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Structural, electronic and thermoelectric properties of the intermetallic materials based on Mg2X (X= Si, Ge, Sn): DFT calculations.

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Abstract – *The scope of this work is the investigation of the physical properties of chalcopyrite materials using ab-initio methods in order to simulate a new structure of thin-films photovoltaic cells with high conversion efficiency. In the first framework, we obtained the results of calculations based on Density Functional Theory (DFT) using the full-potential linearized augmented plane wave method (FP-LAPW) as involved in the WIEN2K computational package. For the exchange-correlation potential, the local density approximation (LDA) was used to calculate the lattice parameters, Bulk modulus and its first derivative as well as the densities of states of the intermetallic semiconductors materials based on Mg2X (X=Si, Ge and Sn). The semi-local Becke-Johnson (mBJ) potential and its modified form proposed by Tran and Blaha (TB-mBJ) were also used for studying the electronic and thermoelectric properties; (merit factor, Seebeck coefficient, electronic conductivity). The achieved results were compared to computational works and other data acquired experimentally.*

Keywords: *FP-LAPW, Science Research, publication*
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I. Introduction

At this work, we will study the structural properties (lattices parameters, bulk modulus and its first derivative), the electronic properties (total and partial density of states) and thermoelectric properties (Seebeck coefficient, thermal and electrical conductivities and figure of merit) for Mg2X(X=Ge, Si, Sn) compounds. The investigation are accomplished by employing a full potential augmented plane wave (FP-LAPW) method framed within density functional theory DFT as implemented in WIEN2K code. To determine the exchange correlation potential, we have used LDA approximation and Tarn et Blaha functional [1] denoted (TB-mBJ), which is modified of Becke-Johnson in the method FP-LAPW.

II. COMPUTATIONAL DETAILS

In the present calculation, full potential augmented plane wave FP-LAPW [2] method within TB-mBJ approximation and LDA approximation are used as incorporated in WIEN2K code [3].

Half-relativistics calculations are performed (spin orbital effect is neglected). We have carried out convergence tests of total energy E_t for Mg_2X (X=Ge, Si, Sn) as function of R_{mt} and $K_{\max}$ parameters and as function of K-points number over reduced Brillioun zone.
The calculations were performed in self-consistent way, using the two approximations mentioned below.
The input parameters are listed in table1.

Table 1. input parameters of FP-LAPW for Mg2X (X=Ge, Si, Sn) compounds

	Rmt*Kmax	K-points	Rmt (Mg)	Rmt X (Ge, Sn, Si)
Mg2Ge	9	1000	1.9	2.5
Mg2Sn	9	1000	2	2.35
Mg2Si	9	1000	2.5	2.5

III. PROPERTIES OF Mg2X COMPOUNDS

III.1. Structural properties for Mg_2X (X= Ge, Si, Sn)

To determine the lattice equilibrium parameters and find how total energy varies as function of those parameters, we have to realize structural optimization on Mg2X. We have performed, employing WIEN2K, a self-consistent total energy calculations. The minimization of total energy was achieved by computing total energy for different lattice parameters around experimental value.

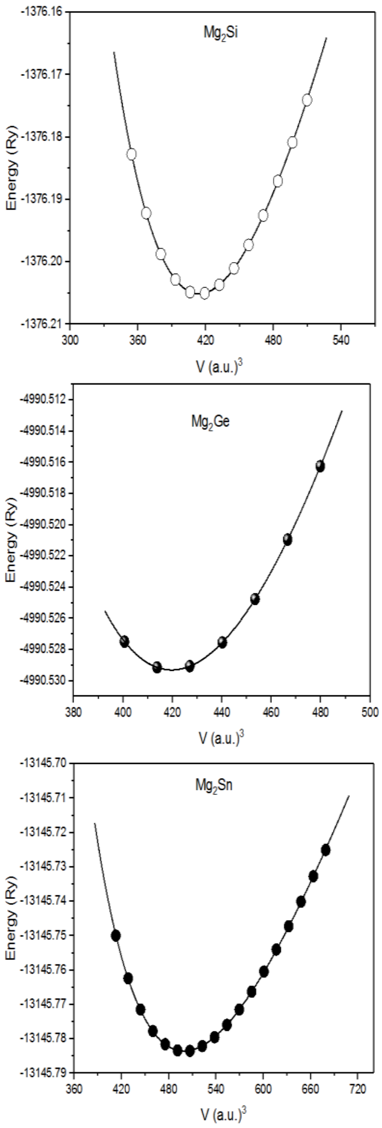


Figure 1. The total energy variation as function of volume for Mg_2X.

The equilibrium volumes for all the investigated compounds were obtained by fitting the total energy as function of Murnaghan's equation state [4]:

$$E(V)= E_0 +\frac{B_0 V}{B_0'}\left[\frac{(V_0/V)^{B_0}}{B_0'+1}+1\right]-\frac{B_0\, V0}{B_0'-1} \quad (1)$$

Where B_0 and B'_0 are respectively the equilibrium bulk modulus and its first derivative of pressure and V_0 being the equilibrium unit cell volume.

The lattice parameter corresponding the ground state is obtained from the minimum of E_{tot} (eV). The total energy was calculated as function of volume (figure 1) for Mg_2X in cubic structure.

Table 2. Lattice parameter a (Å), bulk modulus B (GPa) and its derivative B′ and minimum energy Emin, for Mg2X (X = Si, Ge, Sn).

		Present Calculations LDA	**Other calculations** (GGA)[5]	**Other calculations**	**Experiment**
Mg_2Ge	a (A°)	6,289	6,420	6,12[a] - 6,286[e]- 6,31[f]	6,38[k]
	B_0(GPa)	56,0866	49,7156	57,6[a] – 55,9[e] – 55,1[f]	44,0 – 54,7[i]
	B_0'	4,3089	4,1955	4,051[e]	-
	E_{min}(Ry)	-4990,529293	-4999,5929	–	–
Mg_2Si	a (A°)	6,261	6,369	6,09[a]-6,26[e]-6,29[f]	6,35[k]
	B_0(GPa)	58,7828	54,1633	59,2[a]-58,3[e]-56,2[f]	46,3-55,0[i]
	B_0'	4,2243	3,5255	4,023[e]	–
	E_{min}(Ry)	-1376,202415	-1381,4461	–	–
Mg_2Sn	a (A°)	6,663	6,818	6,825[c]	6,765[k]
	B_0(GPa)	45,6374	40,3594	–	–
	B_0'	4,5973	4,1668	–	–
	E_{min}(Ry)	-13145,78347	-13159,657	–	–

[9][i]. [7][e]. [10][c]. [6][a]. [8][f] .[11][k].

III.2. Electronic properties

The total and partial density of states for Mg2X(X=Ge, Si, Sn) obtained by using mBJ method in cubic structure, are shown in figure 2.

We can deduce that Mg2X compounds have semiconducting character according to the density of states.

The valence band is divided into two bands; the lower one is dominated by X-s orbital with no neglected contribution of Mg-3s and Mg-3p orbitals. The second is between (-9 and -7ev) for Mg2Si and Mg2Sn, between (-10and -8ev) for Mg2Ge below Ef, is dominated by Ge-4s, Si-3s and Sn-5s contribution.

After gap of 2.5ev for Mg2Si and Mg2Sn and 3.5ev for Mg2Sn, it appears that the contribution of states Mg-3s and Mg-3p predominate in this range of (-4.5and 0ev).

In the conduction band, it emerges that the contribution of states Mg-3s, 3p and X-3p are dominated.

According to our decomposition of total and partial densities, we have shown that the valence electrons are mainly around the X (Ge,Si, Sn). Although, there is a weak covalence between Mg and the X

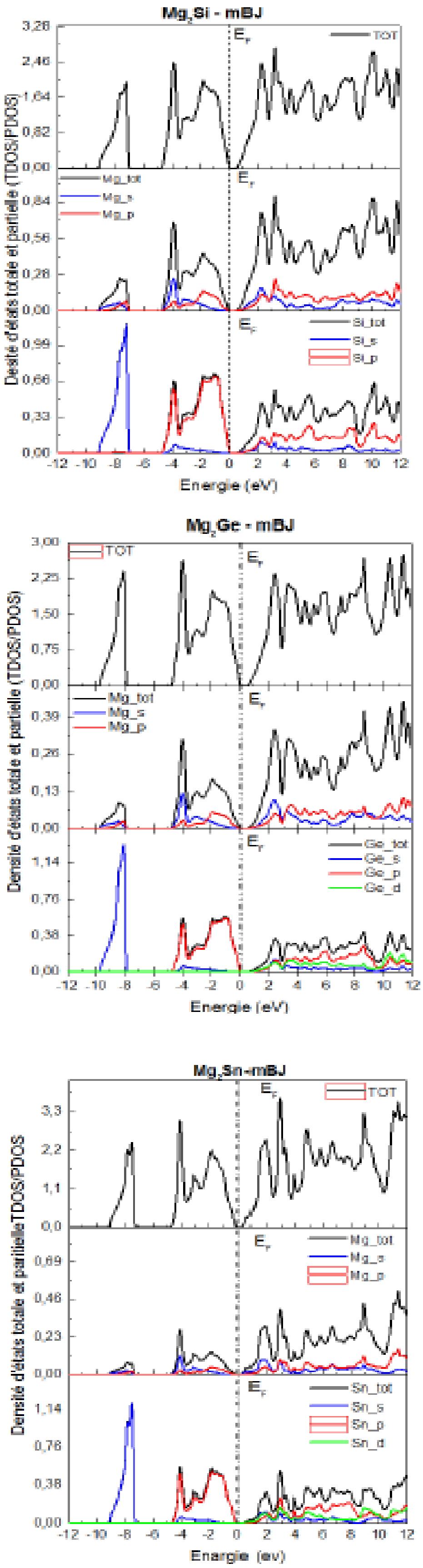
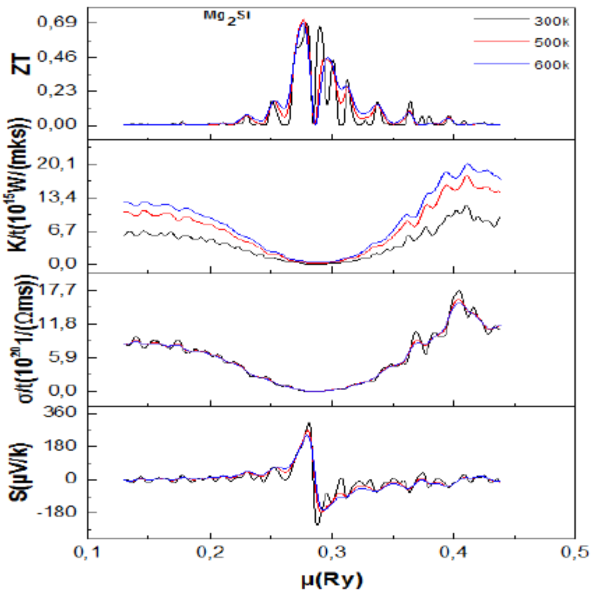


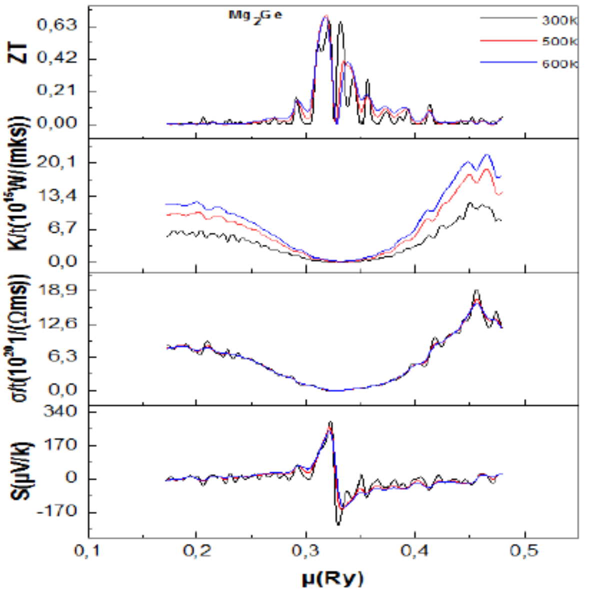
Figure 2. Total and partial density of states for Mg_2X(X=Ge, Si, Sn).

III.3. Thermoelectric properties

The calculation of transport properties such as electrical conductivity, electronic thermal conductivity and Seebeck coefficient are performed using BoltzTrap, which is tool for evaluating those properties, by solving Boltzmann transport equation in the constant relaxation time approximation.

The efficient thermoelectric materials (Figure 3) of Mg2X(X=Ge, Si, Sn) compounds, have obvious attractive characteristics that makes them promising as thermoelectric energy converters in the range of medium temperature between (300-800).





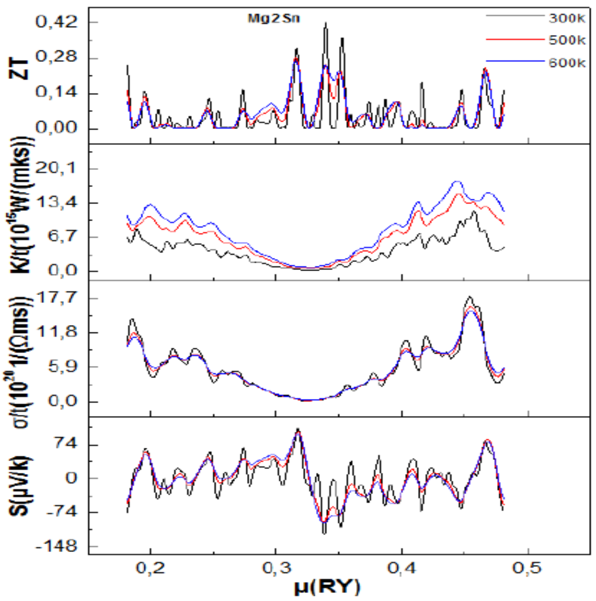


Figure 3. Variation of Seebeck coefficient, electrical conductivity and electronic thermal condutivities with respect to chemical potential for Mg2X(X=Ge, Si, Sn).

IV. CONCLUSION

The purpose of this research work is to investigate the structural, electronic and thermoelectric properties of intermetallic materials based on Mg2X. We have utilized the all-electron FP-LAPW method with LDA for optimizing the lattice constants, the related bulk modulus and its first pressure derivative. The achieved results concerning the structural constants show an excellent agreement with the experimental data and other theoretical values. To calculate the densities of states (PDOS/TDOS) we used the new modified semi-local mBJ approximation, we found that this approach brings the calculated energy gaps close to the experimental values and much better than the previous simulated results. Based on this good agreement, the thermoelectric properties were predicted and discussed in details by using Boltz-Trap code. The results signify that our studied binary compounds are attractive materials for the optoelectronic devices area and thermoelectric applications.

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