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Structural and Electronic Properties Analysis of Cs2XBr6 (X=Ge and Si) Perovskite Compounds for Photovoltaic Applications

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Structural and Electronic Properties Analysis of Cs_2XBr_6 (X=Ge and Si) Perovskite Compounds for Photovoltaic Applications

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Abstract

In this study, we investigated the structural and electronic properties of Cs_2GeBr_6 and Cs_2SiBr_6**,** which belong to the perovskite family and are promising materials for photovoltaic applications. The calculations were carried out using the *ab-initio* method known as linearized augmented plane waves (FP-LAPW) within the framework of Density Functional Theory (DFT).

Our results regarding the structural properties, such as the lattice constant for Cs2GeBr6 (a=10.6032Å) and Cs2SiBr6 (a=10.5666Å), and the compressibility modulus and minimum energy obtained by LDA, are in agreement with theoretical values. These properties indicate significant structural stability, a key factor in improving the performance of these materials in photovoltaic applications.

The study of the electronic structure showed that the energy gap is direct for both Cs2GeBr6 and Cs2SiBr6, making these materials suitable candidates for solar cell applications, as direct energy gaps enhance light absorption efficiency. However, the calculated values of the energy gaps using LDA and GGA approximations were lower than experimental values, which is attributed to known deficiencies in Density Functional Theory (DFT). Nevertheless, the results for Cs2GeBr6 (GGA, Eg = 0.959eV) and Cs2SiBr6 (GGA, Eg = 0.933eV) were consistent with theoretical data.

We also studied the total and partial densities of states (DOS) for the two compounds, allowing us to identify the type of atoms and orbitals formed between the different elements in the compound. This deep understanding of the electronic properties helps improve the design of materials for use in solar cells.

We used the linearized augmented plane wave method (FP-LAPW) based on Density Functional Theory (DFT) to calculate the structural and electronic properties. We employed the Local Density Approximation (LDA) and Generalized Gradient Approximation (GGA) to calculate the exchange-correlation potential (XC) in order to obtain the structural properties such as the lattice constant and compressibility modulus, and the resulting values were consistent with the available practical results.

When using the LDA and GGA approximations to calculate electronic properties (energy bands and density of states), we observed significant improvement in the results with the GGA approximation compared to LDA, which increases the potential for using these materials in photovoltaic applications with higher efficiency.

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Keywords: semiconductors, GGA, LDA, (FP-LAPW), DFT, WIEN2K, perovskite, solar cells.