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Ab-Initio Study of Optoelectronic Properties of $BaLiI_3$ Perovskite

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ABSTRACT

In this work, we have performed ab-initio calculation to study structural, electronic and optical properties of the perovskite compound $BaLiI_3$, which is crystallized in the cubic structure with space group pm-3m. Using the full potential linearized augmented plan wave (FP-LAPW) method within the framework of the density functional theory (DFT) implemented in the WIEN2K code. Exchange correlation potential for the structural and electronic properties have been computed using the LDA and GGA-PBE approximations, whereas the optical properties were computed using the GGA-PBE approximation. The results of the electronic properties show that the compound exhibits semiconductor behavior, while the optical properties indicate that it is characterized by a high absorption coefficient. Thus, is suitable for photovoltaic applications.

Keywords: Perovskite, DFT, WIEN2K, Optoelectronic properties.

1. Introduction

Recently, halide perovskites have emerged as promising candidates for the next generation of clean energy harvesting technologies, due to their low cost, ease of fabrication and exceptional electronic and optical properties [1]. The aim of this work is to investigate the structural, electronic and optical properties of $BaLiI_3$ compound by the DFT using FP-LAPW. Firstly, we computed the ground state properties of cubic $BaLiI_3$ compound like lattice constant and bulk modulus. Then, we calculated the electronic structure including band structure. Finally, we studied the optical properties of our compound.

2. Computational Method

All calculations were carried out using the WIEN2K code [2],which incorporates the full potential linearized augmented plane wave (FP-LAPW) method based on the density functional theory (DFT). The exchange-correlation potential is treated by the local density approximation (LDA) and the generalized gradient approximation (GGA) developed by Perdew-Burke-Ernzerhof (PBE). In our work, the kenitic energy cut off which separated the core and the valence states is chosen to be -6 Ry, the $R_{MT}*K_{max}$ value was assumed to be 7 (Where R_{MT} is the smallest of all MT sphere radius and K_{max} is the maximum value of the wave vector K) and K-points in the first Brillouin zone is selected as 2000. Furthermore, the muffin-tin radii (R_{MT}) values are 2, 2 and 2.25 Bohr for Ba, Li and I, respectively.

3. Results and Discussion

3.1. Structural properties

From Table I we can observe that values of lattice parameter and bulk modulus calculated by GGA-PBE are well in agreement with the available theoretical work. On the other hand, LDA underestimates the lattice constant and overestimates the bulk modulus, which is in line with the general trend of these approximations.

Table 1: *Calculated values of structural parameters for $BaLiI_3$ at the optimized state.*

	Lattice constant (A)		Bulk modulus (GPa)	
	LDA	**GGA-PBE**	**LDA**	**GGA-PBE**
Present work	5.4442	5.6644	27.7407	20.3370
Theoretical work	---	5.66 [3]	---	20.67 [3]

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3.2. Electronic properties

The energy band structure along a high symmetry line of our compound obtained by LDA and GGA-PBE is shown in Figure1. The valence band maximum occurs at the R point, while the conduction band minimum occurs at the Γ point; so $BaLiI_3$ has an indirect gap (R-Γ) of 2.32 eV and 2.60 eV for LDA and GGA-PBE approximations, respectively. This indicates that the GGA-PBE overestimates the band gap compared to the LDA approximation

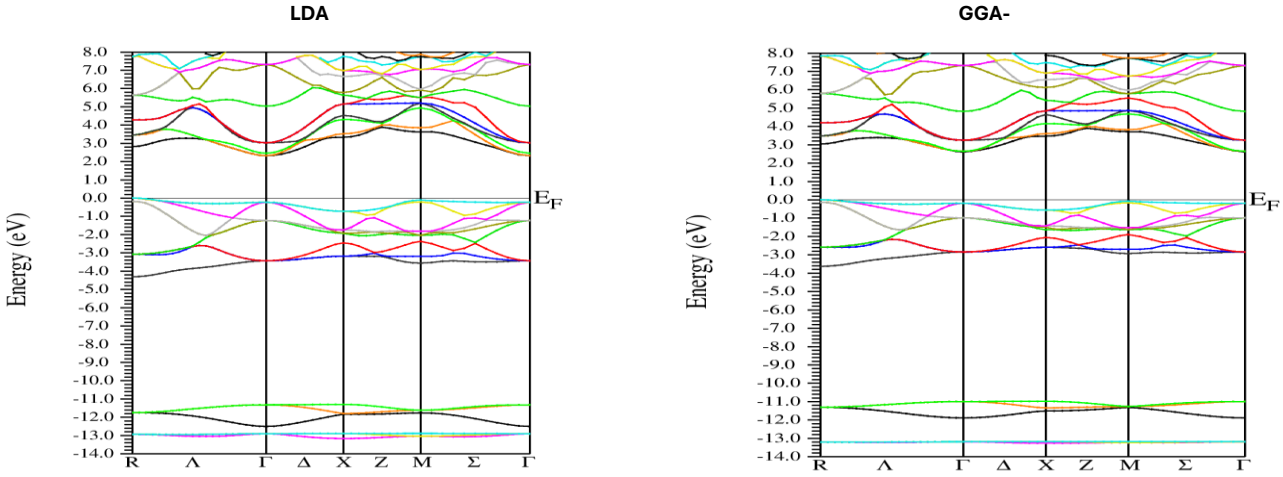

Figure 1: *Band structure of $BaLiI_3$.*

3.3. Optical properties

Significant values were achieved by studying the optical properties of our material. Firstly, from the real part of the dielectric function $\varepsilon_1(\omega)$, we obtained a static dielectric constant of 4.42. Secondly, from the imaginary part, the threshold energy determined at 2.57 eV was found to be almost identical to the band gap obtained by our analysis. In addition, the static refractive index, recorded at 2.1, and the high absorption coefficient at 30 eV.

4. Conclusions

In this work, we have investigated the structural, electronic and optical properties of BaLiI3 compound using the full potential linear augmented plane wave (FP-LAPW) within the framework of DFT based on LDA and GGA-PBE approximations. The optimized lattice constant achieved via GGA-PBE approximation is in accordance with the available theoretical result. From the electronic properties, the band structure indicates a semiconductor behavior with an indirect gap according to the two approximations: LDA and GGA-PBE. Furthermore, optical parameters were also determined over the energy range 0-40 eV. Our results suggest that this compound can be useful for photovoltaic applications.

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