

# Ab Initio Study of Structural, Electronic, Magnetic Alloys: XTiSb (X =Co, Ni and Fe)

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**Abstract.** Structural, electronic and magnetic properties of three semi-Heusler compounds of CoTiSb, NiTiSb and FeTiSb were calculated by the method (FP-LAPW) which is based on the DFT code WIEN2k. We used the generalized gradient approximation (GGA (06)) for the term of the potential exchange and correlation (XC) to calculate structural properties, electronic properties and magnetic properties. Structural properties obtained as the lattice parameter are in good agreement with the experimental results available for the electronic and magnetic properties was that: CoTiSb is a semiconductor NiTiSb is a metal and FeTiSb is a half-metal ferromagnetic.

**Keywords:** ab-initio calculation, DFT, FP-LAPW, Half-Heusler.

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## INTRODUCTION

Half-Heusler compounds are ternary intermetallic compounds that have the general composition XYZ. In this class, X and Y represent d-electron transition metals, and Z denotes an sp-electron element [1]. In recent years, Half-Heusler and Heusler compounds have been extensively studied, and motivated by their gained importance due to advancements in spintronics [2–6]. In contrast to half-metallic ferromagnets (HMFs) [7], only a few Heusler compounds (all of them with a rare earth metal at the Y position) have been successfully implemented as superconductors [8]. Pd<sub>2</sub>YSn is the Heusler compound with the highest critical temperature (4.9K) [9]. The coexistence of antiferromagnetism and superconductivity demonstrating the manifoldness of the Heusler family, was reported for Pd<sub>2</sub>YbSn [10] and Pd<sub>2</sub>ErSn [11].

Many of the Heusler compounds have been reported to be HMFs [12,13], and several Co<sub>2</sub>-based Heusler compounds have been used as electrodes in magnetic tunnel junctions [14,15]. The hexagonal compound Pd<sub>2</sub>CeIn orders antiferromagnetically at 1.23 K [16]. D. B. de Mooij *et al.* [17] reported that Pt<sub>2</sub>GdSn and Pt<sub>2</sub>ErSn exhibit ferromagnetic (T<sub>c</sub>= 20 K) and paramagnetic behavior, respectively. Generally, Heusler compounds (X<sub>2</sub>YZ) crystallize in the cubic L2<sub>1</sub> structure (space group Fm3m), the X<sub>2</sub> atoms form a primitive cubic sublattice and adjacent cubes of this X<sub>2</sub> sublattice are filled by alternating Y or Z atoms. If the number of 3d electrons of Y atom is more than X atom, we can observe CuHg<sub>2</sub>Ti-type

structure with the space group F43m. In this structure, X atoms occupy the nonequivalent 4a(0,0,0) and 4c(1/4,1/4,1/4) positions, while Y and Z atoms are located at 4b(1/2,1/2,1/2) and 4d(3/4,3/4,3/4) positions, respectively [18].

In the present paper, the structural, electronic, and magnetic properties of XTiSb (X = Co, Ni and Fe) are reported. The aim of this work is to evaluate the validity of the predictions of half metallicity for XTiSb half-Heusler compounds. The calculations are performed using ab-initio full-potential linearized augmented plane wave (FP-LAPW) within the density functional theory (DFT) with the generalized gradient approximation GGA-WC. In this paper, we organized the theoretical background as it showed in Section 2. The results and discussions are mentioned in Section 3. The summary of our results is given in Section 4.

## METHOD OF CALCULATIONS

First principles calculations [19, 20] with both full potential and linear augmented plane wave (FP-LAPW) method [21] as implemented in the WIEN2k code [22] have been employed. The exchange-correlation effects were described with the parameterization of the generalized gradient approximation (GGA) by Wu and Cohen (GGA-WC) [23]. In these calculations the parameter RMTKmax=9, which determines matrix size (convergence), that is to say that Kmax is the plane wave cut-off and Rmt is the smallest of all atomic sphere radii. The muffin-tin radii (MT) are for Sb to be 2.25 and Ti, Co, Ni, Fe to be 2.4 (a.u), respectively. Within the spheres, the charge density and potential are expanded in terms of crystal harmonics up to angular momenta L=10 and a plane wave is used in the interstitial region. The value of Gmax=14, where Gmax is defined as the magnitude of largest vector in charge density Fourier expansion. The Monkhorst-Pack special k-points were performed using 1000 special k-points in the Brillouin zone. The cut off energy, which defines the separation of valence and core states, was chosen as -6 Ry. We select the charge convergence as 0.0001e during self-consistency cycles.

## RESULTS and DISCUSSION

Structural data on the equilibrium is obtained by adjusting the total energy as a function of volume (at T = 0K) using the equation of state of Murnaghan [24, 25].

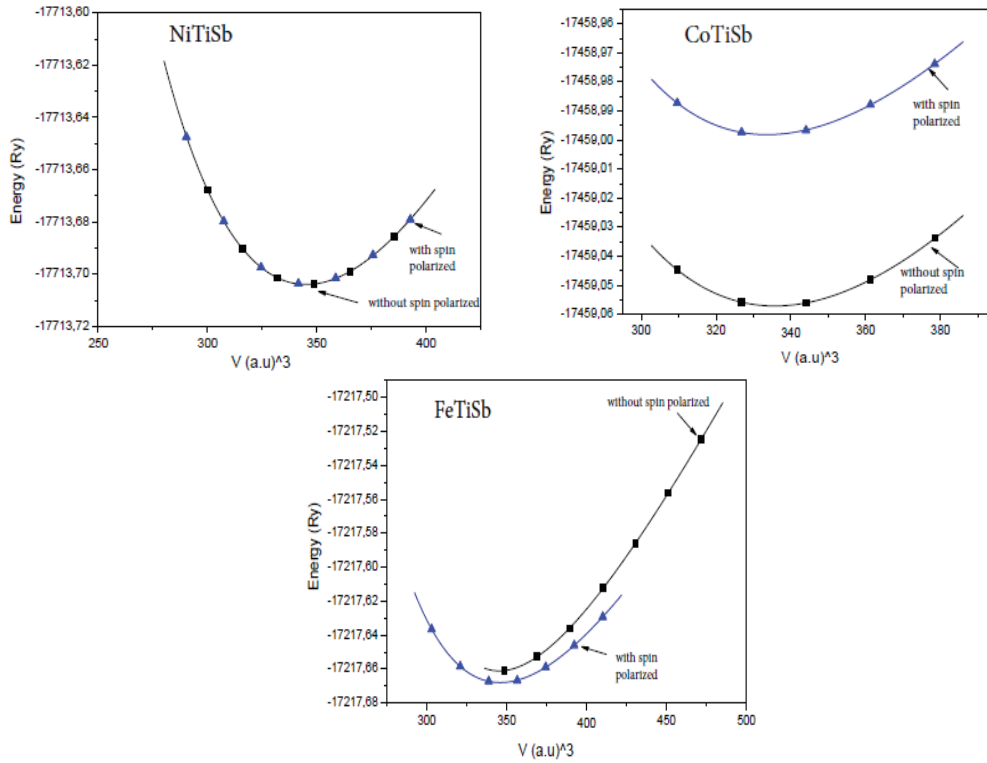
Figure 1 shows the total energy of the XTiSb (X = Co, Ni and Fe) as a function of volume with and without spin polarized in the GGA (06) approximation.

We note the stable phase corresponds to the non-magnetic state of CoTiSb. But the stable phase is the same in the magnetic state or the non-magnetic state NiTiSb. While the stable phase corresponds to the magnetic state of FeTiSb.

The Table 1 shows the structural parameters such as the lattice parameter, the bulk modulus and the minimum of Energy obtained in the calculations.

**Table 1.** Lattice Parameter  $a$  (Å), bulk modulus  $B$  (GPa), its derivative  $B'$  and the minimum of total energy  $E$  (Ry).

	CoTiSb		NiTiSb		FeTiSb	
	Non-magnetic	magnetic	Non-magnetic	magnetic	Non-magnetic	magnetic
$a$ (Å)	5.838	5.826	5.893	5.892	5.893	5.897
	5.886[26]	5.886[26]	5.964[27]	5.964[27]	5.997[27]	5.997[27]
	5.884[24]	5.884[24]	5.87 [25]	5.87 [25]		
$B$ (GPa)	155.60	155.30	139.51	138.34	177.00	132.53
$B'$	4.52	4.60	4.29	4.36	6.71	4.95
$E_{\min}$ (Ry)	-17459.0571	-17459.0570	-17713.7039	-17713.7037	-17217.6611	-17217.6680



**FIGURE 1.** The total energy as a function of volume, with and without spin polarized, of CoTiSb, NiTiSb and FeTiSb.

Figure 2 shows the energy bands of CoTiSb which present an energy gap (indirect) of 0.95 eV, the energy gap occurs between the top of the valence band at  $\Gamma$  point and the bottom of the conduction band at X point. The band structure of CoTiSb with spin-polarized (spin "up" and spin "down") are similar, which confirms that CoTiSb compound is a semiconductor. Figure 3 shows the band structure of NiTiSb with spin-polarized (spin "up" and "down"). We observed that two energy bands (spin "up" and "down") for NiTiSb are similar and an overlap was found between the energy bands

and the Fermi level  $E_F$ . This overlap confirms that NiTiSb is a metal. Figure 4 shows the bands structures of FeTiSb with spin-polarized (spin "up" and "down") these bands are not similar. We observe that spin up having a gap energy equal to 0.9 eV. While an overlap between the energy bands and the Fermi level was found in the spin down. This confirms that FeTiSb is half-metal.

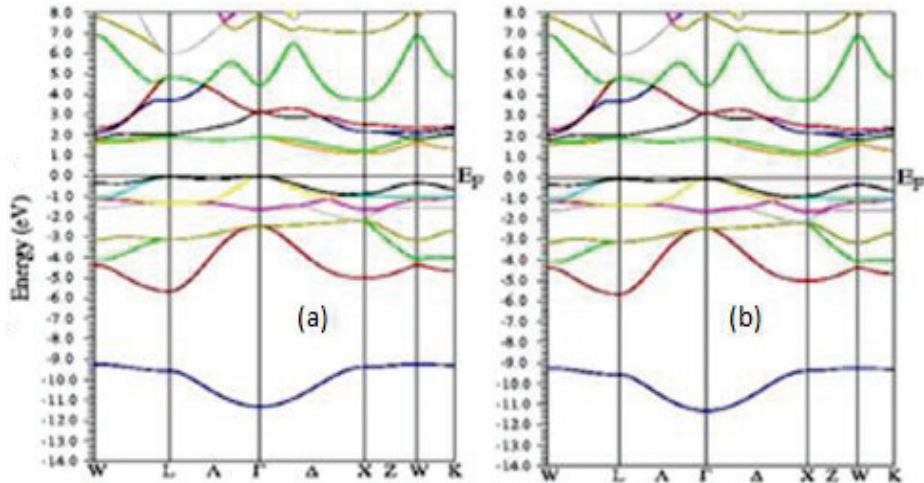


FIGURE 2. Band structure of CoTiSb with spin-polarized (a) "up" ( $\uparrow$ ) and (b) "down" ( $\downarrow$ ).

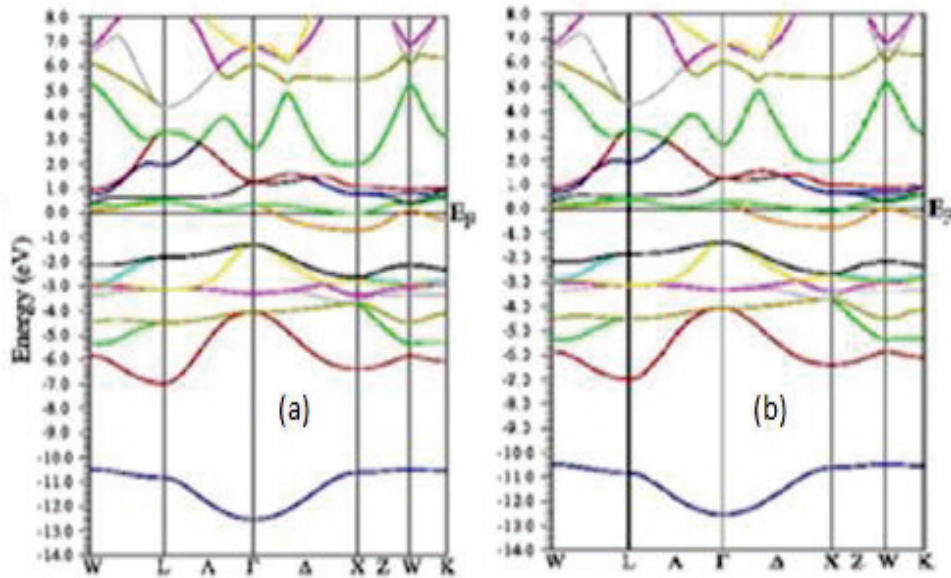


FIGURE 3. Band structure of NiTiSb with spin-polarized (a) "up" ( $\uparrow$ ) and (b) "down" ( $\downarrow$ ).

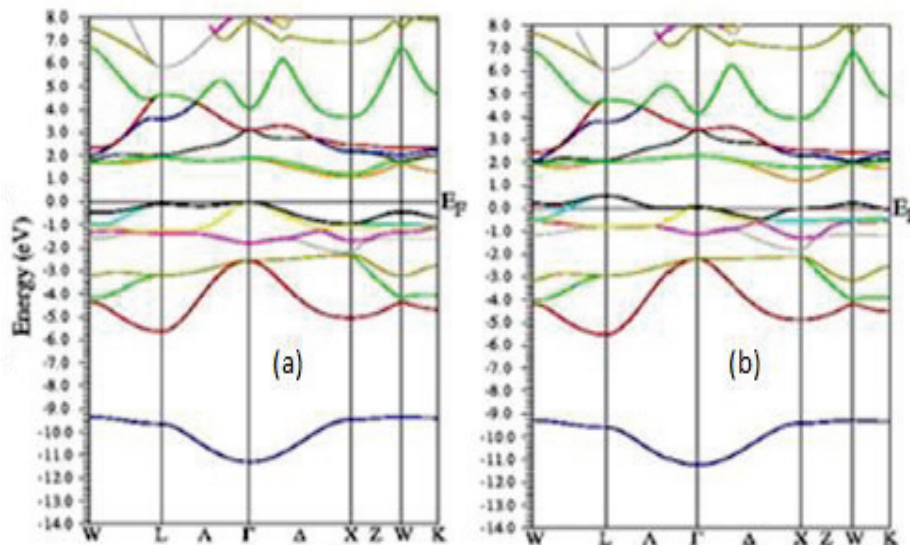


FIGURE 4. Band structure of FeTiSb with spin-polarized (a) "up" ( $\uparrow$ ) and (b) "down" ( $\downarrow$ ).

Figure 5 shows the total density of states of XTiSb ( $X = \text{Co, Ni and Fe}$ ). For CoTiSb and NiTiSb compounds we note that there is a symmetry between spin up ( $\uparrow$ ) and spin down ( $\downarrow$ ). However, in the composite FeTiSb there is no symmetry; this indicates that this element has a magnetic property.

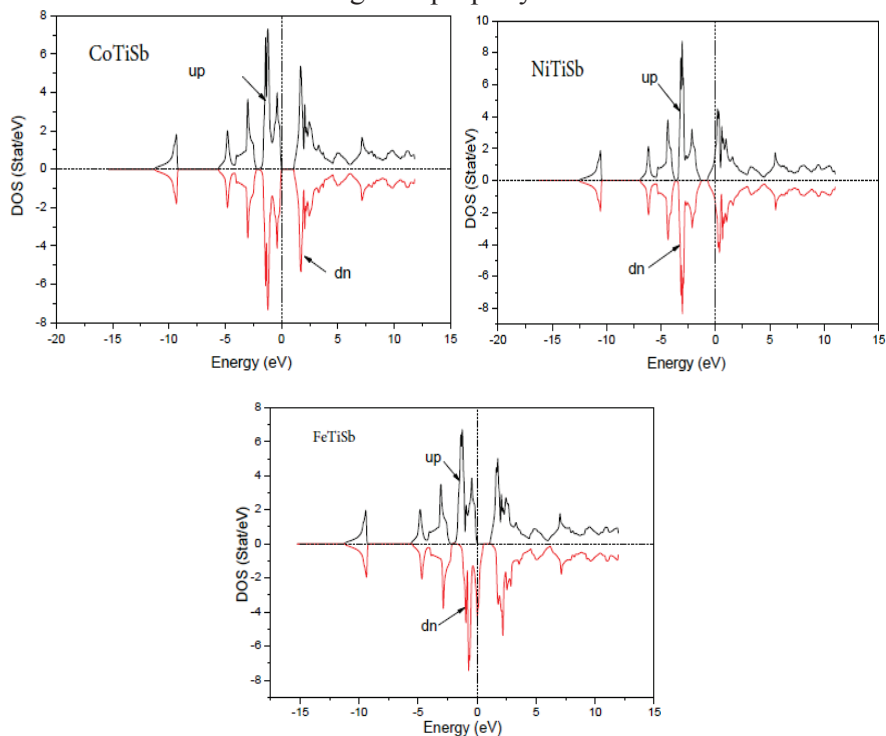


FIGURE 5. Total density of states for XTiSb ( $X = \text{Co, Ni and Fe}$ ) with spin-polarized "up" ( $\uparrow$ ) and "down" ( $\downarrow$ ).



## CONCLUSION

For the XTiSb (X = Co, Ni and Fe) Heusler compounds, the electronic structure and magnetic properties have been calculated using the first principles full-potential linearized augmented plane waves (FPLAPW) method. The main results are: The structural properties show that the values of the lattice parameters (a) calculated are in good agreement with the experimental data. The stable state of FeTiSb is the magnetic state; the stable phase of CoTiSb and NiTiSb is the non-magnetic state. Our calculations of the electronic structure and DOS show that : NiTiSb is a metal; CoTiSb is a semiconductor and FeTiSb is a half-metal ferromagnetic.

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