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FERROMAGNETIC HALF-METAL FOR SPINTRONIC APPLICATIONS: AB-INITIO CALCULATION

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Article Info	Abstract
Received: 21.10.2020 *Accepted: 16.02.2021* **Keywords:** DFT, GGA, FP-LAPW, half-metallic	The density functional theory (DFT) is used to study the structural, electronic, magnetic properties of Heusler Alloy compounds PdCoMnAl. The calculations are performed via FP-LAPW computational approaches as part of the generalized gradient approximation GGA and modified Becke–Johnson TB-mBJ for exchange-correlation potential. The prediction of the structure of the energy bands and of the densities of states shows a strong hybridization between the states d of the atoms of the transition metals of high valence (Pd) and the states d of the atoms of the transition metal of low valence (Mn) and (Co), which generates a half-metallic gap. In addition, the densities of total and partial states (PDOS) and the results of magnetic spin moments reveal that this compound is stable and ideal half-metallic ferromagnetic. The effects of the unit cell volume on the half-metallic and magnetic properties are crucial. It is interesting to note that our results of the total magnetic moment for PdCoMnAl equal to 5 µB per unit cell, nicely follow the rule µtot = Zt-18.

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1. Introduction

Spintronics is a new branch in nanotechnology research, which is the combination of the charge of the electron, the spin of the electron and the photon [1-2]. We also note that the spin of electron is very important in this technology, so it can be named spin electronics [3]. Spintronic Applications started appearing in the 1980s [4]. For example the first application of spintronics is the giant magneto resistive effect (GMR) used in the read heads of hard disks [5], in this application uses ferromagnetic metals like iron Fe and coblate Co, but the quantum property of spin offers new application possibilities in particular the realization of very sensitive sensors which have revolutionized the magnetic storage of information.

In 1983 de Groot discovered new class of materials called half-metal [4], in these Materials the valence band for one spin orientation is partially filled that is to say this substance acts as

a conductor to electrons of one spin orientation but is a gap in the density of states for the other spin orientation [6], all half-metals are ferromagnetic so have attracted some interest for their potential use in spin electronics [7].

The rest of this work has been divided in three parts. In Section 2, we briefly describe the methodology and details of calculations used in this study. The purpose of this study is to predict the structural, electronic, and magnetic properties of PdCoMnAl Heusler alloy [8] In Section 3. Finally, we summarize this study in Section 4.

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2. Methodology and details of calculations

The calculations were performed using the full potential linear-augmented-plane wave FP LAPW method [9]. Within the density functional theory DFT [10] as implemented in the WIEN2K package [11]. Energy of exchange and correlation XC [12] were treated within the generalized gradient approximation GGA [13] and modified Beck Johnson TB-mBJ [14]. which is based on XC energy optimization to calculate the total energy. The parameter RMT × Kmax is the smallest muffin-tin radius multiplied by the maximum k value in the expansion of plane waves in the basis set[14]. We chose RMT × Kmax = 8 The muffin-tin radius (RMT) used in these calculations are 2.4,2.4,2.4 and 2.26 atomic units for Pd, Co, Mn, and Al, respectively. we sampled the Brillouin zone using a Monkhorst-Pack grid (14x14x14) containing 120 k points, corresponding to 3000 k points in the Brillouin zone. The valence wave functions internal the muffin-tin spheres were extended up to Lmax=10, while the charge density was Fourier extended up to Gmax=14 atomic units (a.u). The self-coherence calculations are estimated when the energy differences between the succeeding iterations is lower than 10^{-4} Ry.

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The electronic configuration are taken: Pd: [Kr] $4d^{10}$, Co: [Ar] $3d^7$ $4s^2$, Mn: [Ar] $3d^5$ $4s^2$ Al: [Ne] $3s^2 5p^1$.

3. Results and Discussions

3.1. Structural Parameters and Magnetic Properties

A Quaternary Heusler alloy (QHA) [15] of composition XX'YZ is classified in space group No 216 (F-43m), with X, Z and Y occupying 4c (1/4, 1/4, 1/4), 4a (0, 0, 0) and 4b (1/2, 1/2, 1/2) respectively, which makes the arrangement of atoms along the diagonal of the Heusler lattice as XY-X'-Z[16]. It has been found that if the number of valence electrons decreases along X, X', Y, Z, then the XX'YZ structure is the most stable. However, there are two other possible non-equivalent configurations if we fix the position of X 'as the 4d site

(3/4, 3/4, 3/4) and swap the occupations of the other three sites. In principle, three non-equivalent atomic arrangements are possible in this type of structure as summarized in Table 1. And show the structures of the three possible types in Figure 1.

Table 1. Unequal site occupancy within the structure of a Quaternary Heusler XX'YZ [17].

Position	4a	4b	4c	4d
Type I	Z	Y	X	X'
Type II	Z	X	Y	X'
Type III	X	Y	Z	X'

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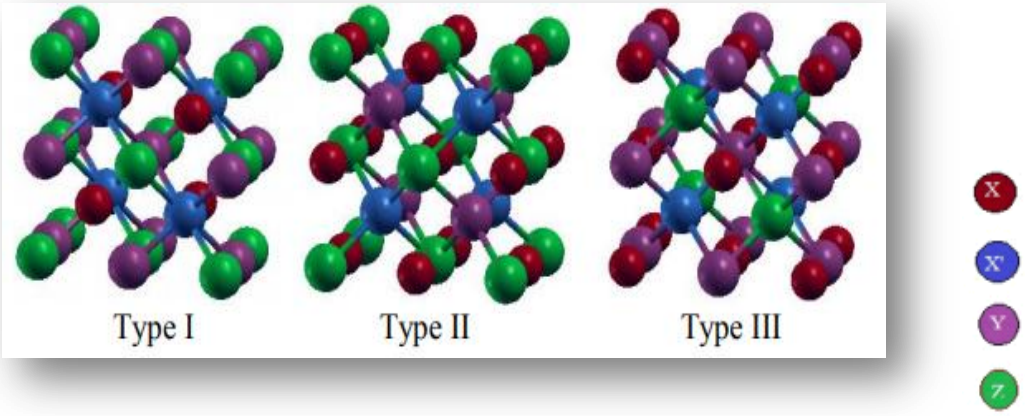


Figure1. The possible structures of a quaternary Heusler XX'YZ

Table 2. Atomic positions of type 1, 2 and 3 in the Heusler alloy PdCoMnAl.

PdCoMnAl	Pd	Co	Mn	Al
Type I	(1/4,1/4,1/4)	(3/4 ,3/4,3/4)	(1/2,1/2,1/2)	(0,0,0)
Type II	(1/2,1/2,1/2)	(3/4 ,3/4,3/4)	(1/4,1/4,1/4)	(0,0,0)
Type III	(0,0,0)	(3/4 ,3/4,3/4)	(1/2,1/2,1/2)	(1/4,1/4,1/4)

The most important step in an ab-initio calculation is the determination of the structural properties of the material being studied. Knowledge of this information allows us to subsequently access other physical properties (electronic, Structural, etc.) To determine the structural properties of the equilibrium state such as the equilibrium parameter a_0, the minimum energy E_0, the Bulk modulus B_0 and B' is its first pressure derivative at zero pressure, we followed the steps below:
The first step we performed an optimization of the three different configurations by

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calculating the total energies as a function of the volume for non-magnetic (NM) and ferromagnetic (FM). The equilibrium lattice constants and the total energies are presented in Table 3 and Figures 2, 3 and 4.

Table 3. The total energy for the three types of the PdCoMnAl at equilibrium

PdCoMnAl	NM	FM
Type I	- 15673,526672 Ry	- 15673,630416 Ry
Type II	- 15673,517717 Ry	- 15673,547248 Ry
Type III	- 15673,543191 Ry	- 15673,579178 Ry

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From Table 3 We deduce that the ferromagnetic phases are the most stable, then the comparison between the FM phases we deduce that type I is the most stable for the structure of PdCoMnAl, (see Figures 5).

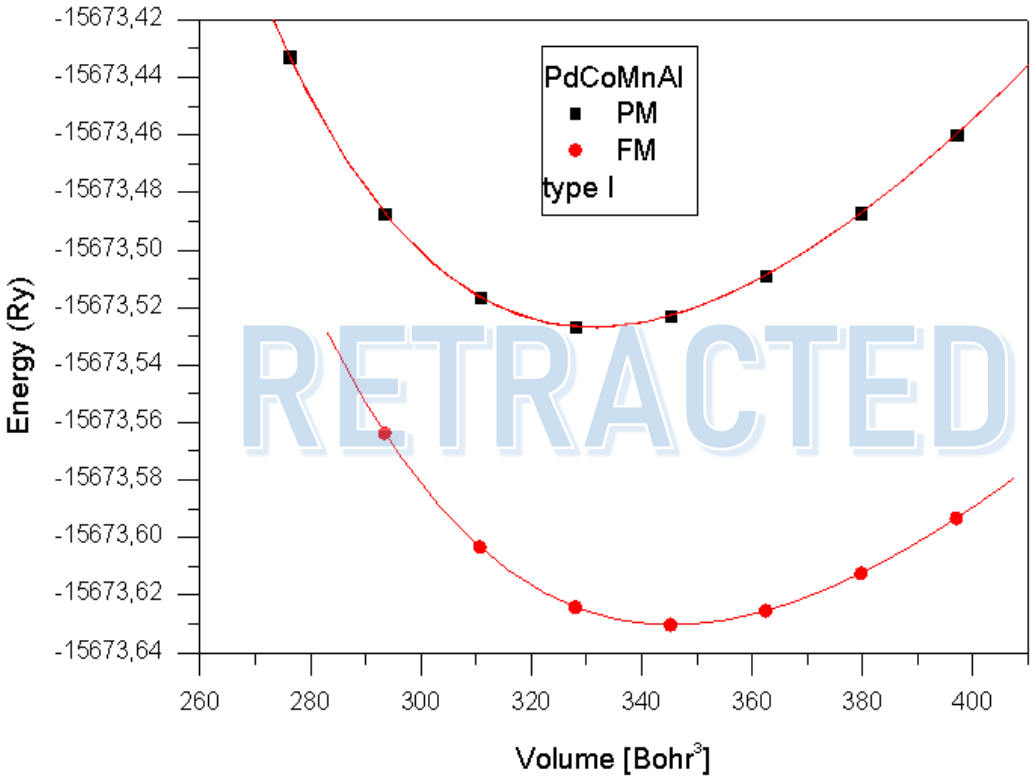


Figure 2. The variation of energy as a function of the volume type 1

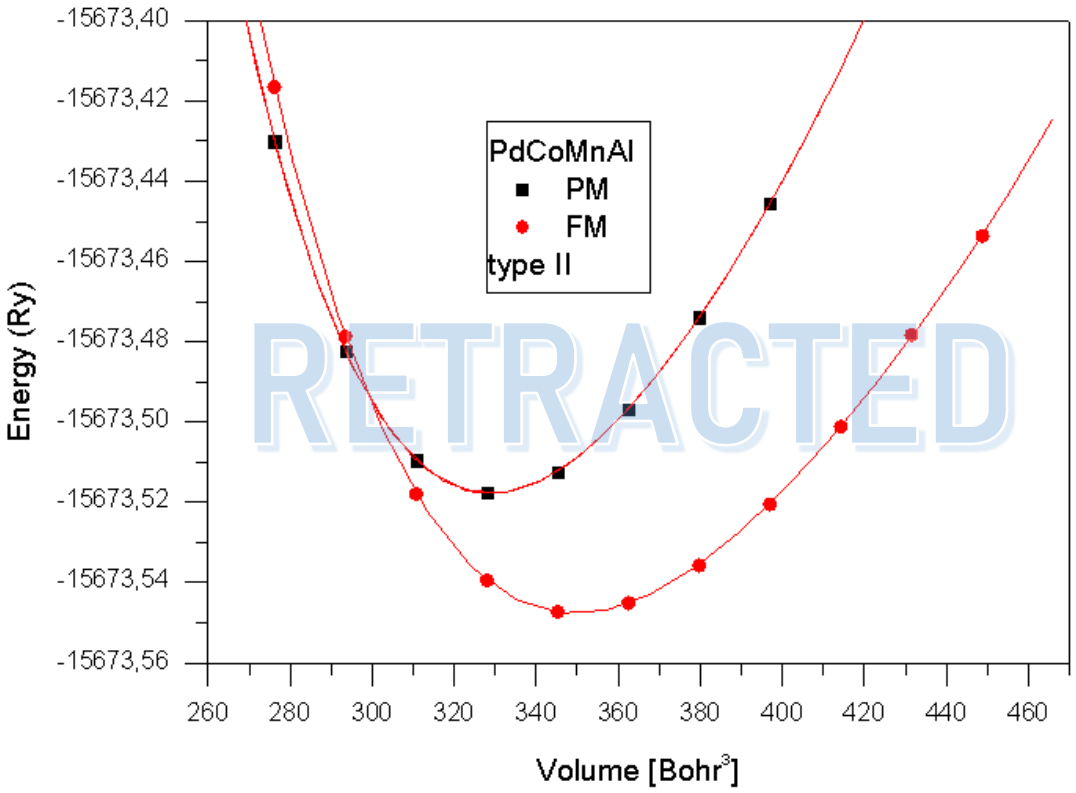


Figure 3. The variation of energy as a function of the volume type 2

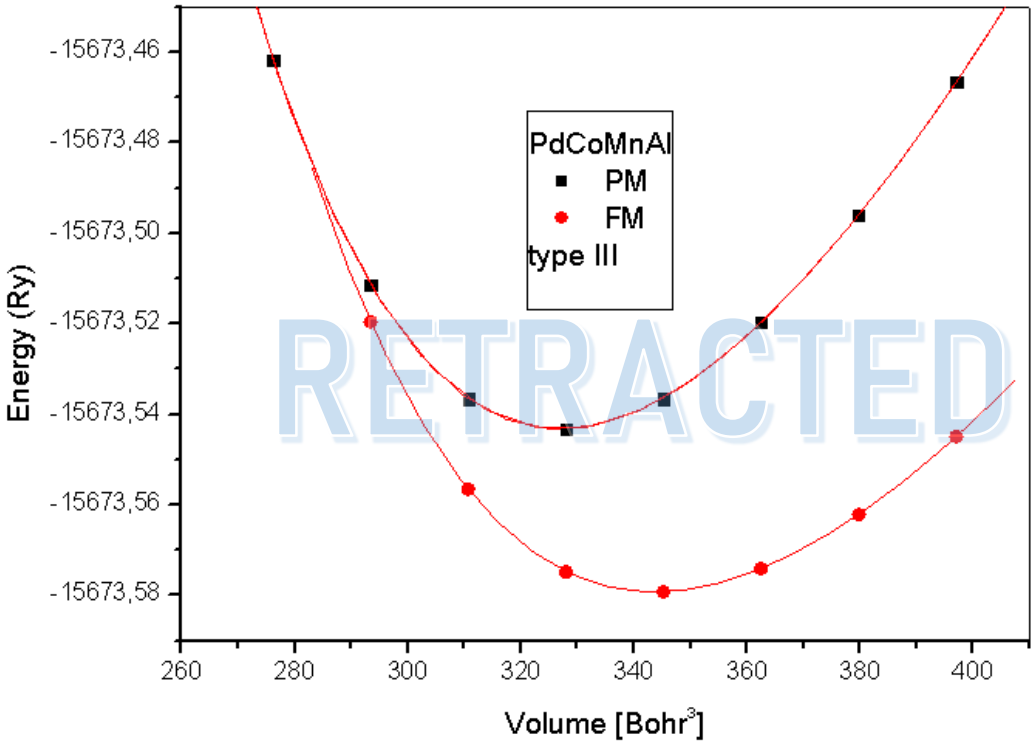


Figure 4. The variation of energy as a function of the volume type 3

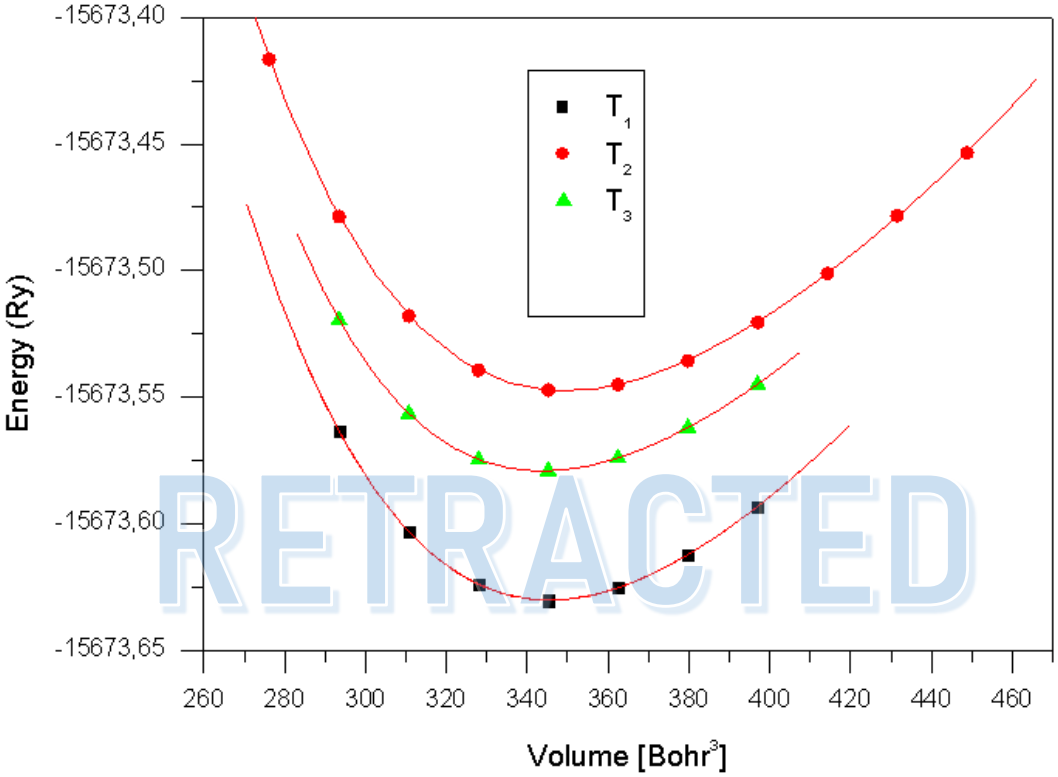


Figure 5. The variation of energy as a function of the volume type 1, 2 and 3 (Fm)

The next step is to determine a_0, V_0, E_0, B_0 and B′. For this, we calculated the total energy E_{tot} for different volume values by the Murnaghan equation of state [18]:

$$E_{tot} = \frac{B_0 V}{B'(B'-1)} * \left[B' \left(1 - \frac{V_0}{V}\right) + \left(\frac{V_0}{V}\right)^{B'} - 1 \right] + E_0 \quad (1)$$

Where V_0 is the unit-cell volume, E_0 is the total energy per primitive cell of the equilibrium state. The volume V_0 and the energy E_0 are given by the minimum of the E_{tot} (V) curve.

The magnetic moment is represented by the magnetic spin moment defined by the total occupancy number of majority spin orbital's minus the total occupancy number of minority spin orbital's [19]. In half-metallic compounds, the spin moment per unit of formula is an integer (in μB).

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Table 4. The structural parameters of the ground state of the compound PdCoMnAl

The structural parameters	a_0 (Å)	E_0 (Ry)	B_0 (GPa)	B'
Value	5.8949	-15673,630416	182.5345	4.5050

Our calculations show that the magnetic moment of the Co atom equal 0.38414 μB, We remark that the Mn and Pd atoms magnetic moments are the highest and equal to 3.41520 μB and 1.28970 μB respectively, where as that of Al atom is the lowest and equal to - 0.04565 μB .As a consequence, the PdCoMnAl exhibits a half-metallic ferromagnetic behavior.

The results of Table 5 are that PdCoMnAl has a total magnetic moment of 5.00 µB, which follows the Slater-Pauling rule of Mt = Zt − 18 = 5.00 μB, where Zt is the number of valence electrons.

Table 5. The total and partial magnetic moments of PdCoMnAl at equilibrium

Compound	Interstitial	Pd (µB)	Co (µB)	Mn (µB)	Al (µB)	Mt (µB)
value	-0.03046	1.28970	0.38414	3.41520	-0.04565	5.0081

3.2. Electronic Properties

The energy bands give the possible energies of an electron as a function of the wave vector [20]. Depending on how these bands are distributed, it is possible to distinguish between a conductor, semiconductor ... etc. We define the energy gap as the difference between the maximum of the valence band and the minimum of the conduction band. We calculated the energy bands of the PdCoMnAl compound along the lines of high symmetry in the first Brillouin zone, the spin-up and spin-down band structure of PdCoMnAl is shown in Figure 6 and 7. Figure 6: valence band and conduction band overlap (i.e. intersect) below Fermi level, indicating that the alloy has a metallic character. Figure 7: the band structure presents a gap between the valence band and the conduction band, which indicates that the compound has a semiconductor behavior with direct gap, where the gap energy equal to 0.38 eV and the half metallic gap energy equal to 0.13 eV.

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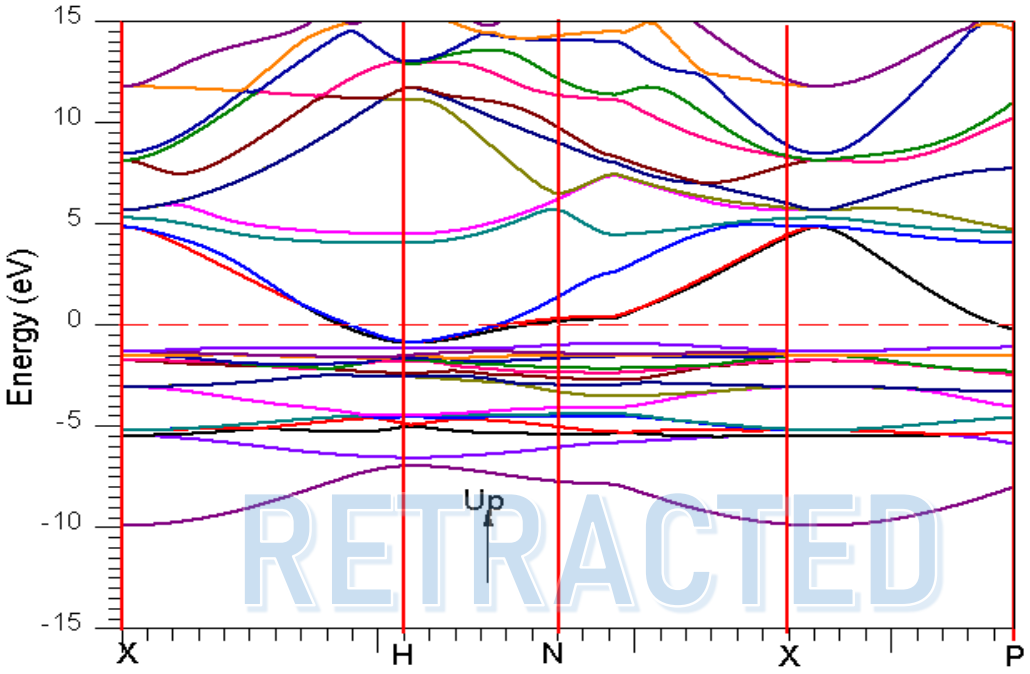


Figure 6. The band structure of majority spin (up)

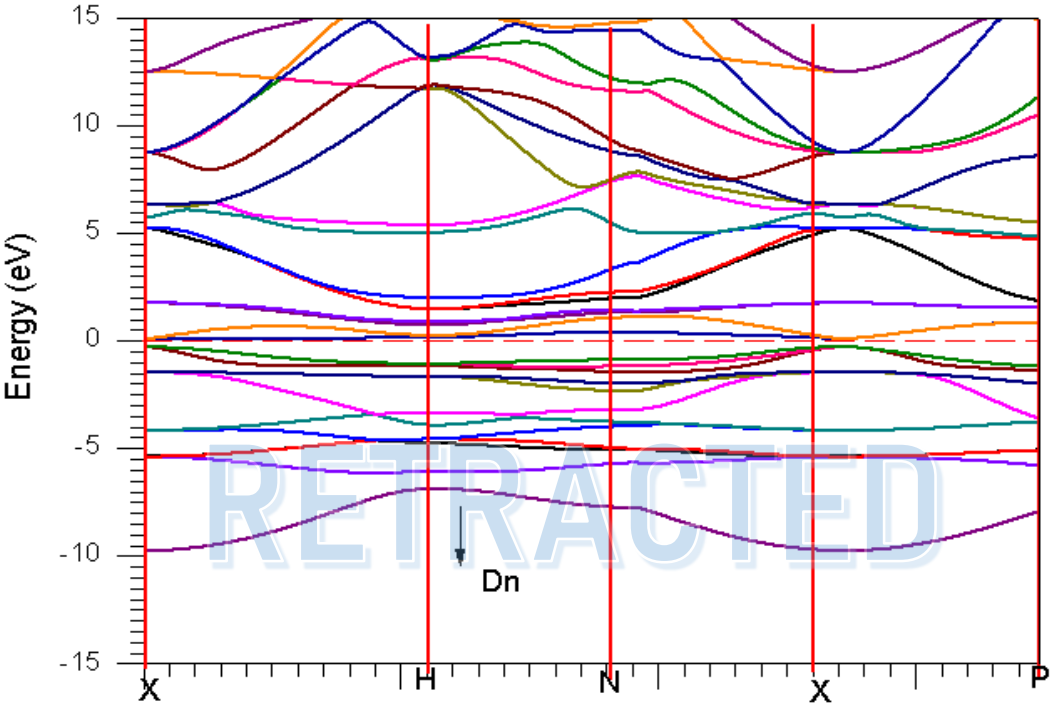


Figure 7. The band structure of minority spin (dn)

The structure of energy bands of a half-metallic material [21] presents an asymmetry between the spin up and spin down states with an energetic gap or pseudo gap at the Fermi

level. This gives rise to polarizations of the conduction electrons at the Fermi level which can reach 100%.

To get a general idea of the origin of the electronic band structure, we calculated the partial and total densities of state (DOS) of the compound PdCoMnAl. The total and partial spin up and spin down densities of states have three sub bands:

For Spin up:

The higher valence sub band comes from the hybridization of the Pd-4d, Mn-3d and Co-3d states.

The conduction sub band is mainly due to a mixture of Pd-4d, Co-3d, Mn-3d and Al-3p states.

The sub band of semi-core or sub-band of lower valence comes from its Al-3p states.

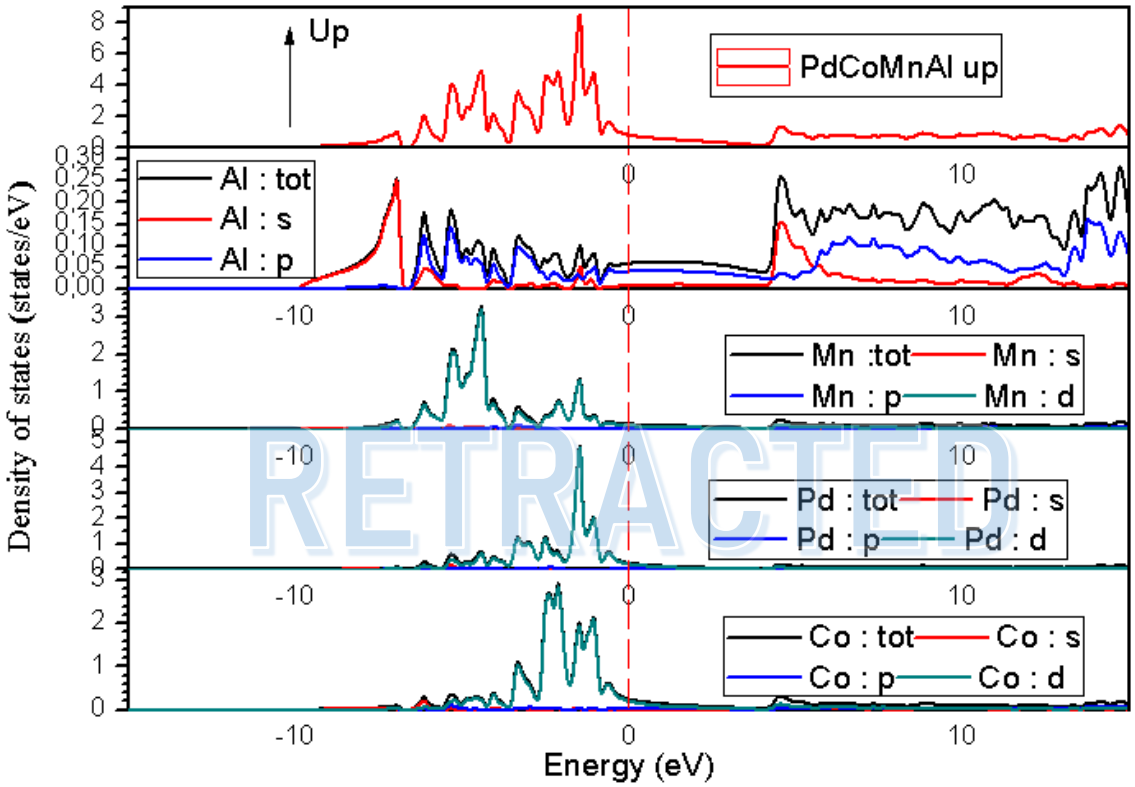


Figure 8. Partial and total densities of states for PdCoMnAl majority spin (up)

For Spin down:

The valence sub band comes from the hybridization of the Pd-4d, Mn-3d and Co-3d states.

The conduction sub band is due to the strong hybridization of the Pd-4d, Mn-3d and Co-3d states.

The semi-core sub band comes from the Al-3p states.

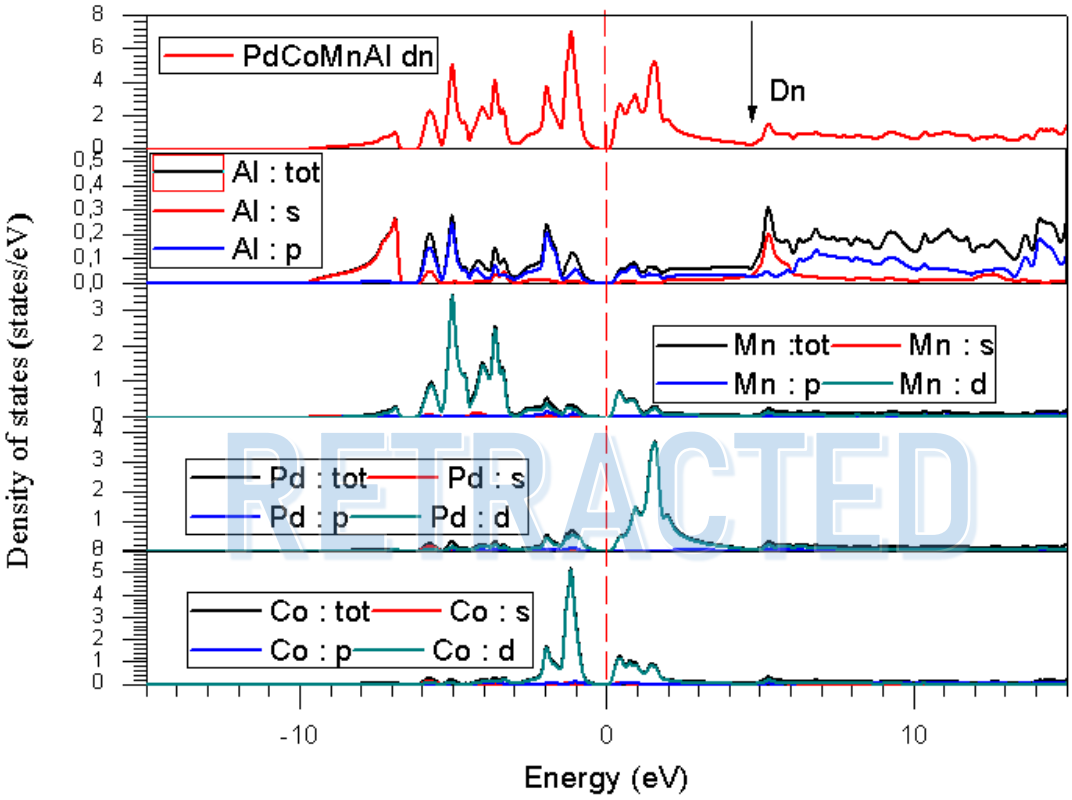


Figure 9. Partial and total densities of states for PdCoMnAl minority spin (dn)

The state densities presented in Figure 10 confirm the metallic character for the majority spins and an absence of electronic states at the Fermi level for the minority spins which brings us closer to the semiconductor character. This indicates a half-metallic behavior for the Heusler alloy PdCoMnAl.

We can distinguish, from the total and partial densities found by the FP-LAPW method, that the region of the valence band is divided into three important energy intervals:

First interval: [-10eV;-0.35eV] we clearly see a strong hybridization of the d orbital of Mn, Co and the Pd in spin and a weak contribution of the p orbital of the Al atom.

Second interval: [-0.35eV; 0.03eV] we observe a band gap, in the minority spin , while there are contributions of state d of Mn as well as very low population of electrons d of Pd at the level of Fermi in majority spin. This confirms that our studied compound is a half-metallic material.

Third interval: [0.03eV; 10eV] the conduction band is formed mainly from the d orbital of Mn in spin up and spin dn and that of Pd and Co in minority spin.

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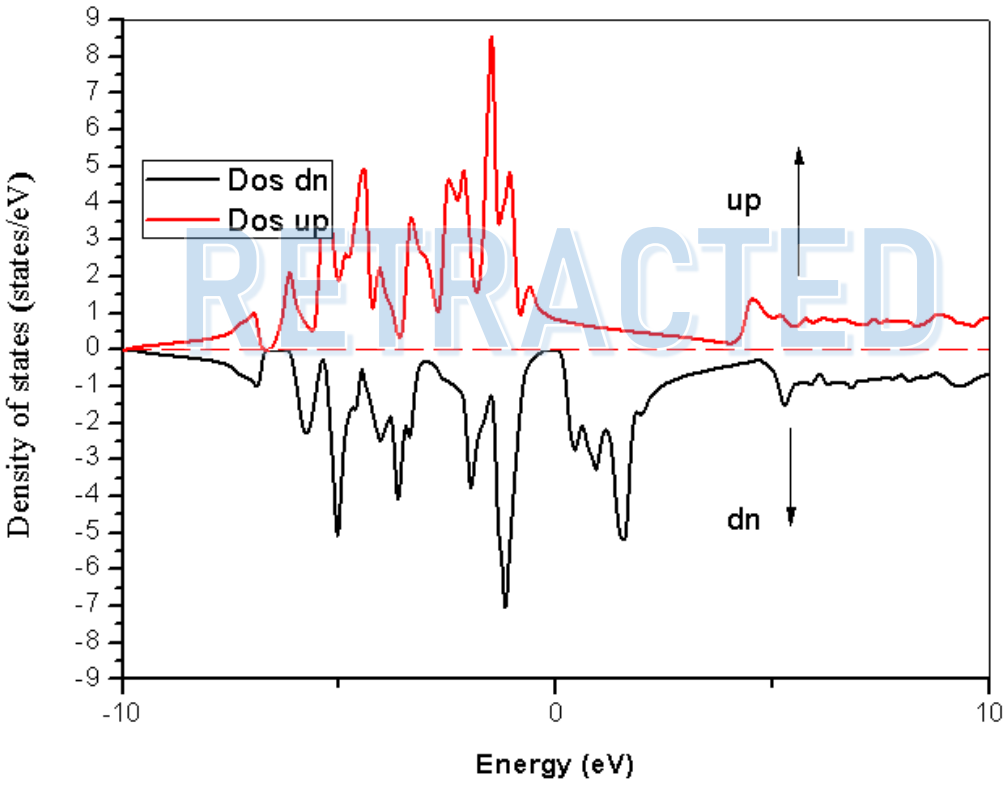


Figure 10. Spin-polarized total density of states for PdCoMnAl of majority spin (up) of minority spin (dn)

4. Conclusion

In this manuscript, we discussed an ab initio calculation of the structural, electronic and magnetic properties of PdCoMnAl compound. Our assessments were performed by the augmented plane wave method FP LAPW founded on the DFT (density functional theory) and introduced in the Wien2k calculation code. This investigation of the electronic band, structural and magnetic properties were performed using a combination of the generalized gradient approximation and modified Becke–Johnson GGA+TB-mBJ for exchange-correlation potential. In our study: The state densities confirm the metallic character for the majority spins and an absence of electronic states at the Fermi level for the minority spins which brings us closer to the half-metallic character. The ferromagnetic behavior of the compound is very clear with magnetic moments of around 5 µB, confirming its half metallicity.

Therefore, these compounds are potential candidates for the field of spin electronics (spintronics technology).

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