DFT Study on Rubidium based Perovskites for Solar Cells Applications

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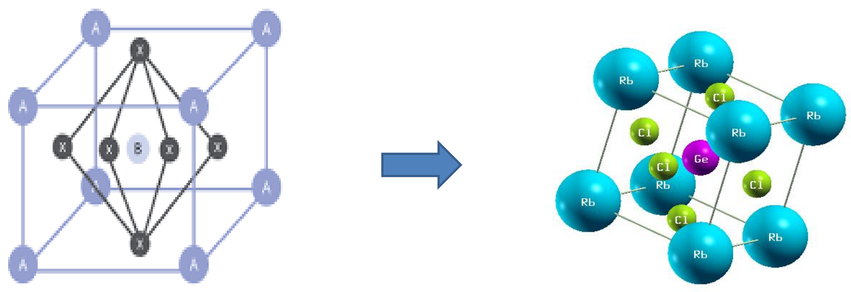
Background

1. Background and Problem Statement

Lead-based perovskites like $CH_3NH_3PbI_3$ pose environmental risks due to toxic PbI_2 by-products formed upon decomposition in water[1]. This necessitates developing environmentally friendly alternatives for sustainable photovoltaic applications. This research investigates lead-free perovskite materials by substituting lead with germanium from group 14 elements. The study focuses on $RbGeX_3$ compounds (where Rb occupies the A-site, Ge the B-site, and halides I, Cl the X-site) across different crystallographic phases (cubic, trigonal, and tetragonal). These germanium-based perovskites are expected to offer reduced environmental toxicity, improved structural stability, and enhanced solar cell efficiency compared to lead-based counterparts, while enabling bandgap optimization for better photovoltaic performance



(a) (b)

Fig. 1 *(a) :The Idealized Cubic Arrangement of the ABX_3 Perovskite Lattice [2] (b) A visual drawing of a $RbGeCl_3$*

Current Work

1.Specific Objectives

1.Determine the energy band gap using DFT.
2.Determine the dynamical stability
3.Estimate the electrical conductivity
4.Determine the optical properties

2. Methodology

This study utilized the Quantum Espresso code to optimize the cubic structure of the compound. The flowchart depicts the iterative process applied to attain self-consistency in DFT calculations, ensuring precise electronic structure outcomes.

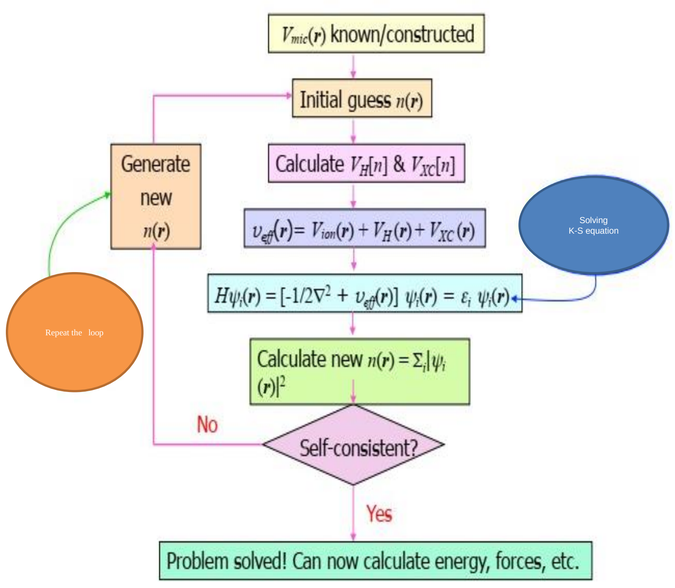


Fig. 2 *:Self Consistent field procedure*

3. Preliminary Results – Structural optimization

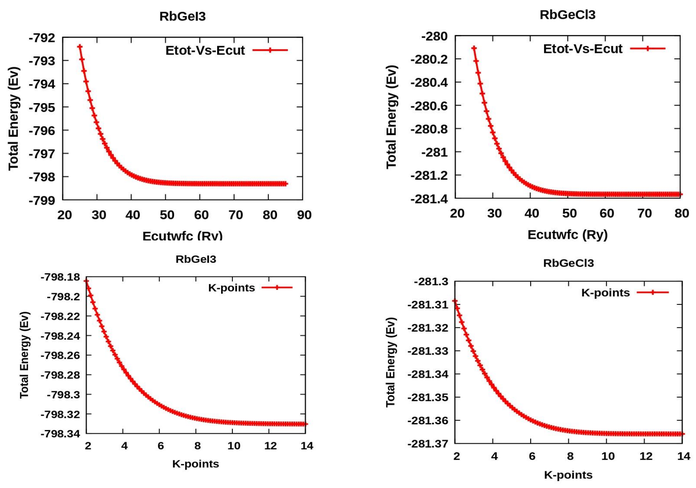


Fig. 3 : *The optimized Ecut and K-point plots for RbGeCl3 and RbGeI3.*

The plot illustrates the convergence behavior of the total energy for both $RbGeCl_3$ and $RbGeI_3$ as a function of increasing Ecut and K-points. The total energy stabilizes at higher values, indicating a threshold beyond which further increases in Ecut and K-points have minimal. The optimal parameters were determined to be an Ecut of 60 Ry and a K-point grid of 10, ensuring reliable computational accuracy for both compounds.

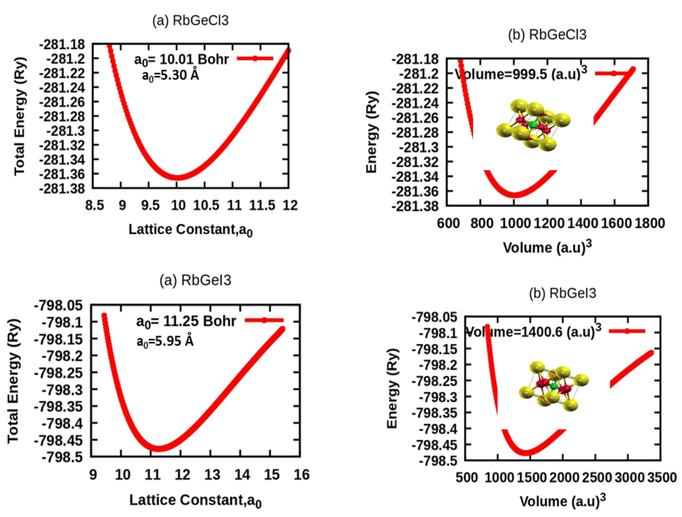


Fig. 4*: Optimized Lattice parameters for $RbGeCl_3$ and $RbGeI_3$.*

The plot presents the optimized lattice parameters for $RbGeCl_3$ and $RbGeI_3$, derived from computational analysis. For $RbGeCl_3$, the equilibrium lattice constant is determined to be 10.01 Bohr (5.30 Å), corresponding to an equilibrium volume of 999.5 (a.u.)³. In contrast, $RbGeI_3$ exhibits a larger equilibrium lattice constant of 11.25 Bohr (5.95 Å) and an equilibrium volume of 1400.6 (a.u.)³. These values highlight the structural differences between the two compounds, reflecting the influence of the halide ion on the lattice dimensions

Conclusion & Expectations

The results offer a comprehensive comparison of the two compounds, highlighting their successful structural optimization and confirming their suitability for further exploration of additional properties.
To advance this research, collaboration with machine learning scientists, solar energy experts, and research funding organizations is anticipated to enhance resources, expertise, and access to international partnerships.

References & Acknowledgment

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