



## The Electronic and Magnetic Properties of New Full-Heusler Compounds: $M_2IrSi$ (M=Ti, Cr and Mn)

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### Abstract

The structural and magnetic properties of  $M_2IrSi$  (M=Ti, Cr and Mn) full-Heusler compounds were investigated using WIEN2k program. The ferromagnetic states (FM) were compared to the non-magnetic states in the  $Hg_2CuTi$  and  $Cu_2MnAl$  structures to determine more stable state as energetically using the optimization curves. For all compounds, FM states are the most stable states in the  $Hg_2CuTi$  type structure. The electronic calculations show that the majority electrons of  $Ti_2IrSi$ ,  $Cr_2IrSi$  and  $Mn_2IrSi$  compounds have metallic feature. For  $Ti_2IrSi$  and  $Mn_2IrSi$  compounds, the minority electrons have semiconducting nature with an energy gap of 0.89 and 0.41 eV, respectively. Finally,  $Ti_2IrSi$  compound is a conventional half-metallic,  $Cr_2IrSi$  compound is metallic and  $Mn_2IrSi$  is a half-metallic ferromagnet within 2.73, 1.0 and 3.0  $\mu_B$ /f.u. magnetic moment, respectively.

## 1. INTRODUCTION

The  $NiMnSb$  compound is the first Heusler compound which was introduced by de Groot et al. in 1983 [1]. According to this prediction,  $NiMnSb$  compound was half-metal material. While one band of half-metallic materials exhibits semiconducting qualities, the other band exhibits metallic properties [2,3]. Half-metallic ferromagnets have attracted a great deal of interest in spintronic applications in recent years due to the increased application areas. Magnetic sensors [4-6], the tunnel junction and spin-injector materials can be given as examples of these applications of semi-conductor materials [7]. It has also been observed that half-metallic materials reduce electricity consumption and integration intensities [8]. It has been reported in the literature that some full-Heusler compounds [9-14], ferromagnetic metal oxides [15-17], half-Heusler compounds [18,19] and zinc-blende structures [20-23] worked both theoretically and experimentally.

The full-Heusler compounds are ternary materials with 2:1:1 atomic sequence. The first two elements of this ternary structure are transition metals and the last one is III-VIA group element [24]. There are two forms of full-Heusler compounds. The first is the  $Cu_2MnAl$  crystal structure, which is the space group  $Fm-3m$ . The second is the  $Hg_2CuTi$  crystal structure, which is the space group  $F-43m$ . In  $Cu_2MnAl$ -type structure, atoms are placed at the Wyckoff positions of X 8c (1/4, 1/4, 1/4), Y 4a (0, 0, 0) and Z 4b (1/2, 1/2, 1/2). In  $Hg_2CuTi$ -type structure, first transition metal is located on 4a (0, 0, 0) and 4c (1/4, 1/4, 1/4) positions, second transition metal is located at 4b (1/2, 1/2, 1/2) and III-VI A atoms are placed on 4d (3/4, 3/4, 3/4) positions [11].

For investigate of electronic and magnetic properties some  $Ti_2$ -based  $Ti_2CoSn$ , the  $Cr_2$ -based  $Cr_2MnSb$  and the  $Mn_2$ -based  $Mn_2ZB$  (Z=Fe, Co and Ni) alloys were studied before [25-27]. Even though some

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Heusler alloys were investigated for their structural and magnetic properties by theoretically and experimentally [9,10,25-31], there are no any studies on the  $M_2\text{IrSi}$  ( $M=\text{Ti, Cr}$  and  $\text{Mn}$ ) full-Heusler compounds until now. In present study, the electronic, structural and magnetic properties of  $M_2\text{IrSi}$  ( $M=\text{Ti, Cr}$  and  $\text{Mn}$ ) full-Heusler compounds were studied firstly.

## 2. CALCULATION METHODS

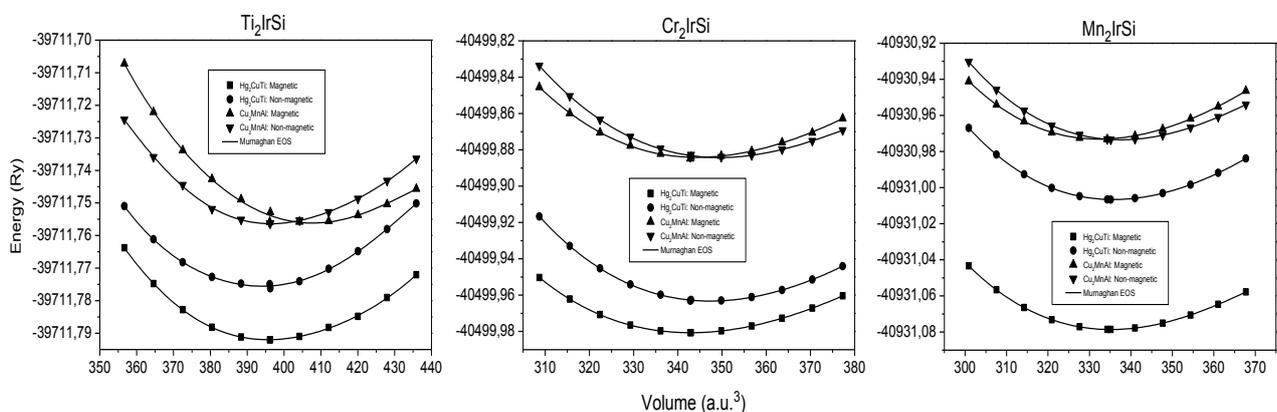
The Full Potential Linearized Augmented Plane Wave (FP-LAPW) method is among the most accurate methods for performing electronic structure calculations for crystals [32]. This method is based on Density Functional Theory (DFT). The calculations of  $M_2\text{IrSi}$  ( $M=\text{Ti, Cr}$  and  $\text{Mn}$ ) compounds have been realized by applying this method and theory to the WIEN2k code [33]. The generalized gradient approximation (GGA) in Perdew-Burke-Ernzerhof (PBE) was used to determine the exchange-correlation correction [34,35]. The electronic structures were plotted by using graphing and data analyses software of OriginPro 8.0.

In FP-LAPW method the space was separated using muffin-tin (MT) spheres so that it can prevent intersection of space with an interstitial region. Inside the MT spheres, basic functions; such as charge density, the wave function and potential, were extended by spherical harmonic functions and plane waves basis set in the interstitial region. The choice of MT spheres is determined to be greater than the radius of each atom it covers. In this way, all the spherical potential values of the targeted atom are kept in the MT sphere to prevent potential leakage to the outside. In  $\text{Ti}_2\text{IrSi}$  compound, the muffin-tin radii were chosen as 2.15 a.u. for Ti(1) and Ti(2), 2.37 a.u. for Ir and 1.86 a.u. for Si. In  $\text{Cr}_2\text{IrSi}$  full-Heusler compound, the muffin-tin radii were selected as 2.16 a.u. for Cr(1) and Cr(2), 2.39 a.u. for Ir and 1.87 a.u. for Si. In  $\text{Mn}_2\text{IrSi}$  compound, the muffin-tin radii were chosen 2.20, 2.20, 2.31 and 1.86 a.u. for Mn(1), Mn(2), Ir and Si, respectively. For all compounds, the spin cut off parameter was set to  $K_{\text{max}}R_{\text{MT}} = 7$ . The magnitudes of largest vectors were selected as  $12 \text{ (a.u.)}^{-1}$ . The energy cut off defines the separation into core and band states. These energy values were chosen as -6 Ry. In these calculations, the charge convergence parameter was adjusted as 0.0001 e. The quantity of the specified Brillouin Zone (BZ) number was selected to determine the most stable, i.e. lowest energy state, in the volume optimization curve. Using the tetrahedron method, the charge density for integration was calculated by taking into account 104 special k-points for  $\text{Cr}_2\text{IrSi}$  and  $\text{Mn}_2\text{IrSi}$  (3000 k-points in BZ) and 165 special k-points for  $\text{Ti}_2\text{IrSi}$  compound (5000 k-points in BZ) [33].

## 3. RESULT AND DISCUSSION

### 3.1. Ground States Properties

In Figure 1, the total energies of  $M_2\text{IrSi}$  ( $M=\text{Ti, Cr}$  and  $\text{Mn}$ ) compounds were plotted as a function of volume for FM and NM configurations in both  $\text{Hg}_2\text{CuTi}$  and  $\text{Cu}_2\text{MnAl}$ -type structures.



**Figure 1.** Structural volume optimization of  $M_2\text{IrSi}$  ( $M=\text{Ti, Cr}$  and  $\text{Mn}$ ) full Heusler compounds for both  $\text{Cu}_2\text{MnAl}$  and  $\text{Hg}_2\text{CuTi}$ -type structures

In Figure 1, it is seen that  $\text{Hg}_2\text{CuTi}$  structures are the most stable structures for FM configurations. Furthermore, the lattice parameters, bulk modulus, its first derivatives, equilibrium energies and volumes are given at Table 1.

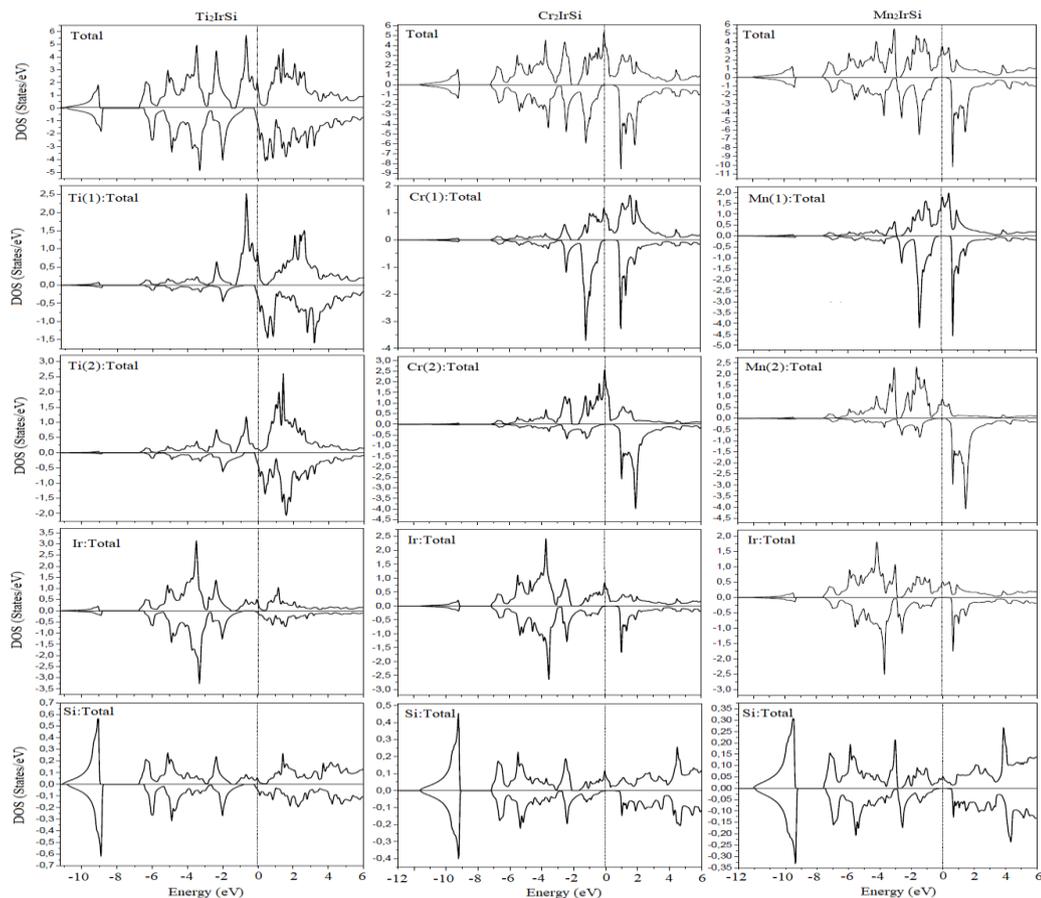
**Table 1.** The lattice parameters, bulk modulus, first derivatives of bulk modulus, equilibrium energies and volumes

Compounds	$a(\text{\AA})$	B(GPa)	$B'$	$E_0(\text{Ry})$	$V_0(\text{a.u.}^3)$
$\text{Ti}_2\text{IrSi}$	6.17	173.3563	4.4887	-39711.7921	396.1274
$\text{Cr}_2\text{IrSi}$	5.88	206.9174	5.7652	-40499.9805	343.6292
$\text{Mn}_2\text{IrSi}$	5.83	234.5151	5.2289	-40931.0785	335.1884

$\text{M}_2\text{IrSi}$  ( $M=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) alloys have never been investigated until now.

### 3.2. Electronic Properties

In Figure 2, the total and atomic density of states (DOS) of  $\text{M}_2\text{IrSi}$  ( $M=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) compounds are plotted.

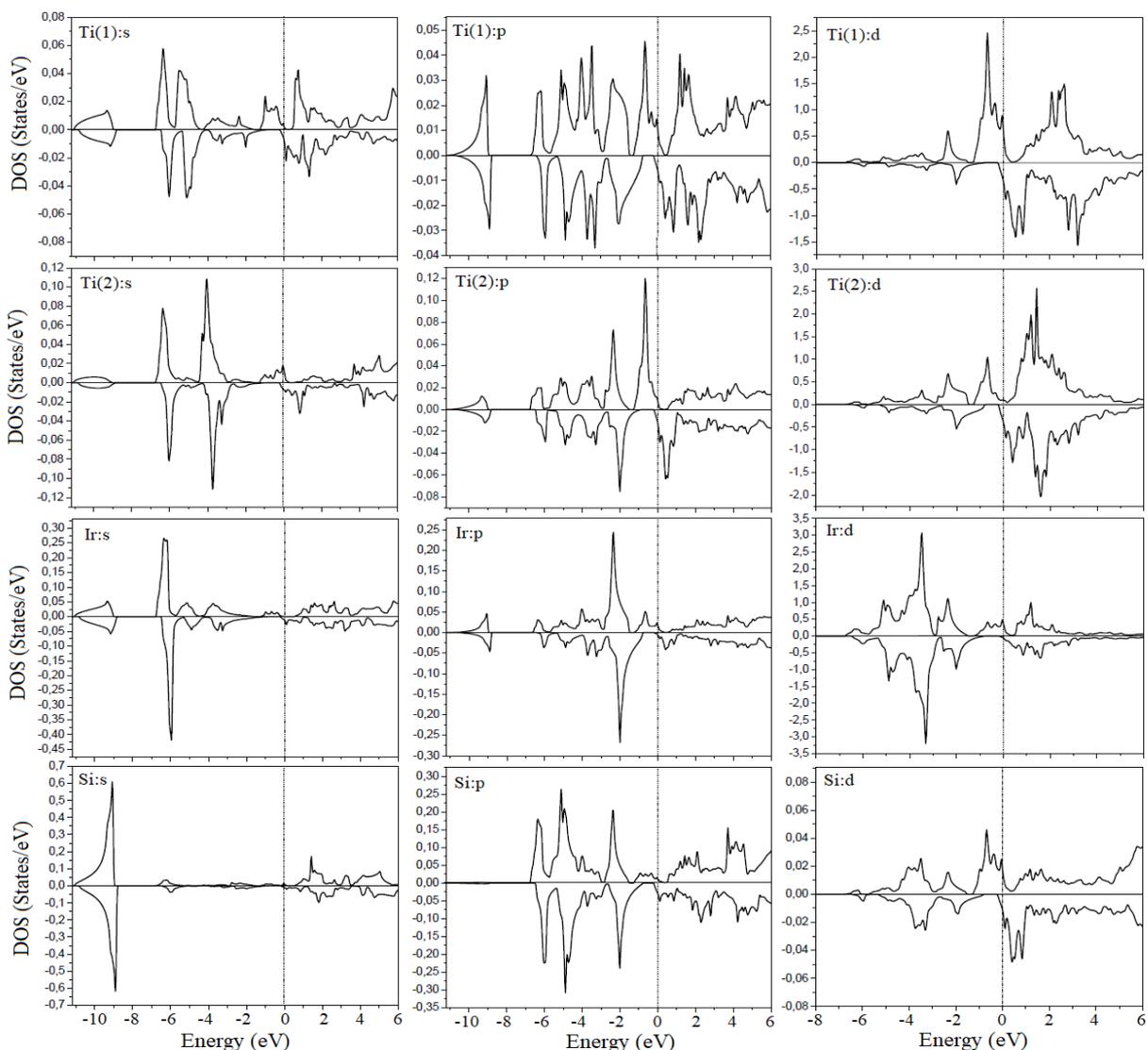


**Figure 2.** The spin-polarized total densities of states (DOS) and atom-projected DOS of the  $\text{M}_2\text{IrSi}$  ( $M=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) compounds

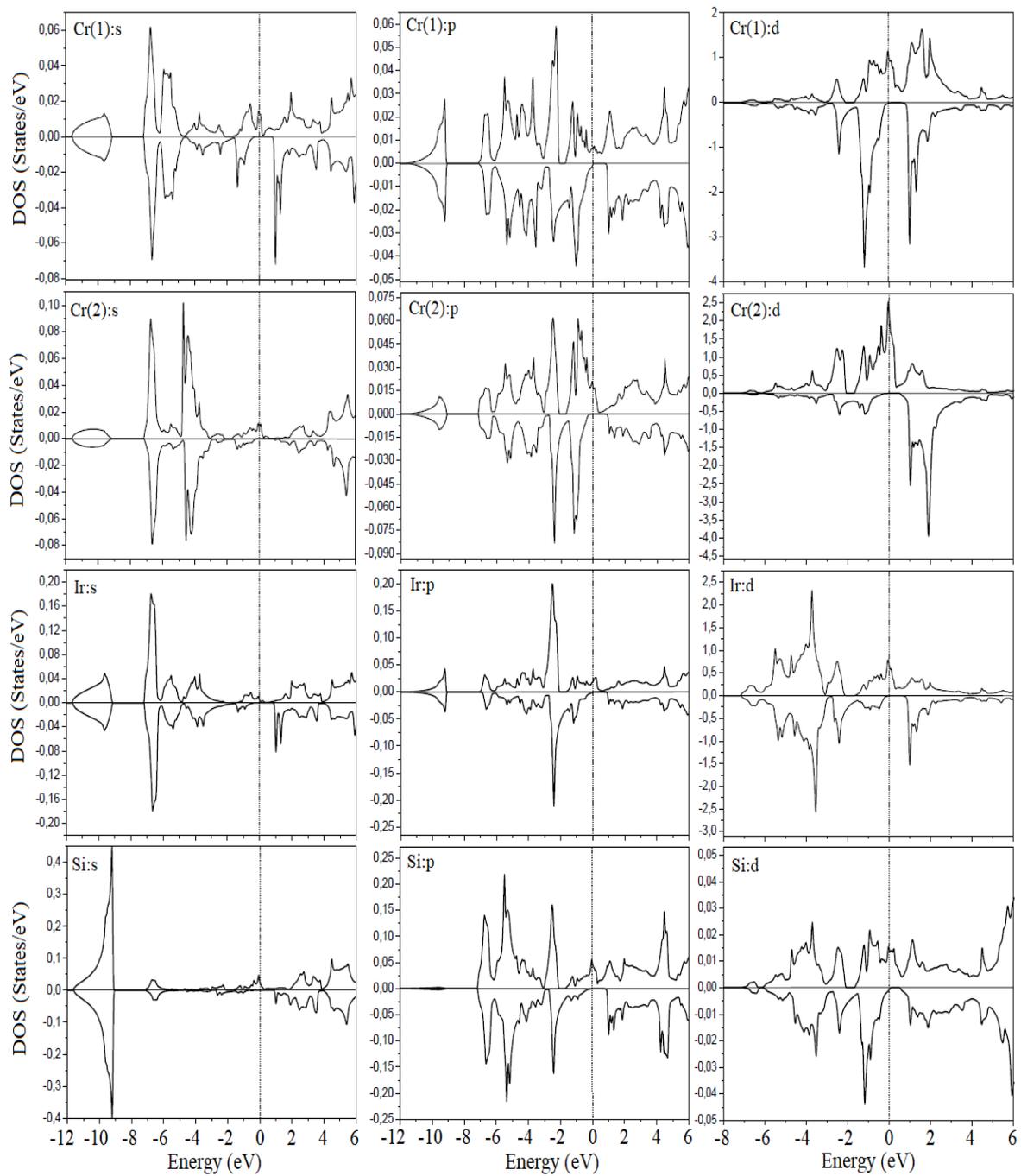
In all compounds, the sharp peaks between energy interval of (-11, -9) eV belong to Si atom and the interval of -6 and -2 eV, the main contribution to total DOS come from transition metal Ir. In spin-up electrons of  $\text{Ti}_2\text{IrSi}$  compound, the sharp peak between -2 and 0 eV relative to Ti(1) atom. In the positive

energy regions, the main contribution to total DOS belong to Ti(1) and Ti(2) atom. For  $\text{Cr}_2\text{IrSi}$ , in the -2 and 0 eV energy range, the contribution to the spin-up electrons is due to the Cr(1) atom and the spin-down electrons to the Cr(2) atom. In the 0 and -6 eV energy range, although the contributions come from all the atoms, the main contributions to total DOS belong to Cr(1) and Cr(2) atoms. In  $\text{Mn}_2\text{IrSi}$  compound, the sharp peaks belong to transition metal around the Fermi level. Although spin-up electrons intercept the Fermi level, there is an energy gap in spin-down electrons. This magnitude of this energy gap is 0.41 eV. This non-zero gap shows that  $\text{Mn}_2\text{IrSi}$  full-Heusler compound has half-metallic feature. Later, the band structure of  $\text{Mn}_2\text{IrSi}$  compound will be examined to confirm this feature.

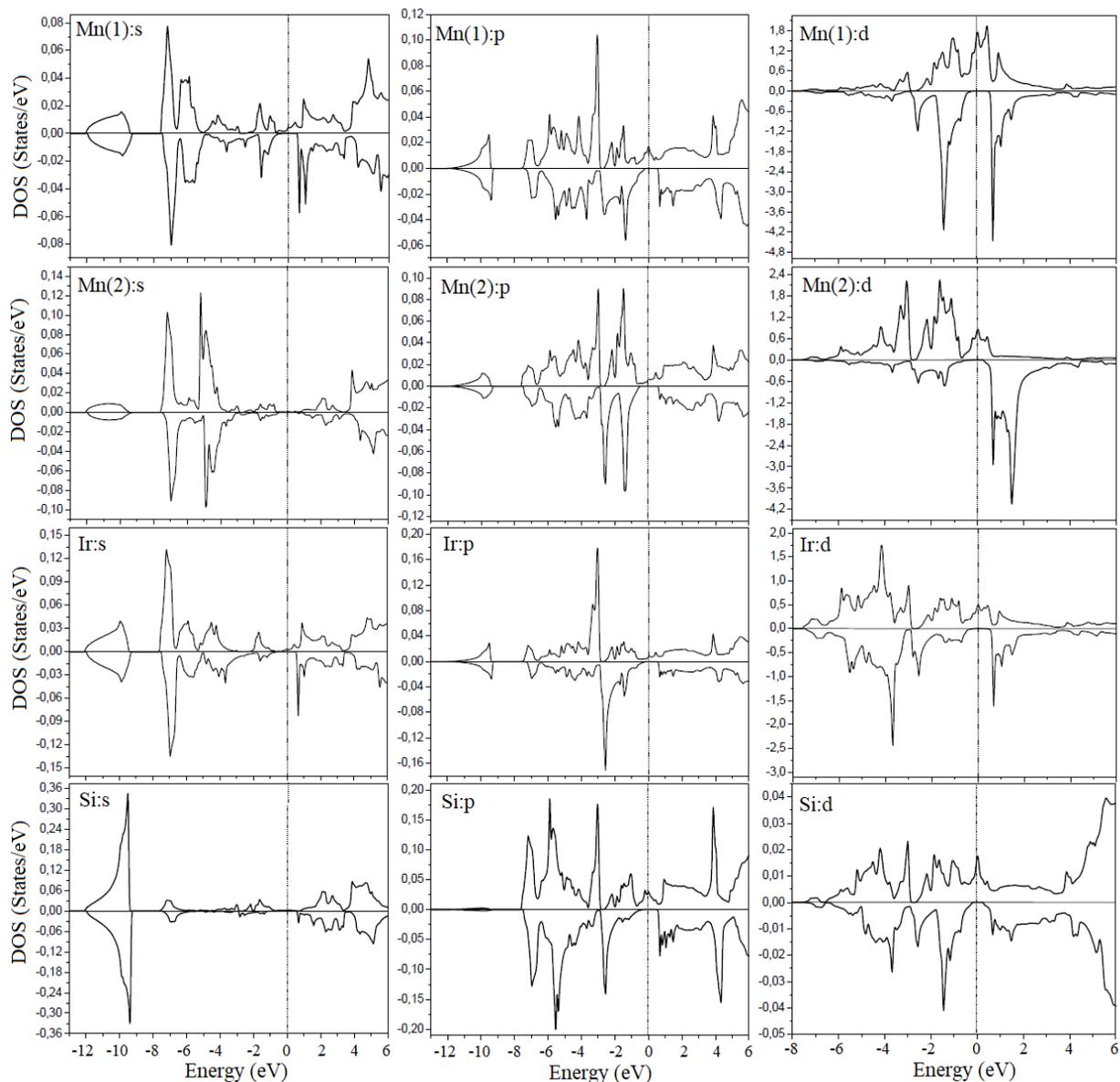
The d orbital is the outermost orbital of electron distribution in transition metals. Therefore, it can be expected that the most contributions to DOS come from d orbitals. The contributions of s, p and d orbitals of  $\text{Ti}_2\text{IrSi}$ ,  $\text{Cr}_2\text{IrSi}$  and  $\text{Mn}_2\text{IrSi}$  full-Heusler compounds have been plotted in Figure 3, Figure 4 and Figure 5, respectively. For all compounds, we mentioned that the sharp peak between -11 and -9 eV energy interval belongs to Si atom. It is clear that these contributions come from Si-s orbital.



**Figure 3.** The densities of states (DOS) of s, p and d orbitals of  $\text{Ti}_2\text{IrSi}$  compound. The zero energy point represents the Fermi level

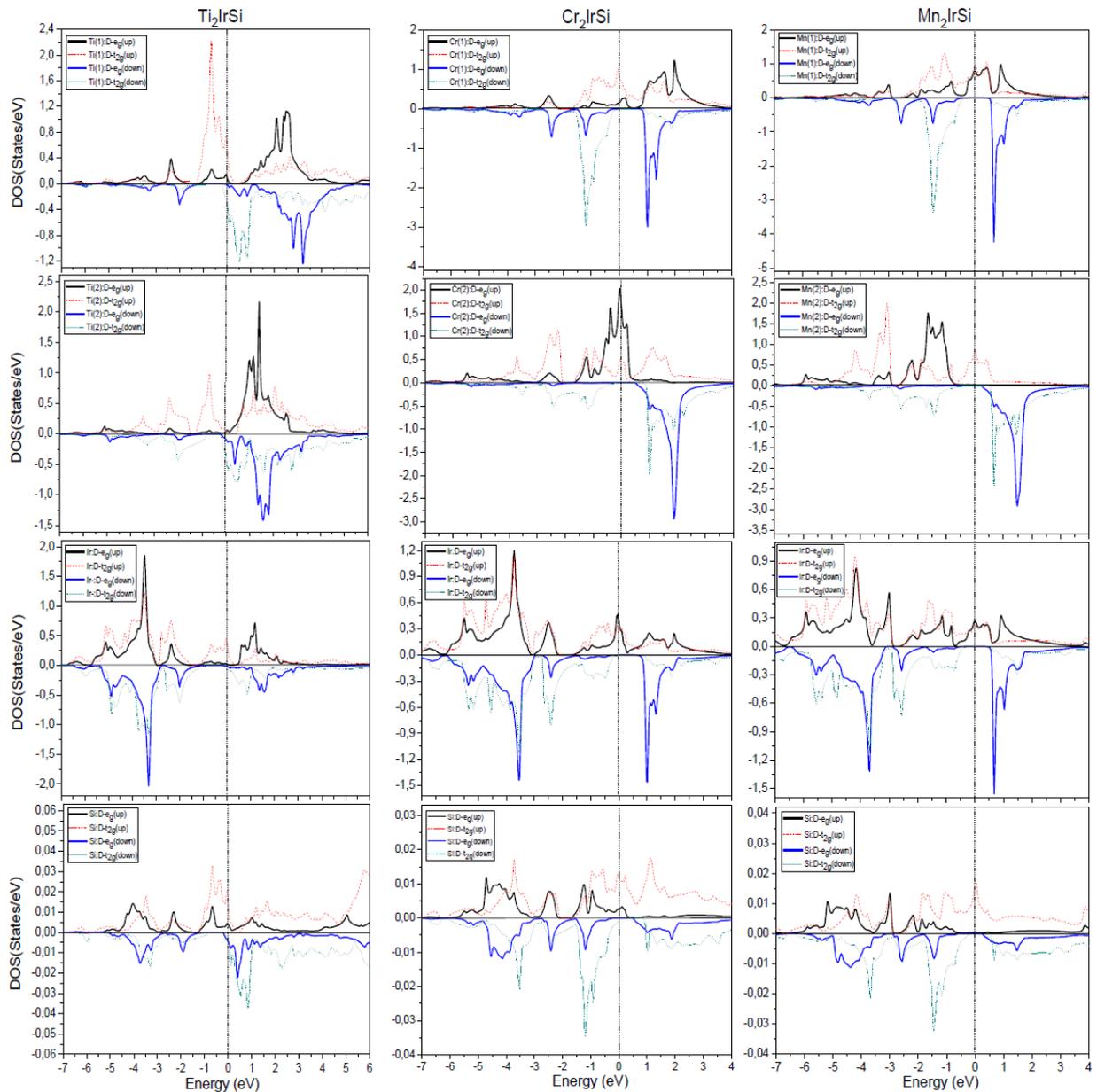


**Figure 4.** The densities of states (DOS) of s, p and d orbitals of  $\text{Cr}_2\text{IrSi}$  compound. The zero energy point represents the Fermi level



**Figure 5.** The densities of states (DOS) of *s*, *p* and *d* orbitals of  $Mn_2IrSi$  compound. The zero energy point represents Fermi level

In  $Ti_2IrSi$  compound, the peaks between -7 and -2 eV belong to the *p* orbital of Ir and Si atom. The sharp peaks, which are intercept the Fermi level, relative mainly to  $Ti(1)$ -*d* orbital. In this energy region, the peaks come from mainly Ir-*d* orbital have been seen in  $Cr_2IrSi$  compound. In  $Mn_2IrSi$  compound, while spin-up electrons intercept Fermi level, there is 0.41 eV energy gap at spin-down electrons. Briefly, the contributions from III-VI A elements are seen in remote energy regions from Fermi level. But as we approach the Fermi energy level, it appears that the main contributions come from transition metals, especially *d* orbitals. This is also an expected result.



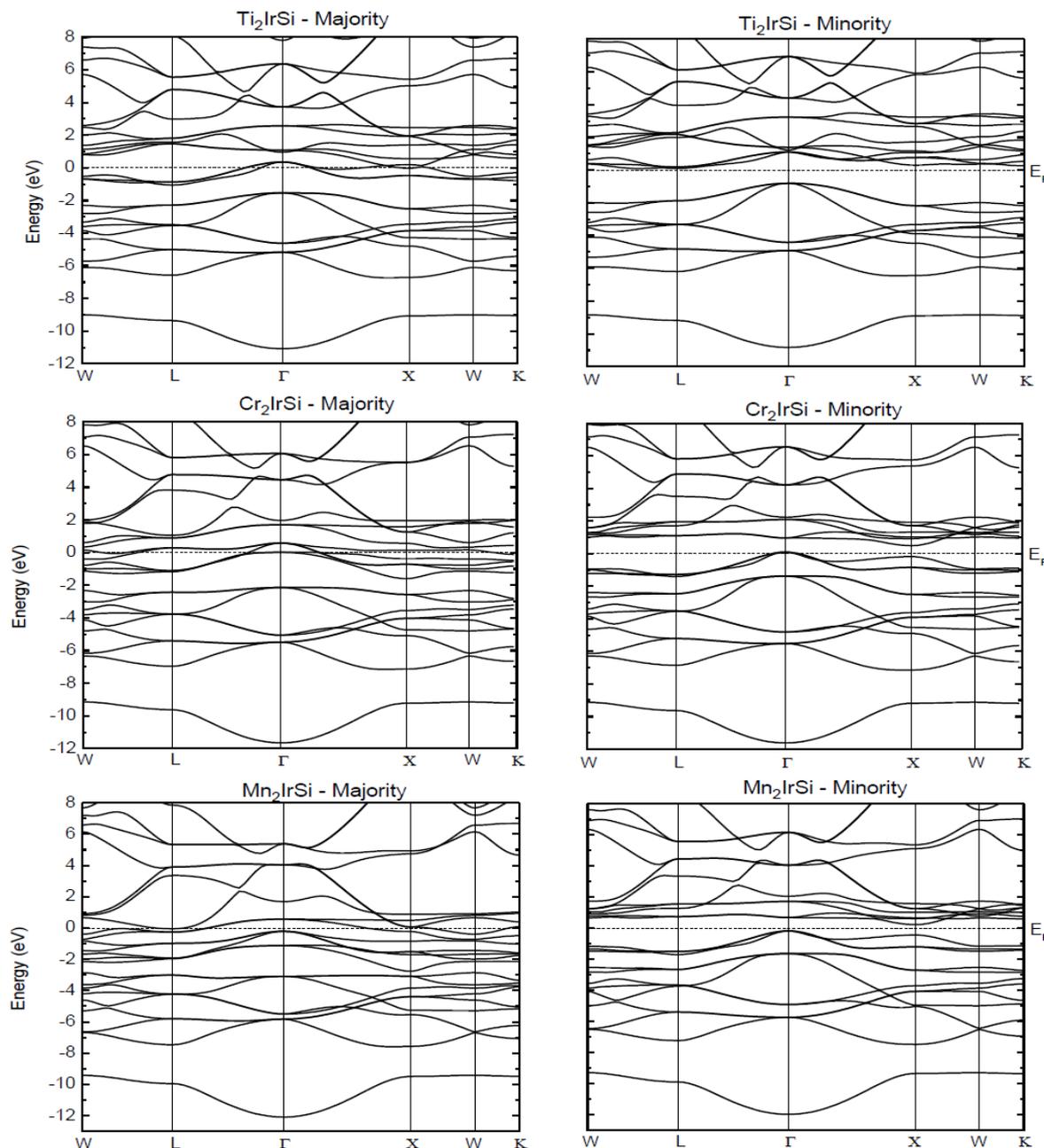
**Figure 6.** The partial DOSs of the  $M_2IrSi$  ( $M=Ti, Cr$  and  $Mn$ ) compounds. The zero energy point represents Fermi level

The hybridizations are one of the reason for energy gap [36]. For example, covalent hybridization between transition metals and bonding/anti-bonding states and d-d hybridization between d orbitals of transition metals may be the cause of these energy gaps [37]. In Figure 6, hybridizations were seemed energy interval of -6 and 5 eV. The majority and minority states for  $Ti_2IrSi$  and  $Cr_2IrSi$  compounds between -6 and -2 eV and for  $Mn_2IrSi$  between -6 and -4 eV energies come from mainly transition metal atom Ir. For  $Ti_2IrSi$  and  $Cr_2IrSi$  full-Heusler compounds, the sharp peak around the energy intervals of -2 and 0 eV belong to Ti(1), Ti(2) and Cr(1), Cr(2) atoms, respectively. In  $Mn_2IrSi$  compound, the hybridization between -2 and 0 eV belong to mainly Mn(1) and Mn(2) atom. The sharp peaks between energy intervals of 0-4 eV for majority and minority states come from mainly Ti(1) and Ti(2) atom in  $Ti_2IrSi$  compound. For  $Cr_2IrSi$  compound, the sharp peaks between the energy intervals of 0-2 eV belong to Cr(1) and Cr(2) atom in minority states. In  $Mn_2IrSi$  compound, the main contribution to DOS come from Mn(1) and Mn(2) atom. Furthermore, between 0-2 eV energy intervals, some contributions come from Ir atom. The  $Mn_2CuSb$  alloy was also studied about its covalent hybridization and band gap [38]. Therefore, both covalent and d-d hybridizations may be one of the reason of energy gap for  $Mn_2IrSi$  alloy.

The total and atomic magnetic moments of  $\text{Ti}_2\text{IrSi}$ ,  $\text{Cr}_2\text{IrSi}$  and  $\text{Mn}_2\text{IrSi}$  alloys are calculated and listed in Table 2. It is obviously seen that for  $\text{Ti}_2\text{IrSi}$ ,  $\text{Cr}_2\text{IrSi}$  and  $\text{Mn}_2\text{IrSi}$  alloys, the biggest contribution to magnetic moments come from Ti(1), Cr(2) and Mn(2) atoms, respectively.

### 3.3. Band Structure

The band structures of  $\text{M}_2\text{IrSi}$  ( $\text{M}=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) compounds for majority and minority electrons are presented in Figure 7.



**Figure 7.** Band structures of the  $\text{M}_2\text{IrSi}$  ( $\text{M}=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) compounds

In  $\text{Hg}_2\text{CuTi}$ -type structure for  $\text{Ti}_2\text{IrSi}$  compound, majority band structure has metallic nature. In minority band structure, energy gap can be seen at the Fermi level so, it has semiconduction behavior. The valance band maximum (VBM) value of the  $\text{Ti}_2\text{IrSi}$  compound is  $-0.80$  eV at  $\Gamma$  and conducting band minimum (CBM) value is  $0.09$  eV at W-L point range. The sum of these two values gives the band gap of  $-0.89$  eV. For half-metal materials, there has to be % 100 polarization around the Fermi level. This feature one of the

critical factor for HM materials. Here, it is clear that there is no %100 polarization so;  $Ti_2IrSi$  compound is conventional half-metallic ferromagnet. For  $Cr_2IrSi$  compound, both majority and minority band structures have metallic nature because of intersections at the Fermi level. Therefore,  $Cr_2IrSi$  compound is metallic ferromagnet. For  $Mn_2IrSi$  full-Heusler compound, the spin-up band structure is metallic while spin-down band structure has semiconduction nature due to energy gap. The sum of the energy gap is 0.41 eV. This energy gap and %100 polarization point out that  $Mn_2IrSi$  alloy is a true half-metallic ferromagnet. Therefore, this non-zero energy gap in band structure confirms of its density of states.

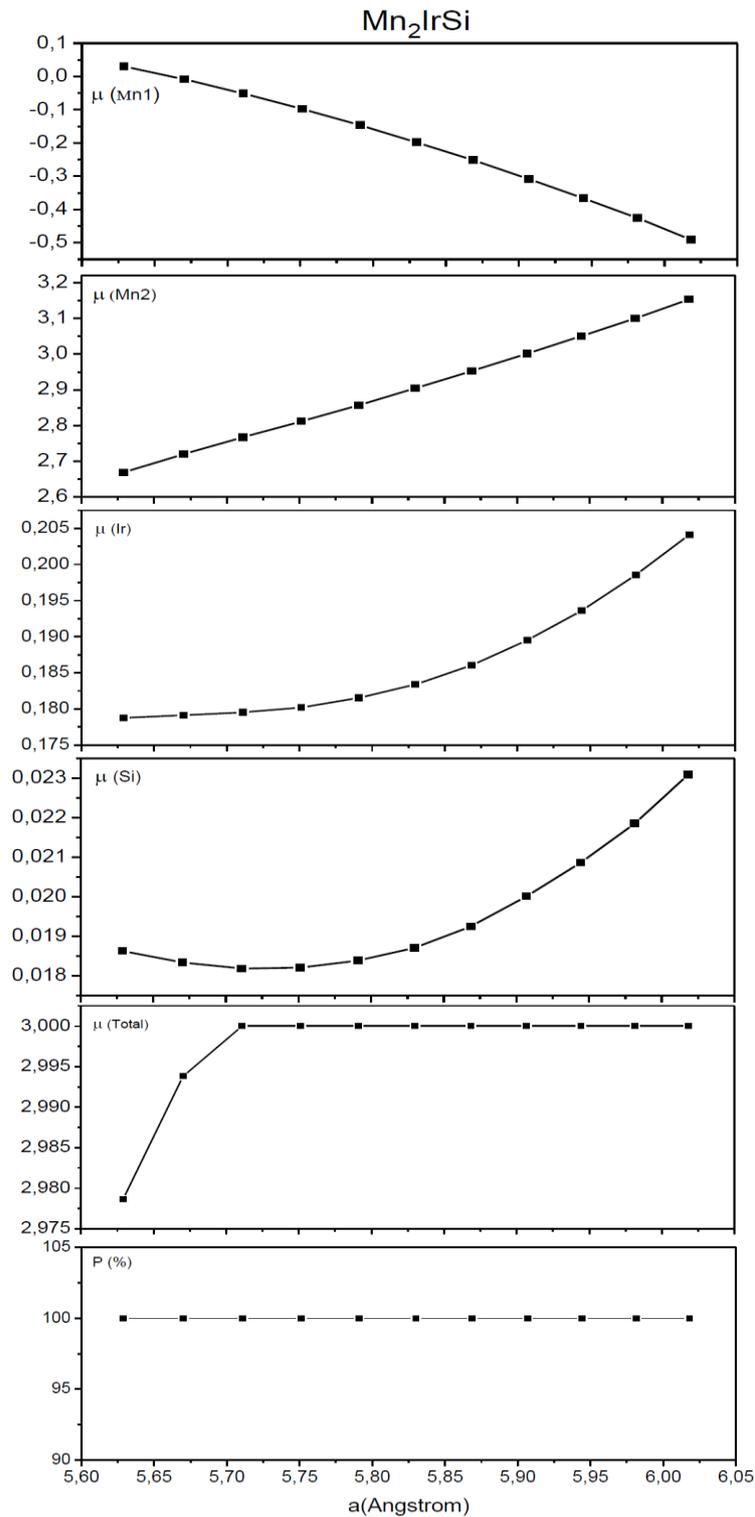
### 3.4. Magnetic Properties

We also calculate the total and atomic magnetic moments of  $M_2IrSi$  (M=Ti, Cr and Mn) compounds and list the results in Table 2.

**Table 2.** The total and atomic magnetic moments of  $Ti_2IrSi$ ,  $Cr_2IrSi$  and  $Mn_2IrSi$  compounds

Compounds	$\mu_{Tot}$ ( $\mu_B/f.u.$ )	$\mu_{X1}$ ( $\mu_B$ )	$\mu_{X2}$ ( $\mu_B$ )	$\mu_{Ir}$ ( $\mu_B$ )	$\mu_{Si}$ ( $\mu_B$ )
$Ti_2IrSi$	2.73	1.28	0.52	0.12	0.009
$Cr_2IrSi$	1.00	-1.08	1.97	0.04	0.001
$Mn_2IrSi$	3.00	-0.20	2.91	0.18	0.020

The Slater-Pauling rule proved to be a direct effect between the total magnetic moment  $M_t$  and the total number of valence electrons  $Z_t$  when examining the half-metallic properties of Heusler compounds [13]. This effect can be formulated as  $M_t=Z_t-18$  and  $M_t=Z_t-24$  [39]. The total numbers of valence electrons  $Z_t$  of  $Ti_2IrSi$ ,  $Cr_2IrSi$  and  $Mn_2IrSi$  Heusler compounds are 21, 19 and 27, respectively. According to SP rule, the total magnetic moments of  $Ti_2IrSi$  and  $Mn_2IrSi$  Heusler compounds are 3.0 and  $Cr_2IrSi$  is 1.0  $\mu_B$ . As a result of our calculations, the total magnetic moments of  $Ti_2IrSi$ ,  $Cr_2IrSi$  and  $Mn_2IrSi$  compounds are observed to be 2.73, 1.0 and 3.0  $\mu_B$ , respectively. Briefly, the work we do is similar to the SP rule in  $Cr_2IrSi$  and  $Mn_2IrSi$  compounds. Although  $Cr_2IrSi$  compound provides the SP rule, it is not a half-metallic material due to the intersections of the band structure. We conclude that  $Mn_2IrSi$  compound is true half-metallic ferromagnet.



**Figure 8.** The total and partial magnetic moment of  $Mn_2IrSi$  full-Heusler compound as a function of lattice constants

Figure 8 shows the computed total and atom-projected magnetic moments of  $Mn_2IrSi$  as a function of lattice parameters between 5.62 - 6.02 Å. According to Figure 8, the intervals of the lattice parameters, calculated total magnetic moment is 3.0  $\mu_B$  for  $Mn_2IrSi$  compound. It is clear that the main additive to magnetic moment comes from Mn(2) atom. The absolute values of magnetic moments increase with increasing lattice constant. This increasing was also seemed in different Heusler compounds [40].

#### 4. CONCLUSION

We studied the structural and magnetic properties of  $M_2\text{IrSi}$  ( $M=\text{Ti}$ ,  $\text{Cr}$  and  $\text{Mn}$ ) full-Heusler compounds for ferromagnetic and non-magnetic states using WIEN2k. All calculations are performed for the FM states of the  $\text{Hg}_2\text{CuTi}$  structure, which is the most stable state as energetically. According to these calculations; majority electrons have metallic nature in all compounds. Around the Fermi level, spin-down electrons of  $\text{Ti}_2\text{IrSi}$  compound have 0.89 eV energy gap while both total and atom-projected DOSs intercept the Fermi level. For  $\text{Cr}_2\text{IrSi}$  compound, spin-down electrons are also intercept the Fermi level. In the minority spin band of  $\text{Mn}_2\text{IrSi}$  full-Heusler compound, there is 0.41 eV energy gap.  $\text{Ti}_2\text{IrSi}$ ,  $\text{Cr}_2\text{IrSi}$  and  $\text{Mn}_2\text{IrSi}$  compounds have 2.73, 1.0 and 3.0  $\mu_B/\text{f.u.}$  magnetic moment, respectively. Furthermore, the total and partial magnetic moments of  $\text{Mn}_2\text{IrSi}$  alloy is computed as a result of lattice parameters intervals of 5.62- 6.02 Å. These results show the main additive to magnetic moments come from Mn(2) atom. Finally,  $\text{Ti}_2\text{IrSi}$  compound is conventional half-metallic,  $\text{Cr}_2\text{IrSi}$  compound is metallic and  $\text{Mn}_2\text{IrSi}$  full-Heusler alloy is a true half-metallic ferromagnet.  $\text{Mn}_2\text{IrSi}$  full-Heusler alloy can be new candidate material for using in spintronic.

#### CONFLICTS OF INTEREST

No conflict of interest was declared by the authors.

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