# Synthesis and Evaluation of a Low-Cost Biopolymer Encapsulant for Lead Sequestration in Halide Perovskite Solar Cells

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In recent years, single-junction perovskite solar cells with lead-halide frameworks have garnered considerable interest for their superior photovoltaic performance, facile fabrication, and tunable optoelectronic properties. However, concerns about lead toxicity and instability in lead-halide perovskite solar cells (LHPSCs) remain. Water infiltration through the perovskite layer along grain boundaries can lead to the formation of PbI2, the primary decomposition product containing lead in highly efficient solar cells. Given that the maximum permissible levels of lead in drinking water in the U.S. are 15 ppb (EPA), it is crucial to effectively control and restrict the release of dissolved lead-containing products into soil and water reservoirs from LHPSCs. In this project, the efficacy of an alginate-L-cysteine (SA-Cys) biopolymer film was explored for mitigating lead leaching from LHPSCs. Alginate, a biocompatible and biodegradable polymer, was functionalized with thiol groups to enhance its adsorption and chelation of lead ions. The modified polymer was integrated outside the perovskite architecture through a multi-layer deposition strategy, resulting in a modified LHPSC that achieved a sequestration efficiency of 80% and retained over 97% of its original lead content under simulated rainfall. Electronic structure calculations using the PCM solvation model showed the SA-Cys monomer had improved lead-binding properties compared to its non-functionalized counterpart. A preliminary analysis of the performance of encapsulated cells demonstrated that SA-Cys had no impact on the PV output of the solar cells. This investigation provides valuable insights into addressing the challenges associated with lead leaching and aims to further enhance the performance of LHPSCs.