ions and an increase in the iodide coordination number, albeit at slightly larger Pb-I bond distances than when using excess MAI. This data is presented in the context of how precursor chemistry and the lead species present in solution affect the final film morphology. This work therefore provides mechanistic insight into how precursor solution chemistry can be tuned in order to readily produce smooth, continuous, dense lead halide perovskite films for use in high efficiency solar cells.

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