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Effect of Selected Dopants (Bi, Sb, and Sn) on the Optoelectronic Properties of Formamidinium based Lead Halide Perovskite materials: An Ab Initio Density Functional Theory Study

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Abstract

Organic-inorganic hybrid perovskite solar cells (PSCs) are promising for next-generation photovoltaics due to their high power conversion efficiency, tunable bandgaps, and cost-effective fabrication [1]. However, lead toxicity and material instability remain key challenges. This study explores the effects of Bismuth (Bi), Antimony (Sb), and Tin (Sn) doping on the optoelectronic properties of formamidinium-based mixed lead halide perovskites using an ab initio Density Functional Theory (DFT) approach.

DFT calculations using the Generalized Gradient Approximation (GGA-PBE) exchange-correlation functional were performed to analyze the structural, electronic, and optical properties of the undoped perovskite. The bandgap of undoped $FAPbI_3$ was calculated to be 1.28 eV, aligning well with values suitable for efficient light absorption in solar cells. Structural relaxation confirmed lattice stability in the pristine material.

Currently, one of the selected dopants, Sn doping simulations are in progress to evaluate its effects on bandgap modulation, defect states, and charge transport properties. Preliminary insights suggest that Sn incorporation could enhance light absorption and improve charge carrier dynamics, contributing to overall device performance. Further analysis, including defect formation energies and optical absorption spectra, will provide deeper insight into the viability of doping for optimizing perovskite solar cell efficiency.

This study aims to determine optimal dopant concentrations for enhanced optoelectronic performance while maintaining structural stability. Further analysis, including defect formation energies and charge transport characteristics, provided deeper insights into the impact of doping on perovskite solar cells.

References

1. R. Rajeswari, M. Mrinalini, S. Prasanthkumar, and L. Giribabu, "Emerging of Inorganic Hole Transporting Materials For Perovskite Solar Cells,"Chem. Rec., vol. 17, no. 7, pp. 681–699, 2017, doi: 10.1002/tcr.201600117.

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