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Computational Approaches to the Design of Lead-Free Perovskite Solar Cells

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Perovskite solar cells (PSCs) have shown significant promise as an efficient alternative in the renewable energy sector, demonstrating impressive results in capturing solar energy. A key component of these materials is inorganic perovskites, such as $CsPbX_3$ (X = Cl, Br, I), which have band gap values ranging from 1.72 eV for $CsPbI_3$ to 2.31 eV for $CsPbBr_3$.
However, the presence of lead (Pb) in these compounds raises environmental concerns, particularly because it can become a contaminant at the end of the cells'; lifespan.
This study aims to explore lead-free alternatives or those with reduced Pb content by focusing on the theoretical and computational investigation of the physical properties of the compounds $CsGe_nPb_{1-n}X_3$ and $CsSn_nPb_{1-n}X_3$ (X = Cl, Br, I; $0 \leq n \leq 1$). We look at key aspects such as formation energy, electronic structure and band gap. To accomplish this, we conducted a series of ab initio calculations based on quantum mechanics using Density Functional Theory (DFT), along with some machine learning techniques for added insight.
Additionally, this research assesses the structural and electronic properties of these compounds, examining their energetic stability, photovoltaic efficiency, and other essential characteristics. We also considered the Jahn-Teller effect and its impact on the structural stability of the cells, exploring different configurations of the octahedral structures in the materials.
Our ab initio calculations were carried out using the Pseudopotential plus Plane Wave method implemented in the Vienna Ab initio Simulation Package (VASP). These calculations were complemented by numerical simulations of solar cell efficiency using SCAPS-1D software to identify the optimal configuration for maximum power conversion efficiency by testing ZnO for the electron transporting layer and Cu_2O hole transporting layer.