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STRUCTURAL AND ELECTRONIC PROPERTIES OF THE COMPOUND Mg2Ge

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ABSTRACT

A calculation method Ab_Initio was used to study the structural and electronic properties of Mg2Ge compound their antifluorite structure by the method of augmented plane wave linearized (FP-LAPW) which is based on the functional theory of density (DFT). We used it for the generalized gradient approximation (GGA) and GGA-MBJ method for the term of the potential for exchange and correlation, although for the structural properties such as minimum total energy E0, setting network a0 (Å), compressive modulus B (GPa), its derivative BP, and for the electronic properties (density of states (DOS) and band structure (GAP). All this is done with the WIEN2k code. According to the results of the electronic properties, we find that Mg2Ge made is a semiconductor with indirect band.

KEYWORDS: *Semiconductor, DFT, Ab_Initio, Mg_2Ge,* generalized gradient approximation (GGA) and GGA-MBJ

1. INTRODUCTION

The compound Mg2Ge "Germanium Magnesium" is a semiconductor that is crystallized in the antifluorite structure (the group Fm-3m space) CaF2-type (Cubic Faces Focused CFC). It is characterized by high mobility of the charge carriers (electrons and holes), which gives an advantage to use this material especially for thermoelectric effects. The calculations were made by the method of linearized augmented plane wave (FP-LAPW) within the framework of the density functional theory (DFT), and to determine the potential for exchange and correlation, we used the GGA approximation and BJ-GGA method that can provide a good description of the electronic structure and allowed us to have a value of indirect energy gap underestimated and close to the experimental value of 0.69 [3]. The experimental values of the structural parameters such as the parameter of the crystal lattice a0 (Å) is 6.393 [4] and the compression modulus at equilibrium which depends on the rigidity of the material B (GPa) equal to 54.7 [5]. The first calculations of Mg2Ge composed of band structures were made in early 1960. The values of the indirect energy gap theoretically obtained for Mg2Ge, are in the range 0.57-.74 eV [1-2].

2. METHOD COMPUTER

The simulation code WIEN2k was developed at the Institute of Materials Chemistry at the Technical University of Vienna. [6] In the following years, this code has been continuously revised and has undergone several updates. WIEN original code versions were developed (called, in the year of their publication, WIEN93, WIEN95 and WIEN97). We used the WIEN2k Version (2012) which underwent a significant improvement, particularly in terms of speed. A new version of the exchange potential, proposed for the first time by Becke and Johnson [7], was recently tested and published by Tran and Blaha [8]. This is the potential mbd "Becke modified Johnson Potential" (also called TB potential Tran-Blaha) which has been implemented in the latest

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version of WIEN2k code. The code parameters must be optimized to have a stable structure of the material. Product RMTmin * Kmax being a dimensionless quantity, where RMTmin means the radius of the smallest atomic spheres present in the mesh to study and Kmax represents the module of the wave vector up to the base plane waves used in the description of the entire system of the electrons present in the space between the atomic spheres. We will make a calculation of the electronic properties of Mg2Ge composed by FP-LAPW method, where we took the number of points K = 900 and product value RMTmin * Kmax = 8.

3. RESULTS AND DISCUSSION

3.1 Structural Properties

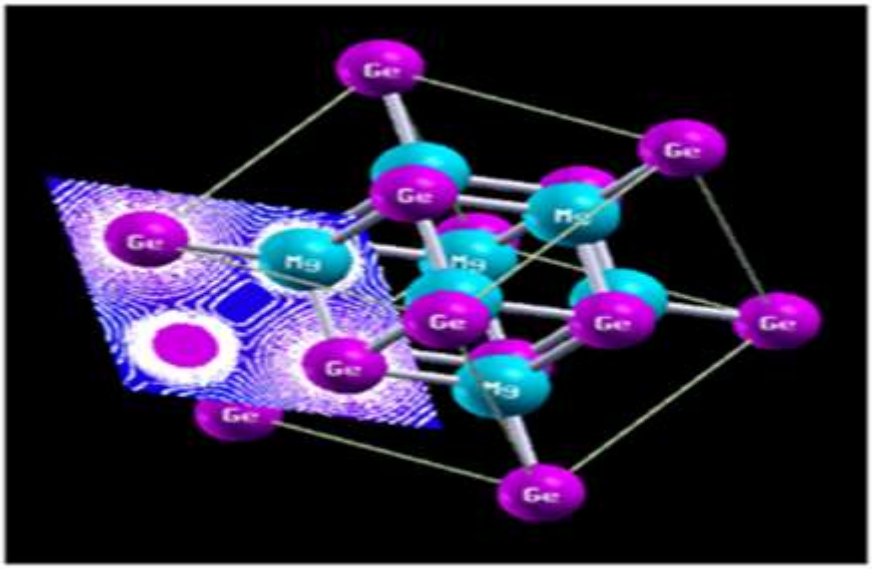

Figure 1: The crystal structure of antifluorite Mg_2Ge compound.

We have found the following parameters: a 0 (Å) represents the parameter of the crystal lattice, V0 (a.u3) is the volume of the unit cell at equilibrium atomic unit B (GPa) and BP are the module respectively compression at equilibrium which depends on the rigidity of the material and its derivative with respect to pressure, E0 (Ry) = -4999.590095 Ry is the minimum energy. These parameters are obtained after volume optimization will help determine the Mg2Ge structure more stable and thus access by following other physical properties.

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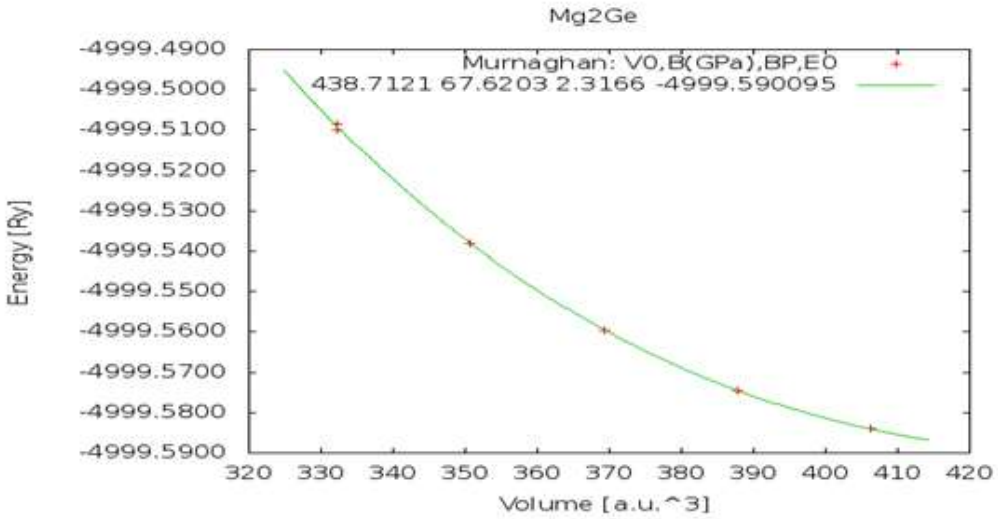
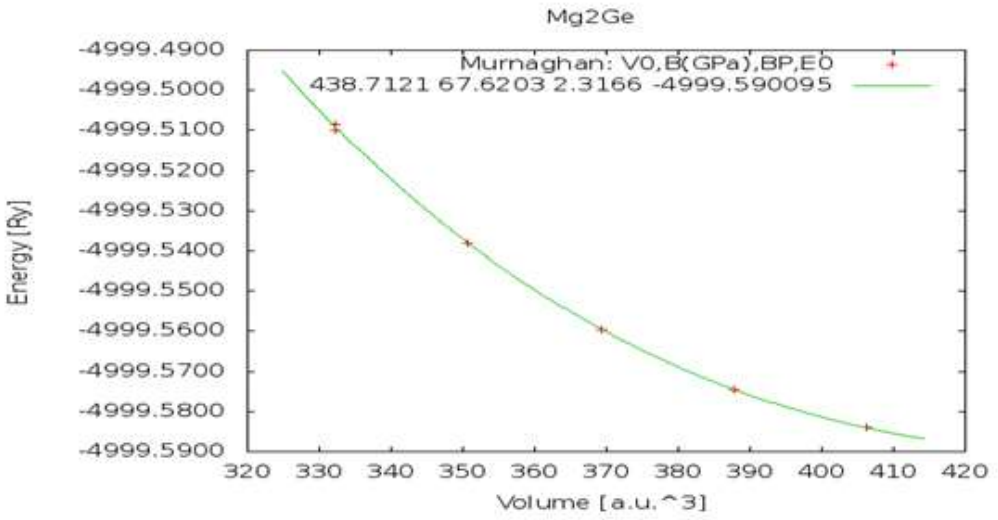
CODEN: IJESS7





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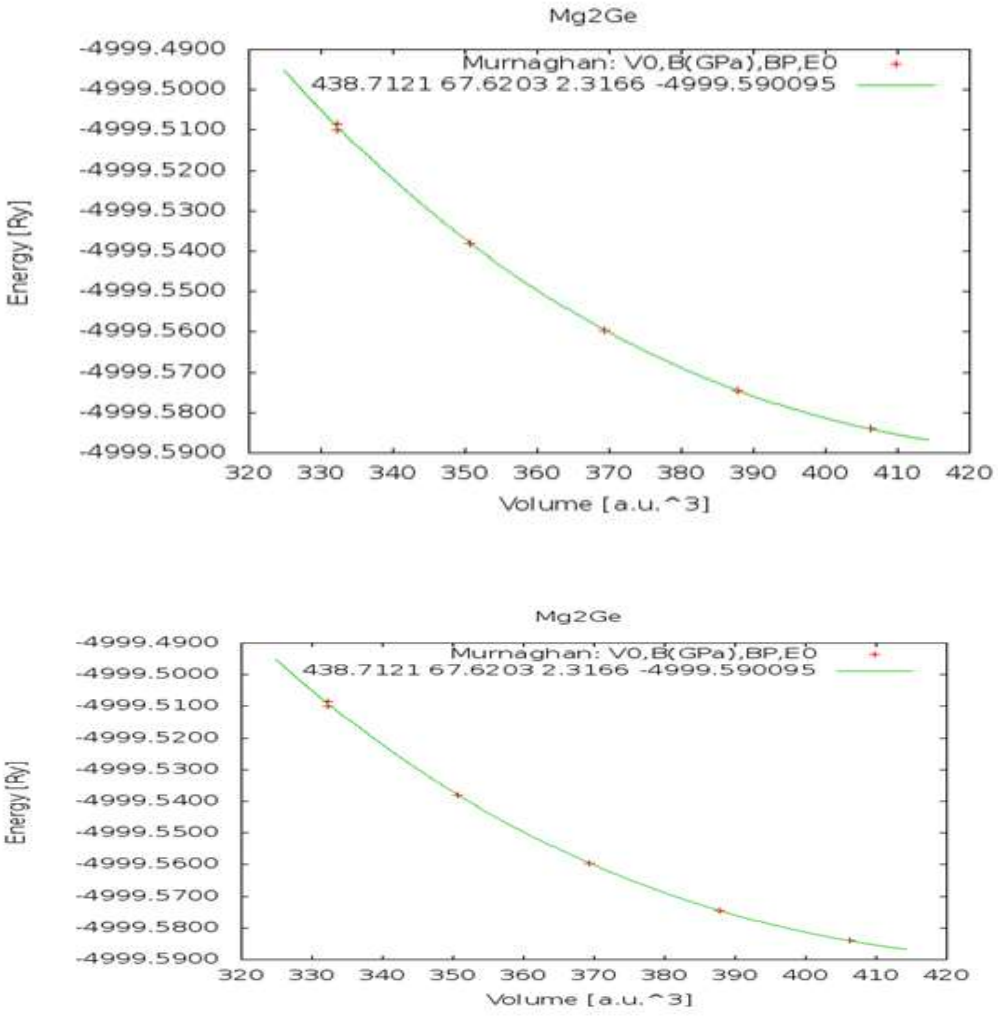

Figure 2:Energy based on volume for Mg2Ge in the GGA approximation.

This table shows a comparison between the structural parameters and we found some theoretical and experimental values available in the literature:

Table 1:Comparison between our values and those found by other authors optimized structure parameters of Mg2Ge compound.

Mg2Ge	Our results byGGA	Other theoretical values	Experimental Values
a_0 (Å)	6.391	6.12 [12], 6.286[13], 6.31 [14]	6.393[4], 6.3849 [9], 6.378[10]
V_0 (a.u^3)	438.7121		
B(GPa)	67.6203	57.6 [12], 55.9 [13], 55.1 [11]	44.0-54.7 [5]
BP	2.3166	4.051[13]	
E_{min}(Ry)	-4999.590095		

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3.2 The electronic properties

The importance of the electronic properties of a material is that they allow us to have the statements for each band and understand the nature of the material based on the band gap (gap) between the valence band from that of the conduction band. These properties include the density of states (DOS) and band structures.

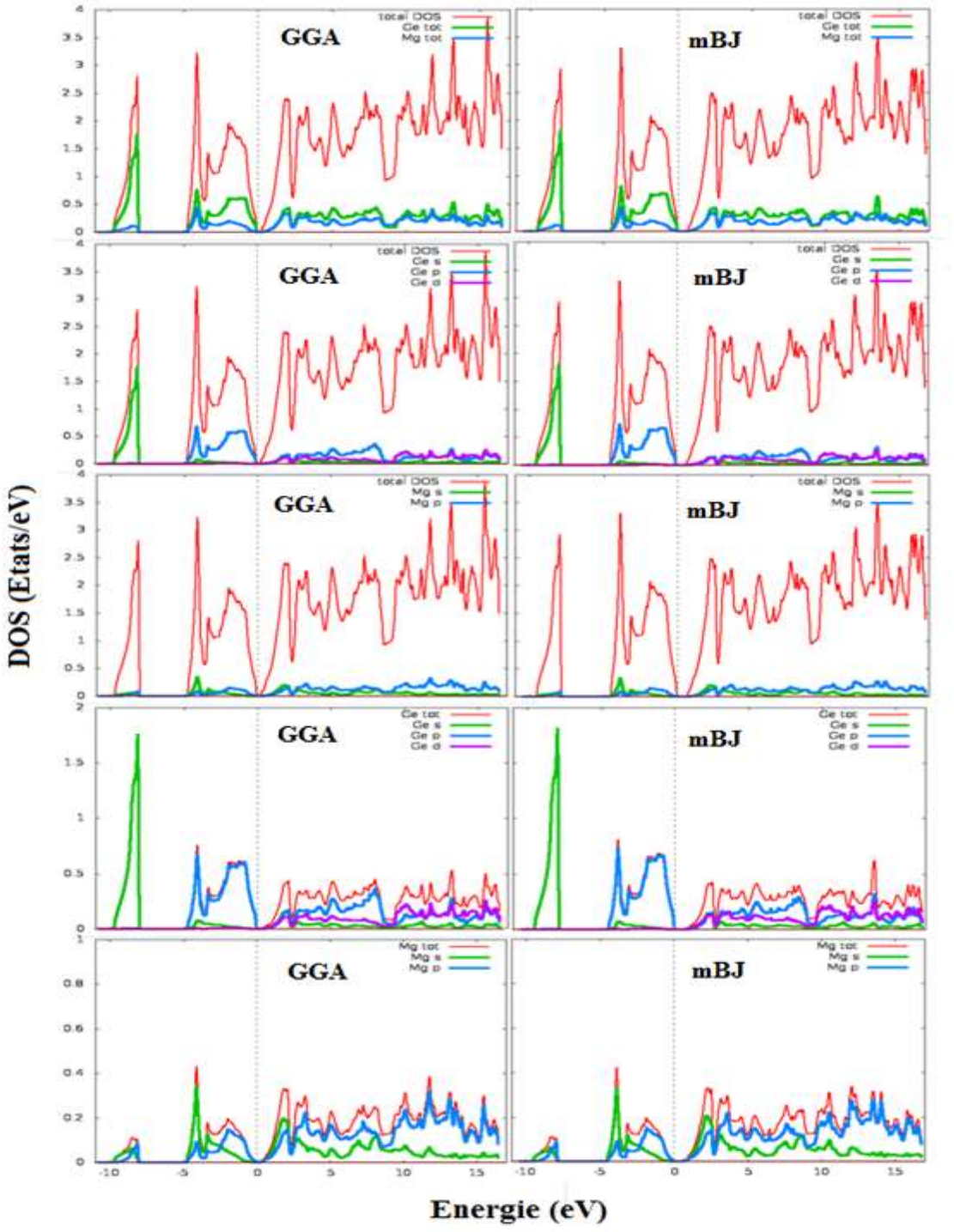

Figure 3: Status Density "DOS" total and partial of Mg2Ge composed by GGA and MBJ-GGA.

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Figure 3 shows that in the phase of antifluorite Mg2Ge compound, we found the use of GGA and MBJ-GGA the same states for each band. The Valencia region is divided into two regions. The first region between -10 and -8 eV, where the main contribution is that from the s state of the atom Ge, with a small contribution of the states s and p of Mg atom. The second region between -5 and 0 eV, which is observed in the statements of contributions of Ge atom p and s and p of Mg atom, with a very small contribution to the state s of the Ge atom . Mg2Ge the conduction region is mainly dominated by the state s and p of Ge atom and the p state of the Mg atom.

We calculated the Mg2Ge composed of band structure along the high symmetry lines in the first Brillouin zone with GGA and MBJ-GGA. The Fermi energy (EF) was reduced to 0 eV in these figures and is indicated with the horizontal line between the valence band to the conduction band. We got the band structure that is present on the Fig.4. From this figure, we see that the minimum of the conduction band and the maximum of the valence band are not found at the same point k, but precisely at the point X to the minimum and the point Γ to the maximum first Brillouin zone. Therefore, the Mg2Ge compound is a semiconductor which has an indirect energy gap (Γ-X) equal to 0.17 eV and 0.58 eV by GGA and BJ-GGA respectively.

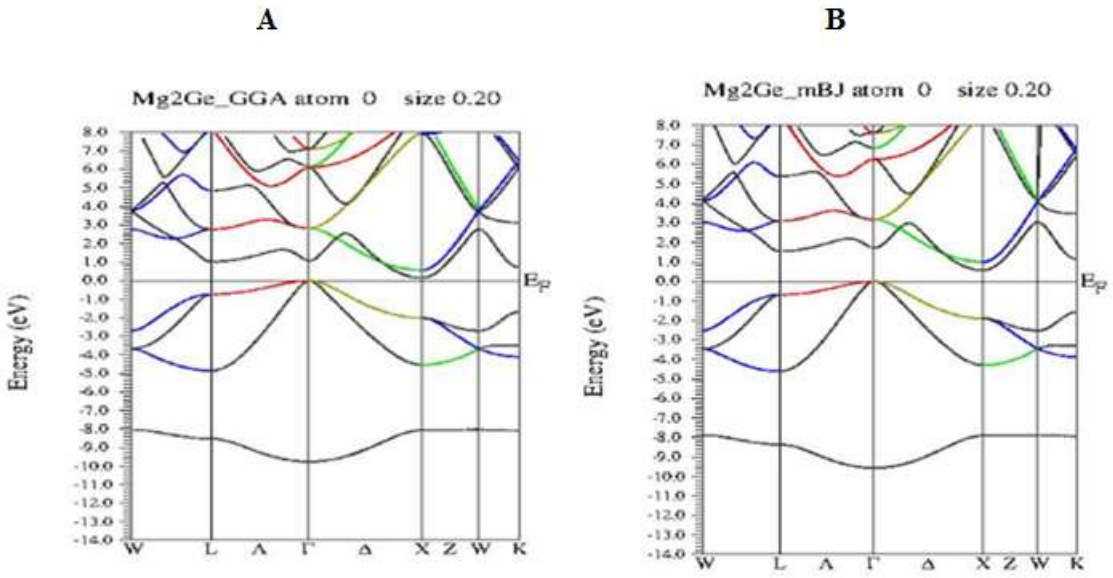

Figure 4: A) Band structure of Mg2Ge composed by GGA. B) Mg2Ge composed of strips structure using MBJ-GGA.

Table 2: Comparison of the results we have achieved by GGA and MBJ-GGA with other work.

Methode	Our results (GGA)	Ourresults (mBJ-GGA)	theoretical values	Experimental Values
Gap indirect (**Γ-X**) (eV)	0.17	0.58	0.166[16], 0.21 [15]	0.69 [3], 0.74 [17], 0.76 [1]

We see from this table that the underestimation compared to the experimental value of the value of the indirect energy gap obtained by BJ-GGA is higher than that obtained by GGA. And the use of the MBD-GGA method gives an increase in the value of the indirect gap of approximately 71% from that calculated by GGA and which is less than about 16% compared to the experimental value 0.69eV [3]. We can explain this improvement and confirmation of the increase of the band gap (gap) by the strong processing electron correlation.

4. CONCLUSION

In this work, we investigated the structural properties and electronic properties such as the density of states and band structure for Mg2Ge compound. The calculations were made by the method of linearized augmented plane wave (FP-LAPW) within the framework of the density functional theory (DFT), and to determine the potential for exchange and correlation, we used the GGA approximation GGA and MBJ-method. Our calculations of the

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electronic structure indicate that Mg2Ge compound is a semiconductor having an indirect gap Γ- X of about 0.17 eV by the GGA approximation and about 0.58 eV by the MBJ method. So using this latter method has allowed us to have a value close to the experimental value which is about 0.69 eV is an underestimation of about 16% with an improvement in the gap value compared to calculated by GGA.

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