Ab-initio Study of the Optoelectronic Properties of $CsXCl_3$ Perovskites (X = Pb, Sn or Ge)

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Introduction

Halide perovskite-based solar cells are very attractive due to their excellent power conversion efficiency and low cost.

Experimental/Theoretical Study

In this work CsXCl3 perovskite alloys (X = Pb, Sn or Ge)are investigated using the ab initio Quantum Espressopackage, which is based on the pseudo-potential and plane wave methods.

Results and Discussion

The calculation of the electronic band structures and the density of states shows that these materials have a direct gap, which is crucial for photovoltaic applications. In addition, the light absorption domain is determined through the examination of the optical properties, allowing us to better understand the photovoltaic behaviorof these compounds.

Conclusion

Our results reveal that these materials are promising photovoltaic candidates.

Keywords: Photovoltaic materials; perovskite structure; DFT;TDDFT; Quantum Espresso; Band gap.

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