An-Najah National University

Faculty of Graduate Studies

STRUCTURAL, ELECTRONIC, MAGNETIC AND ELASTIC PROPERTIES OF THE FULL-HEUSLER COMPOUNDS: SC_2TIAL, SC_2TISI USING FP-LAPW METHOD

By

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Dr. Khaled Ilaiwi	_____
Internal Examiner	Signature

Dedication

I am highly grateful to my beloved parents for all sacrifices they have made to make my future better. May Allah bless them. To my lovely sisters and my brother, who always encourage me and give me powerful support.

Acknowledgments

All thanks to Allah, who gives me health, knowledge and patience to complete my thesis. I would like to acknowledge the following people who helped me in many aspects that made it possible to write this thesis. First, I address a special thanks to my supervisor and instructor Prof. Dr. Mohammed Abu-Jafar and Dr. Mahmoud Farout for their continuous support, effortless help, valuable discussions and humble guidance. They always encourage my work and allow me to think and execute my plans independently. I really feel so lucky to have them as my supervisors. Never forget my faculty members of the physics department in my university for their help and encouragement.

Declaration

I, the undersigned, declare that I submitted the thesis entitled:

STRUCTURAL, ELECTRONIC, MAGNETIC AND ELASTIC PROPERTIES OF THE FULL-HEUSLERR COMPOUNDS: Sc2TiAl, Sc2TiSi USING FP-LAPW METHOD

I declare that the work provided in this thesis, unless otherwise referenced, is the researcher's own work, and has not been submitted elsewhere for any other degree or qualification.

Student's Name: _____

Signature: _____

Date: _____

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STRUCTURAL, ELECTRONIC, MAGNETIC AND ELASTIC PROPERTIES OF THE FULL-HEUSLER COMPOUNDS: SC_2TIAL, SC_2TISI USING FP-LAPW METHOD

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ABSTRACT

In this study, we investigate the structural, electronic, magnetic and elastic properties of the normal and inverse Heusler Sc_2TiAl and Sc_2TiSi compounds using a full potential linearized augmented plane wave (FP-LAPW) method, within the density functional theory. The band structure and DOS calculations are made within the generalized gradient approximation (GGA) and modified Becke Johnson approaches (mBJ-GGA), employed in the Wien2K code. The density of states (DOS) and band structure (BS) show metallic nature. We calculate the structural properties such as the lattice constants, bulk moduli and elastic properties like Poisson ratio v, shear modulus S, Young modulus (Y) and B/s ratio. Results are in agreement with previous studies so these properties provide a road map for its possible uses in electronic devices.

Chapter One

Introduction

The discovery of Heusler compounds has been greatly applied in Spintronic [1], Shape memory [2], thermoelectric [3] and a wide range of functionalities [4-8]. Heusler alloys can be divided into two groups comprising half-Heusler alloys (XYZ-type) which normally crystallize in C1b-type and full-Heusler alloys (X_2YZ-type) which normally crystallize in L21-type. The normal X_2YZ-type Heusler alloys have a face-centered cubic lattice and space group of 225Fm3-m. X_2 atoms are in the positions of (0.25, 0.25, 0.25), (0.75, 0.75, 0.75) and Y atom occupies the position of (0.5, 0.5 0.5) and Z atom occupies the position of (0, 0, 0). In addition, the inverse Heusler alloy has a composition of X_2YZ with 216- F-43Mspace group. X_2 atoms are in the positions of (0.25, 0.25, 0.25),(0.5, 0.5 0.5) and Y atom occupies the position of (0.75, 0.75, 0.75) and Z atom occupies the position of (0, 0, 0). The d-states hybridization should be remodulated in different surroundings of X atoms. Changing elements gave Heusler alloys multiple functionalities, which led to a wide interest [9, 10].

The major purpose of this study is a study consisting of investigating and predicting structural, magnetic, electronic, and elastic properties of Sc_2TiAl and Sc_2TiSi in the cubic phase for possible applications such as spintronic. Spintronics have a high possibility for next generation information technology (IT). Half-metallic ferromagnetism is the main active component of spintronics. Spin polarization characterizes half-metallic compounds. They have metallic behavior in spin-up, while they are semiconductors or insulators in spin-down [11].

Many previous studies have worked on Heusler compounds by various methods. In 2019 Han et al. [12] made a study on scandium based full Heusler compounds. They found that the $L2_1$-type structure (normal structure) is more stable than XA structure (inverse structure) since the difference of energy between the structures ($\Delta E = E_{XA} - E_{L21}$) > 0. This means that $L2_1$- type structure is more likely to synthesize. They calculated the band structure of Sc_2TiAl and Sc_2TiSi alloys. The calculated electronic structures of the $L2_1$- type structure and the XA structure of Sc_2TiAl and Sc_2TiSi are ferromagnetic. The two possible structures, $\Delta E = E_{XA}$ –

E_{l2}, lattice constants, magnetic moments, and the stable structure of Sc based full Heusler alloys are listed in Table 1.

Table 1

The two possible structures, ΔE, lattice constants, magnetic moments and the stable structure of Sc based full [12].

compound	Structure	ΔE (eV /cell)	a(A)	M_t (μB/ f.u)	MSc1 (μB)	MSc2 (μB)	MY (μB)	MZ (μB)	Stable structure	E_F
Sc_2TiAl	XA (inverse)	0.3	6.83	2.24	0.24	0.68	1.55	-0.23	$L2_1$	-0.65
	$L2_1$ (normal)		6.87	2.92	0.47	0.47	2.23	-0.25		
Sc_2TiSi	XA (inverse)	0.34	6.64	2.51	0.23	0.9	1.58	-0.21	$L2_1$	-0.98
	$L2_1$ (normal)		6.69	2.96	0.44	0.44	2.29	-0.2		

In 2020, Abu Baker *et al*. [9] investigated the structural, electronic, magnetic and elastic properties of half metallic ferro magnetism full-Heusler alloys: normal Co_2TiSn and inverse Co_2TiSn using the FPLAPW method. The lattice parameter for the normal Co_2TiSn and inverse Zr_2RhGa are respectively 6.094 A^0 and 6.619A^0. In addition, the total magnetic moments for these compounds are 1.9786μ_B and 1.99μ_B respectively. Also, these compounds have energy gaps 0.482eV and 0.573eV. Furthermore, they are mechanically stable.

In 2021, Yotong, et al. [10] screened the half metallic X_2Y (Al/Si) full Heusler alloys based on the first principle calculations. Ten of these alloys are half-metallic.$(Co/Mn)_2YZ$alloys are magnetic and half metallic. Moreover, they predicted that $(Mn/Co)_2Y(Al/Si)$ alloys can be use in spintronic applications.

This work is formulated with 4 sections, the first one exposes an introduction which highlights the importance of Heusler alloys and literature review about Sc_2TiAl and Sc_2TiSi specifically and Heusler alloys generally and the main purpose of this work. The second section is methodology and the full potential linearized augmented plane wave (FP-LAPW). The third one which encompasses the results obtained by making reference to other results available in the literature review, so all the results obtained are compared. The last section is a conclusion, which shows the physical properties of the normal and inverse Sc_2TiAl and Sc_2TiSi compounds.

Chapter Two

Methodology

To study solids by considering periodic potential with multi-atomic unit cells, quantum mechanics is used to solve the Schrodinger equation for the given solid. Schrodinger equation doesn't have an exact solution. There are some approximations to solve this problem such as density functional theory which allows the proper treatment of the Coulomb correlation as it introduces an exchange correlation term within the one-electron approximation. Also, The local density approximation (LDA) (Parr and Yang, 1989) represents the simplest approach to the exchange-correlation energy $\varepsilon_{xc}[\rho(\vec{r})]$ per electron of a homogenous electron gas whose electronic density is precisely $\rho_o(r)$ at each point **r.** The term "local" refers to the absence of any $\rho_o(r)$ derivative in the expression for $\varepsilon_{xc}[\rho(\vec{r})]$ which implies that the LDA approximation will be valid when the electronic density varies very slowly with the position. Moreover generalized gradient approximation (GGA) improves the LDA definition of the exchange-correlation energy by including the first derivatives of the electronic density. Whereas LDA uses the exchange energy density of the uniform electron gas, regardless of the homogeneity of the real charge density, the generalized gradient approximation takes care of such non-uniform charge density by including the gradient of the electron density in the functional. GGA uses the gradient of the charge density $\vec{\nabla}\rho(\vec{r})$.

The full potential linearized augmented plane wave (FPLAPW) approach is taken into account for performing the theoretical calculations. The WIEN2k software operating within the FPLAPW method is used, which is based on the density functional theory (DFT). The exchange and correlation potentials (ECP) were considered using generalized gradient approximation (GGA) proposed by Perdew. Burke. Emzerholf (PBE). It is well known that the GGA often underestimate the band gap and to overcome this problem the Becke .Johnson potential (mBJ-GGA) was used to improve the calculating band gaps of semiconductors and insulators. In the FPLAPW method, space around the atoms in the unit cell is divided into two regions. The first region is a spherical muffin tin (MT) around the nuclei in which the radial solutions of the Schrödinger equation and their energy derivatives are used as basic functions. The

second region is the interstitial region between the MTs, in which the basis set consists of plane waves [13-15].

$$\phi_{\vec{K}}^{\vec{k}}(\vec{r},E)=\begin{cases}\sum_{l.m}\left(a_{lm}^{\alpha,\vec{k}+\vec{K}}u_l^{\alpha}(r',E)+b_{lm}^{\alpha,\vec{k}+\vec{K}}\dot{u}_l^{\alpha}(r',E)\right)Y_m^l(\hat{r}'), & Inside\ sphere\\ \frac{1}{\sqrt{V}}e^{i(\vec{k}+\vec{K}).\vec{r}}, & Outside\ sphere\end{cases} \quad (1)$$

Where $Y_{lm}(r)$ is Spherical harmonic, $u_l(r,E_l)$ is the regular solution of the radial Schrödinger equation for energy E_l and the spherical part of the potential inside the sphere, and $\dot{u}_l^{\alpha}(r',E)$ is the energy derivative of u_l taken at the same energy E_l. The well-converged solutions of energy in GGA approximation were obtained with $R_{MT}K_{max.}= 8.0$ (where R_{MT} is the smallest muffin-tin radii and K_{max} is the plane wave cut off for the basis function and the largest magnitude of k vector was with $L_{max} = 10$ and $G_{max} = 14$ (a.u.)$^{-1}$[16].

Chapter Three

Results and Discussion

3.1 Computational Method

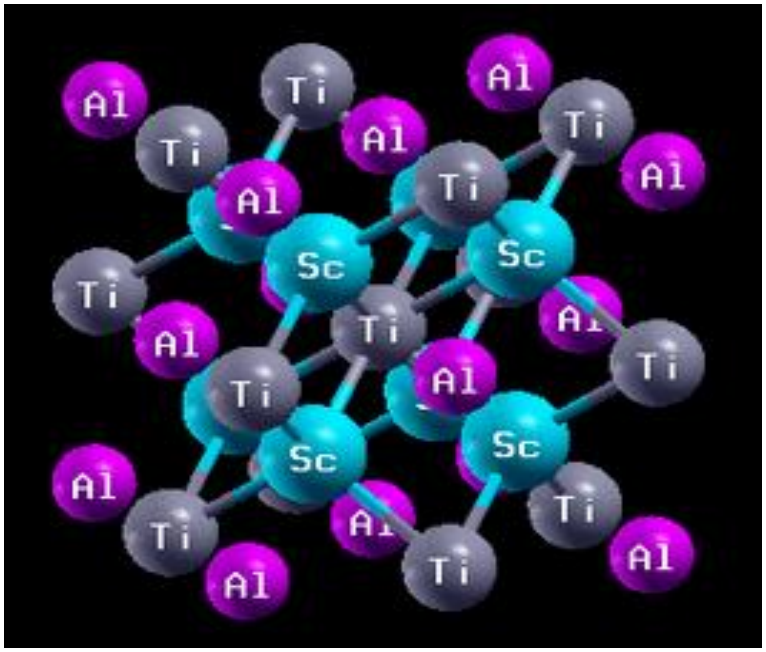
In reporting calculations in this thesis, we used the full potential linearized augmented plane wave implemented in the WIEN2k package [16-20]. According to the compound Sc_2TiAl, the MT radii (R_{MT})of Sc,Ti and Al atoms are 2.50, 2.50 and 2.39 a.u. respectively. Also, for the compound Sc_2TiSi, R_{MT} of Sc, Ti and Si atoms are 2.45, 2.45 and 2.14 a.u. respectively. Moreover, to obtain self consistency for Sc_2TiAl and Sc_2TiSi there are 47 special k points in the irreducible Brillion zone (IBZ)with grid$10\times 10 \times 10$ (equivalent to1000k points in the Full BZ)were used [16]. Furthermore, the expansions of the wave functions were set by l=10 inside the MT spheres and the number of plane waves was restricted by $K_{MAX}R_{MT} = 8$. But the self-consistent calculations are considered to converge only when the calculated total energy of the crystal converges to be less than 10^{-5} Ry. Finally, using second-order derivative within formalism WIEN2k code, the elastic constants of the cubic phase were calculated.

3.2 Structural Properties

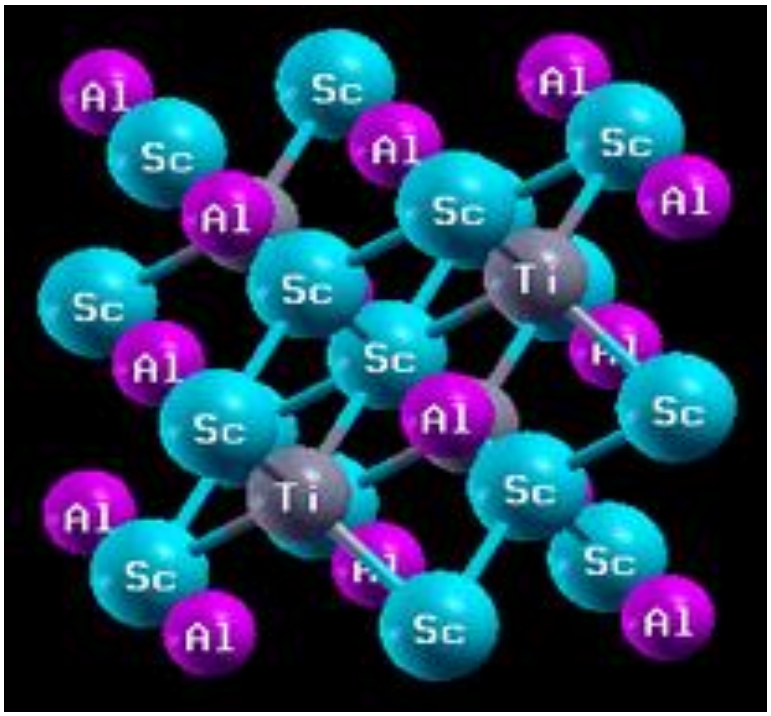
The normal Heusler Sc_2TiAl and Sc_2TiSi compounds have space group Fm-3m L21 (225) and inverse Heusler Sc_2TiAl and Sc_2TiSi compounds have space group F-43m X (216) [9]. The crystal structures of Full-Heusler Sc_2TiAl and Sc_2TiSi compounds are shown in figure 1. In optimized volume calculation we use a guess value of lattice parameter for each compound then the total energy versus the volume for Heusler Sc_2TiAl and Sc_2TiSi compounds are drawn as shown in figures 2 and 3. From figure 2 it is clear that the normal of Sc_2TiAl has minimum energy E0 lower than the inverse of Sc_2TiAl, so the normal structure of Sc_2TiAl is more mechanically stable than the inverse structure of Sc_2TiAl. Also, from figure 3 it is clear that the normal of Sc_2TiSi has minimum energy E0 lower than the inverse of Sc_2TiAl, so the normal structure of Sc_2TiSi more mechanically stable than the inverse structure of Sc_2TiSi.

Figure 1.a

Crystal structures of a) Sc_2TiAl normal Heusler structure, Fm-3m L21 (225) b) Sc_2TiAl inverse Heusler structure, F-43m X (216)



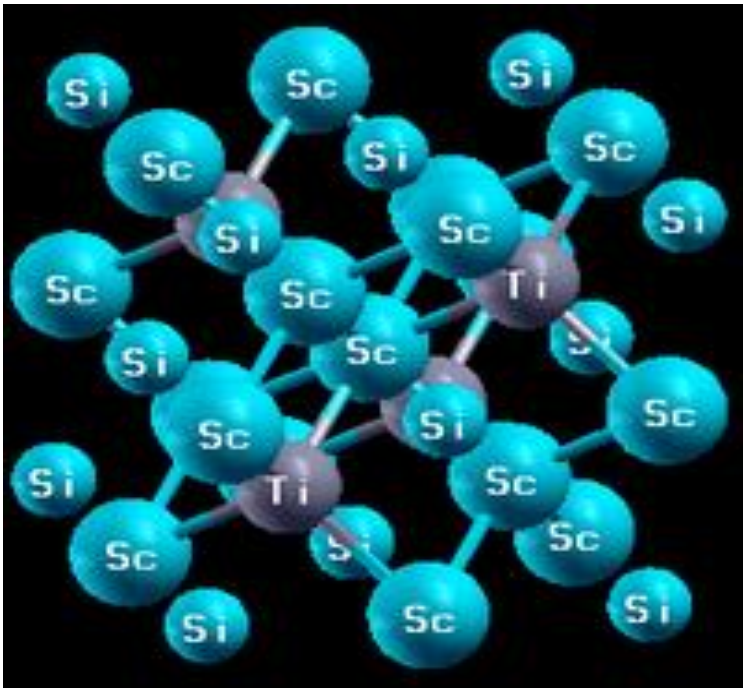
(a)



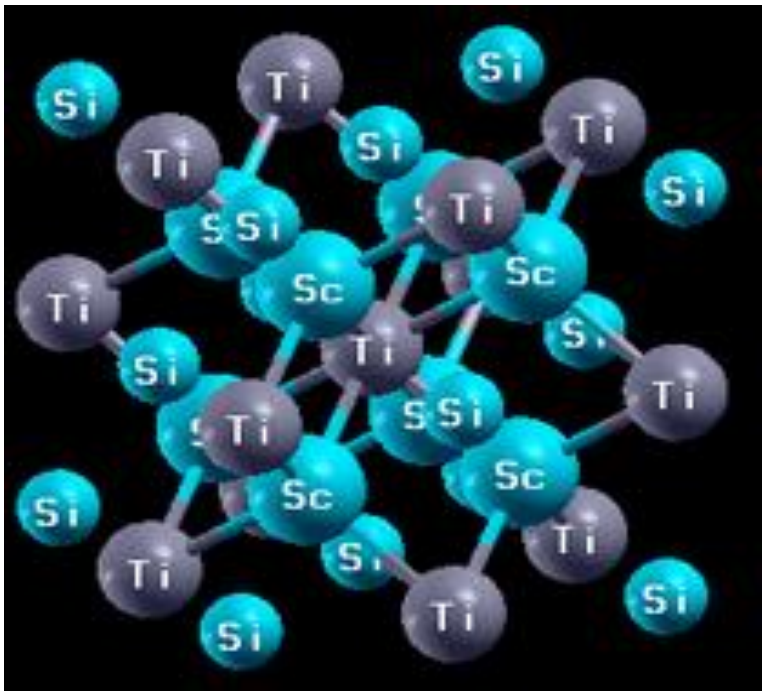
(b)

Figure 1.b

Crystal structures of c) Sc_2TiSi normal Heusler structure, Fm-3m L21 (225) d) Sc_2TiSi inverse Heusler structure, F-43m X (216).



(c)



(d)

Figure 2

The total energy (Ry) versus volume (a.u^3) for normal Sc_2TiAl Heusler and inverse Sc_2TiAl Heusler.

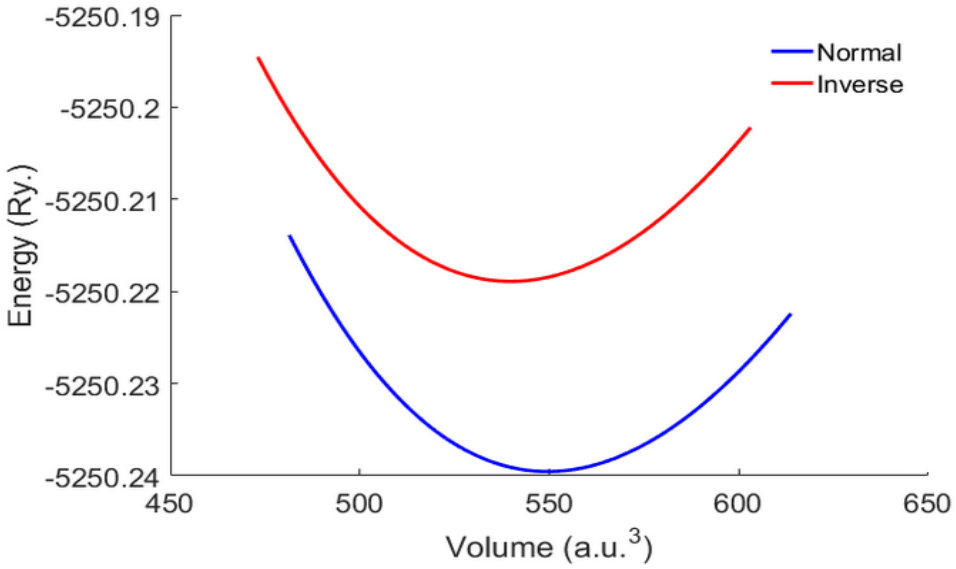
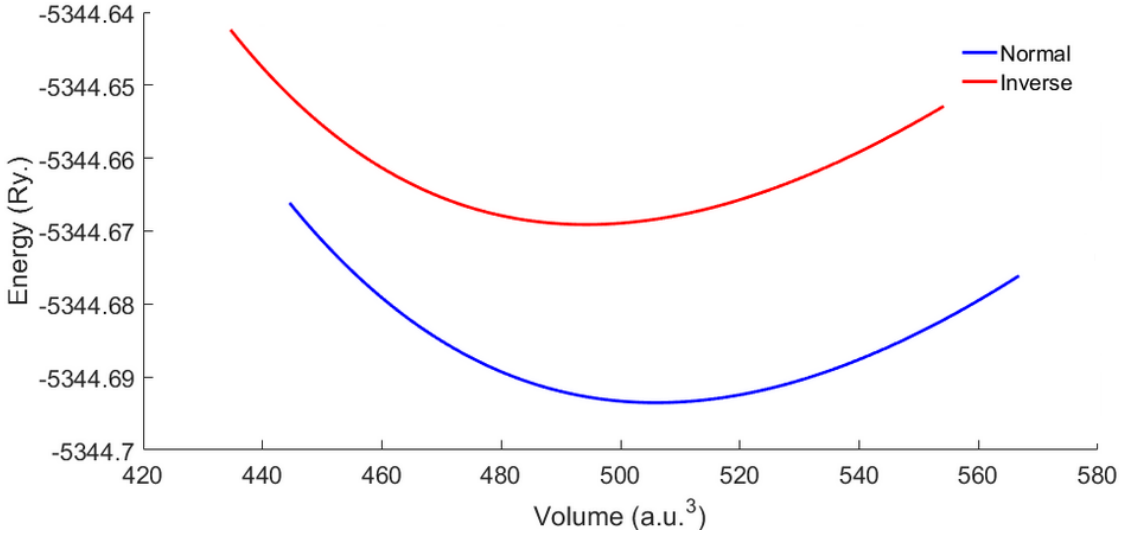


Figure 3

The total energy (Ry) versus volume (a.u^3) for normal Sc_2TiSi Heusler and invers Sc_2TiAl Heusler.



To calculate the structural properties; optimized lattice constant (a), bulk modulus (B), its pressure derivative (B'), and minimum energy E_0. The total energy (Ry) versus volume (a.u^3) graphs were fitted by using Murnaghan's [21, 22]. Murnaghan's equation of state (EOS) is given by:

$$E(V) = E_0 + \frac{VB}{B'}\left\{\left[\frac{\left(\frac{V_0}{V}\right)^{B'}}{B'-1}\right] + 1\right\} - \left[\frac{BV_0}{B'-1}\right] \quad (2)$$

where Pressure, **P= -** $\frac{dE}{dV}$, Bulk modulus, **B= - V** $\frac{dP}{dV}$ **= V** $\frac{d^2E}{dV^2}$

These structural properties of the normal and the inverse Sc_2TiAl and Sc_2TiSi are listed in table(2).

Table 2

Calculated lattice parameter(a),bulk modulus (B),first pressure derivative of the Bulk modulus(B')and minimum energy E_0 for normal and inverse Heusler Sc_2TiAl and Sc_2TiSi compounds.

compounds	reference	Lattice Parameter(a) A^0	B(GPa)	B′(GPa)	E_0 (eV)
normal Sc_2TiAl	present	6.8807	75.8990	2.5917	-5250.239
	theoretical	6.87[12]	-	-	-
inverse Sc_2TiAl	present	6.8369	73.9513	3.3006	-5250.218
	theoretical	6.83[12]	-	-	-
normal Sc_2TiSi	present	6.6935	85.2808	4.3534	-5344.963
	theoretical	6.69[12]	-	-	-
Inverse Sc_2TiSi	present	6.6415	82.7864	5.2583	-5344.669
	theoretical	6.64[12]	-	-	-

In Table 2 it shows that the present calculated lattice parameters are compatible with the theoretical lattice parameters of normal and inverse HeuslerSc_2TiAl and Sc_2TiSi compounds [12].

3.3 Magnetic Properties

The total and partial magnetic moment for the normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi are calculated, and the results of other theoretical works are compared as shown in tables 3 and 4. It turned out that the normal and inverse Heusler Sc_2TiAl and Sc_2TiSi are ferromagnetic compounds. We concluded that the calculated

total magnetic moment of normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi results are in good agreements with theoretical results [12], as shown in tables 3 and 4.

Table 3

Total, atomic and interstitial magnetic moment for inverse and normal Sc_2TiAl compound.

Compounds		**Magnetic Moment**					
		Sc1 (μ_B)	Sc2 (μ_B)	Ti (μ_B)	Al (μ_B)	Interstitial	Total magnetic moment $(M^{tot})(\mu_B)$
Normal Sc_2TiAl	Present result	0.28350	0.28350	1.50006	-0.02116	0.67425	2.72015
	Theoretical result [12]	-	-	-	-	-	2.29
Inverse Sc_2TiAl	Present result	0.17455	0.41469	0.90719	-0.02462	0.60050	2.07231
	Theoretical result [12]	-	-	-	-	-	2.24

Table 4

Total, atomic and interstitial magnetic moment for inverse and normal Sc_2TiSi compound.

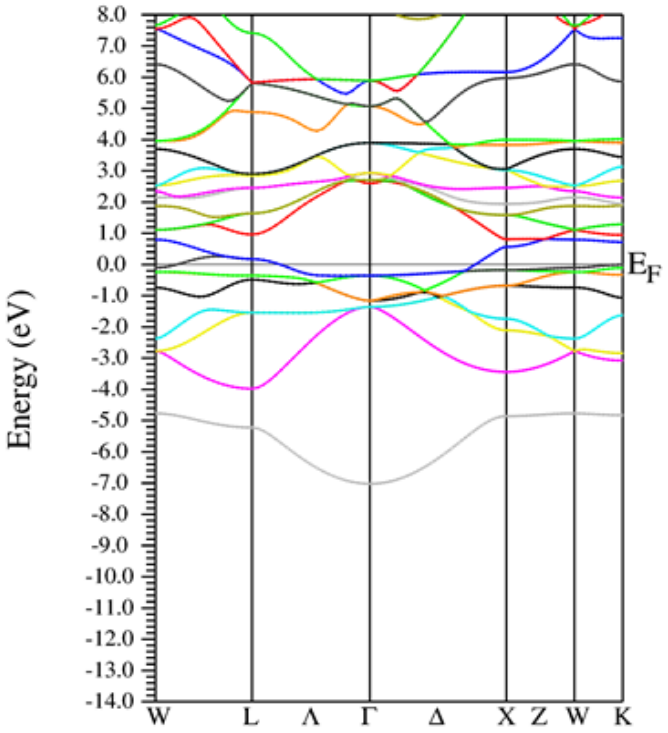
Compounds		**Magnetic Moment**					
		Sc1 (μ_B)	Sc2 (μ_B)	Ti (μ_B)	Si (μ_B)	Interstitial	Total magnetic moment $(M^{tot})(\mu_B)$
Normal Sc_2TiSi	Present result	0.27795	0.27795	1.61519	-0.03812	0.67466	2.80764
	Theoretical result [12]	-	-	-	-	-	2.96
Inverse Sc_2TiSi	Present result	0.16182	0.57086	0.90862	-0.04172	0.60463	2.20421
	Theoretical result [12]	-	-	-	-	-	2.51

3.4 Electronic Properties

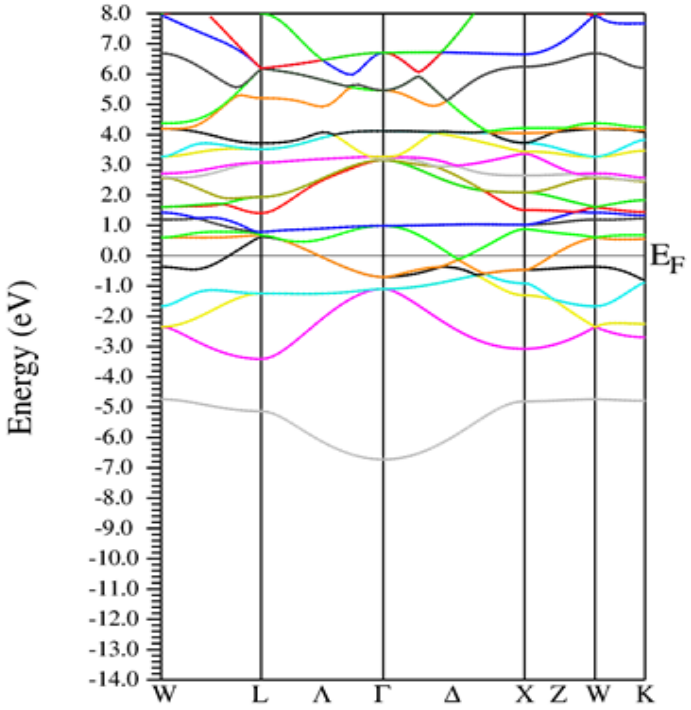
Here, DOS, PDOS, band structure for normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi were drawn. According to the band structure that the normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi are metallic for the spin-up and spin-down band structures within the PBE-GGA method with zero energy gap as shown in figures 4, 5, 6 and 7. In addition, figures 8, 9, 10 and figure 11 in appendix A show metallic behavior of the spin up and spin down BS using mBJ-GGA method for the normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi with zero energy gaps.

Figure 4

The BS for normal Heusler Sc_2TiAl compound by using PBE-GGA method for (a)spin-up (b)spin-down.



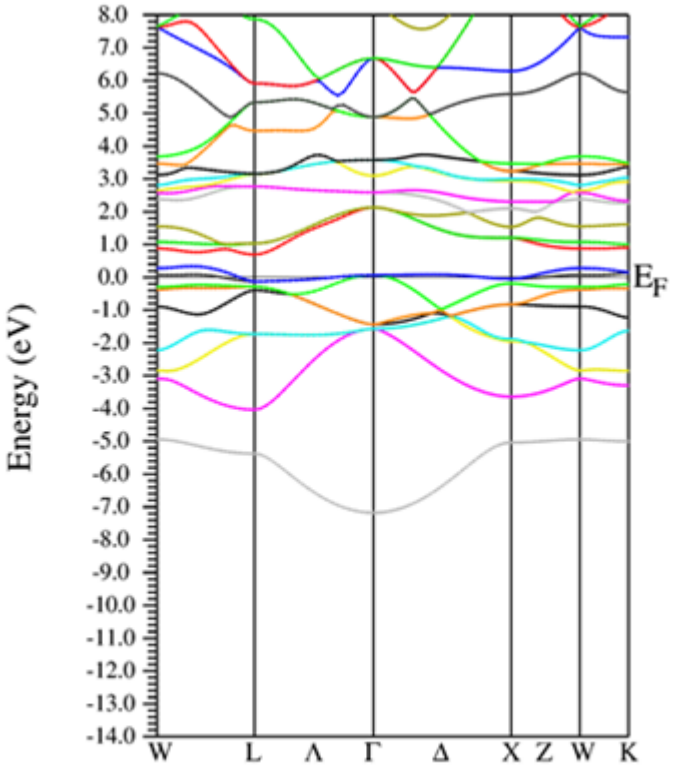
(a)


Energy (eV)
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
-3.0
-4.0
-5.0
-6.0
-7.0
-8.0
-9.0
-10.0
-11.0
-12.0
-13.0
-14.0
E_F
W
L
Λ
Γ
Δ
X
Z
W
K

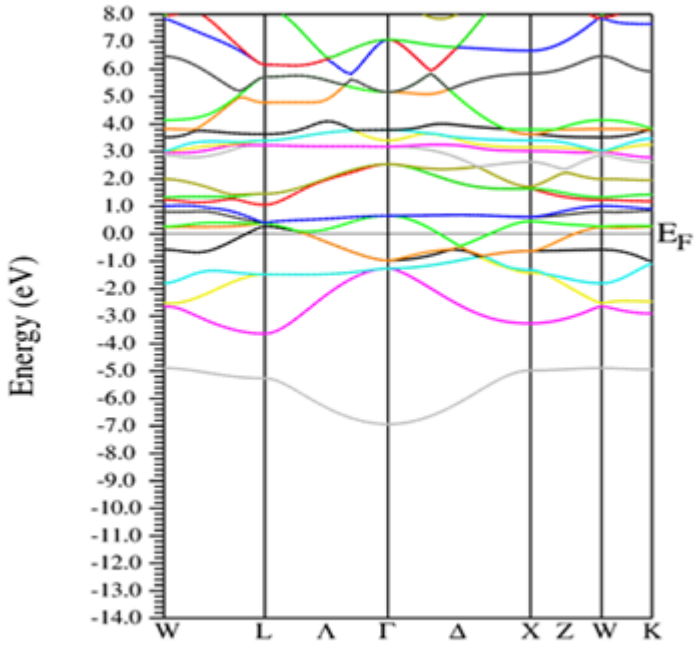
(b)

Figure 5

The BS for inverse Heusler Sc_2TiAl compound by using PBE-GGA method for (a)spin-up (b)spin-down.



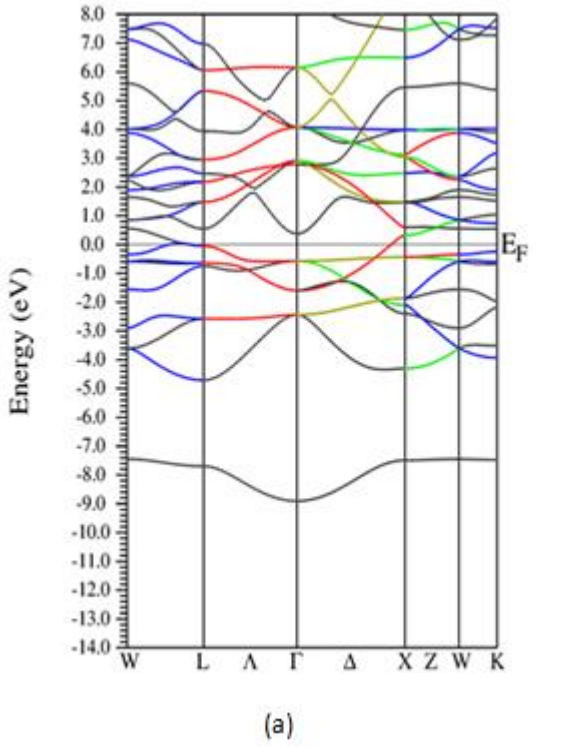
(a)



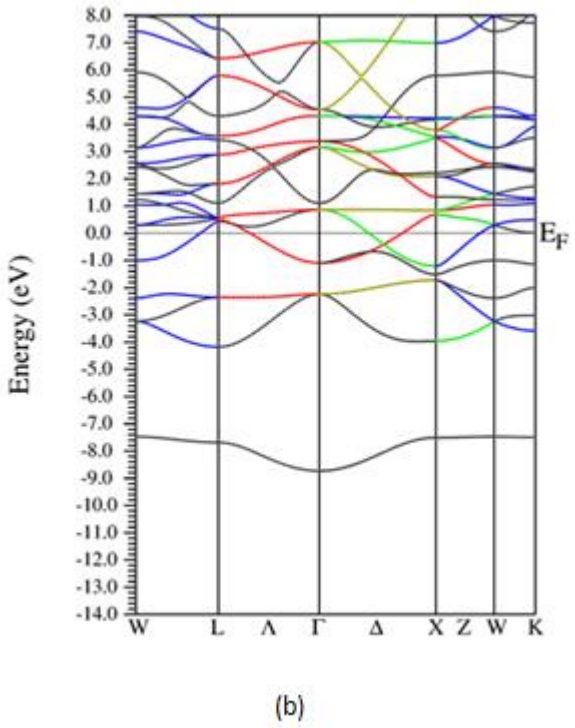
(b)

Figure 6

The BS for normal Heusler Sc_2TiSi compound by using PBE-GGA method for (a)spin-up (b)spin-down.



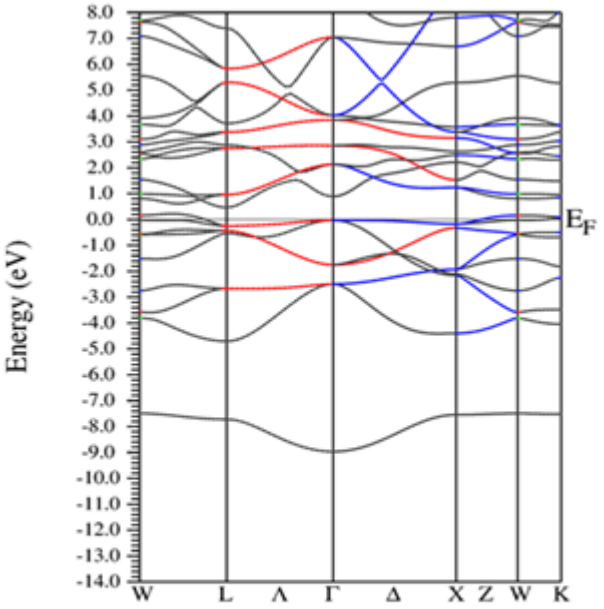
(a)



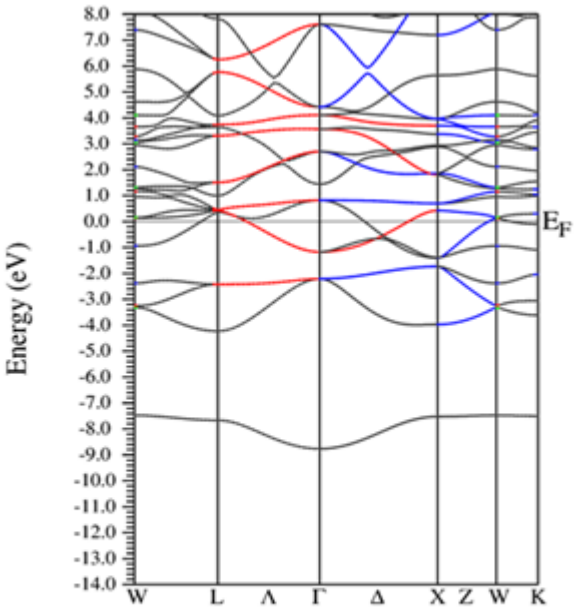
(b)

Figure 7

The BS for inverse Heusler Sc_2TiSi compound by using PBE-GGA method for (a) spin-up(b)spin-down.



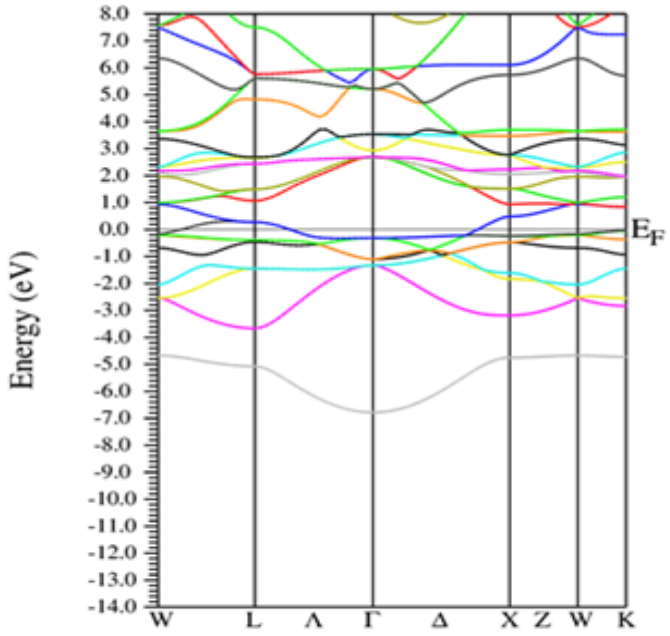
(a)



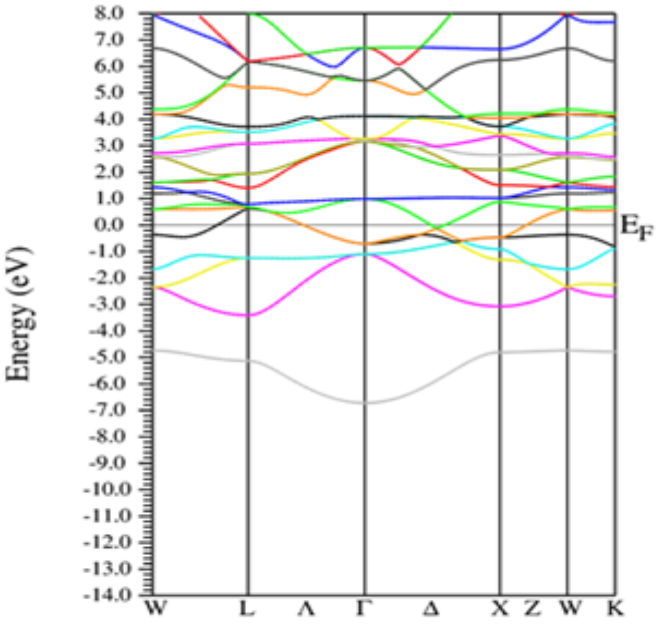
(b)

Figure 8

The BS for normal Heusler Sc_2TiAl compound by using mBJ-GGA method for (a)spin-up(b)spin-down.



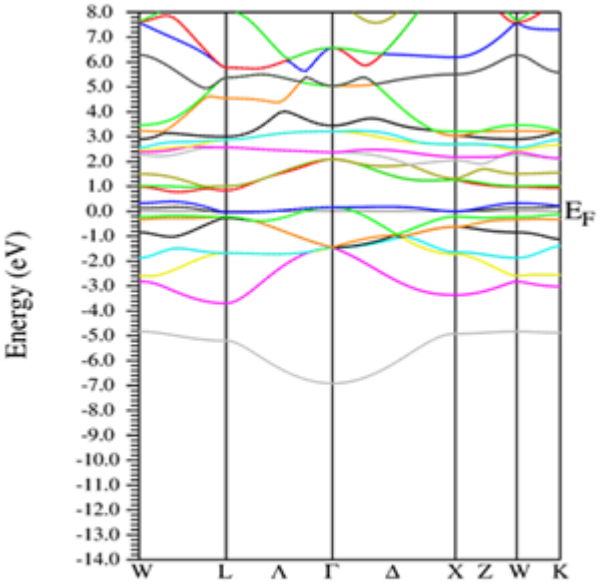
(a)



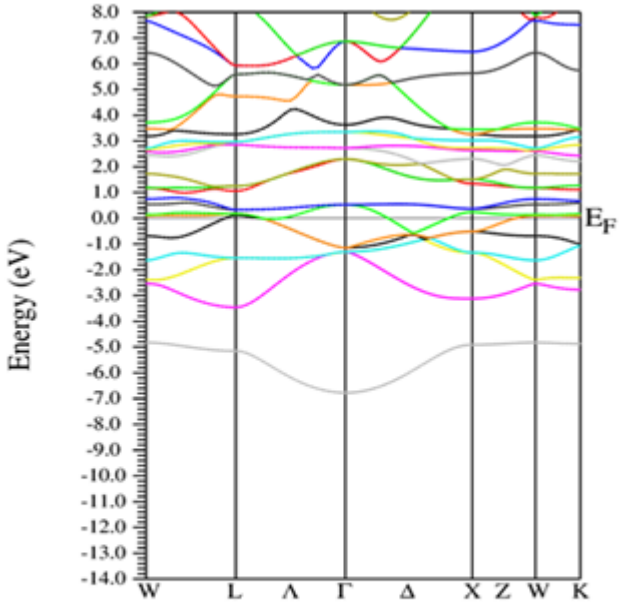
(b)

Figure 9

The BS for inverse Heusler Sc_2TiAl compound by using mBJ-GGA method for (a)spin-up (b)spin-down.



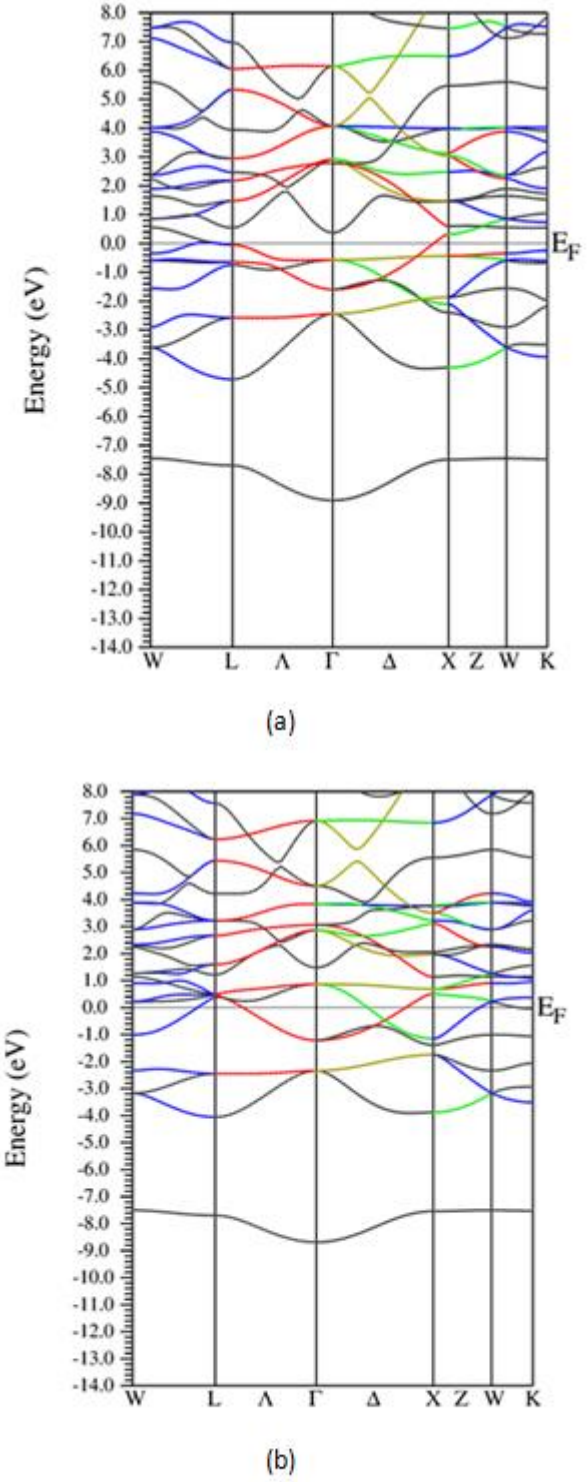
(a)



(b)

Figure 10

The BS for normal Heusler Sc_2TiSi compound by using mBJ-GGA method for (a)spin-up (b)spin-down.



Figures 12-19 in appendix A show DOS, PDOS for spin-up and spin-down of the normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi. These figures show also metallic behavior for the normal and inverse Heusler compounds Sc_2TiAl and Sc_2TiSi.

In the spin up of normal Sc_2TiAl (figure 12), the main contributions in valence band come from d orbits of Sc, d orbits of Ti and the s and p orbits of Al, and the main contributions come from Ti atom then Sc atom then small contribution from Al atom in this compound. Also, the main contributions in conduction band come from d orbits of Sc, d orbits of Ti and the s and p orbits of Al, the main contributions come from Sc atom then Ti atom then small contribution from Al atom in this compound. In spin down of normal Sc_2TiAl (figure 13), the main contributions in valence band come from d orbits of Sc, d orbits of Ti and the s and p orbits of Al, and the main contributions come from Sc atom then small contribution from Al atom then Ti atom in this compound. While the main contributions in conduction band come from d orbits of Sc, d orbits of Ti and the s and p orbits of Al, in addition the main contributions come from Sc atom then Ti atom then small contribution from Al atom in this compound.

In the spin up and spin down of inverse Sc_2TiAl (figures 14 and 15), the main contributions in valence band come from d orbits of Sc, d orbits of Ti, and the s and p orbits of Al, and the main contributions come from Sc atom and Ti atom then small contribution from Al atom in this compound. Also, the main contributions in conduction band come from d orbits of Sc, d orbits of Ti, and the s and p orbits of Al, and the main contributions come from Sc atom and Ti atom then small contribution from Al atom in this compound.

In the spin-up and spin-down of the normal and inverse Sc_2TiSi (figures 16, 17, 18, 19), the main contributions in the valence and the coduction bands come from d orbits of Sc, d orbits of Ti, and the s and p orbits of Si.

3.5. Elastic properties

Elasticity is a property of matter that explains the deformation of materials. Whenever a force is exerted on a solid it undergoes deformation. For investigating elasticity the stability can be used. There are three symmetry elements for cubic bulk alloys C_{11}, C_{12}, and C_{44},. The conditions of mechanical stable are as follows [9, 10], [21-24]:

$$\begin{matrix} C_{11} > 0 \\ C_{44} > 0 \\ C_{11} + 2C_{12} > 0 \\ C_{11} - C_{12} > 0 \\ C_{12} > \mathrm{B} > C_{11} \end{matrix} \quad (3)$$

B: bulk modulus.

For the compounds investigated and according to the above stable conditions, the normal, inverse Sc_2TiAL and the normal Sc_2TiSi alloys are mechanically stable, while the inverse Sc_2TiSi alloy is mechanically unstable, as shown from Table 5.

After that, the ductile behavior and the type of chemical bonds were investigated. The compounds with ratio B/S>1.75 and Poisson ratio v> 0.26 are ductile and others are brittle [25-27]. The Voigt shear modulus S_v, the Reuss shear modulus S_R, the Hill shear modulus S_H and the bulk modulus B were calculated as follows [28-30]:

$$S_v = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \quad (4)$$

$$S_R = 5C_{44}(C_{11} - C_{12})/(4C_{44}+3(C_{11} - C_{12})) \quad (5)$$

$$S_H = 0.5(S_v+S_R) \quad (6)$$

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \quad (7)$$

The nature of bonding is calculated by the Poisson's ratio v. Compounds with covalent bonds have Poisson ratio v smaller than 0.25, while for ionic bonds compounds is 0.25 <v< 0.5[24-27]. From Table 6, the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds are ductile and have ionic bonds.

$$v = \frac{3B-2S}{2(3B+S)} \quad (8)$$

The definition for the ratio of the stress to strain, the Young modulus (Y),is given by the following:

$$Y = \frac{9BS}{(S+3B)} \quad (9)$$

Anisotropic factor is given by the following:

$$A = \frac{2C_{44}}{C_{11}-C_{12}} \quad (10)$$

The hardness of materials is measured by the Bulk modulus and the shear modulus [21], while the stiffness of materials is measured by the Young modulus (Y). Likewise, the elastic anisotropy A is a parameter to measure the degree of anisotropy of materials [22].A is one for an isotropic alloy. Otherwise, the material is elastic anisotropy [21]. The inverse and normal Heusler Sc_2TiAl and Sc_2TiSi compounds are elastic anisotropy as shown in Table 5.

Table 5

Elastic constants (C_{ii}), bulk modulus (B) and anisotropic factor(A) of the normal and inverse Heusler Sc_2TiAl and Sc_2TiSi compounds.

Compounds	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	B (GPa)	A
Normal Sc_2TiAl	92.6833	65.5877	65.5761	74.619	4.840
Inverse Sc_2TiAl	76.1917	73.5691	62.8489	74.443	47.929
Normal Sc_2TiSi	104.8203	78.3970	65.3312	87.204	4.945
Inverse Sc_2TiSi	68.6086	69.7097	65.0067	69.342	-118.07

Table 6

Shear modulus (S), B/S ratio, Voigt Poisson ratio ($\boldsymbol{\nu}$) and Young modulus (Y) of the normal and inverse Heusler Sc_2TiAl and Sc_2TiSi compounds.

Compounds	S (GPa)			B/S (GPa)			Y (GPa)			V		
	Voigt	Reuss	Hill	Voigt	Reuss	Hill	Voigt	Reuss	Hill	Voigt	Reuss	Hill
Normal Sc_2TiAl	44.764	25.856	35.310	1.666	2.885	2.113	111.913	69.536	91.497	0.25	0.344	0.295
Inverse Sc_2TiAl	38.233	3.178	20.705	1.947	23.424	3.595	97.933	9.400	56.844	0.280	0.478	0.372
Normal Sc_2TiSi	44.482	25.341	34.911	1.960	3.441	2.497	114.053	69.309	92.402	0.282	0.367	0.323
Inverse Sc_2TiSi	38.784	-1.394	18.695	1.787	-49.74	3.709	98.068	-4.210	51.460	0.264	0.510	0.376

Chapter Four

Conclusion

In this thesis, the structural, magnetic, electronic and elastic properties of the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds are investigated. The results are found as the following: according to the electronic properties the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds are metals with zero energy band gaps in both methods PBE-GGA and mBJ. Therefore, the mBJ method does not improve the energy band gap in metals, but it can only in semiconductors and insulators. While for magnetic properties, the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds are ferromagnetic compounds with total magnetic moment of M^{tot} =2.72, 2.07,2.80, 2.20 $\mu_B$respectively. In addition, elastic properties of these compounds emphasize that the normal and inverse of Sc_2TiAL and the normal of Sc_2TiSi are mechanically stable, but the inverse of Sc_2TiSi is mechanically unstable. B/S results show that the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds have ductile natures. In addtion, it is clear from the Poisson ratio values that the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds have ionic bonds. Finally, the normal and inverse Heusler Sc_2TiAL and Sc_2TiSi compounds are elastic anisotropy.

List of Abbreviations

Abbreviation	Meaning
BS	Band structure
GGA	Generalized gradient approximation
DFT	Density functional theory
LDA	Local density approximation
mBJ	Modified Becke Johnson
FP-LAPW	full potential linearized augmented plane wave
DOS	Density of state

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Appendices

Appendix A

Figures of Study

Figure A.1

The BS for inverse Heusler Sc_2TiSicompound by using mBJGGAmethod for (a)spin-up (b)spin-down.

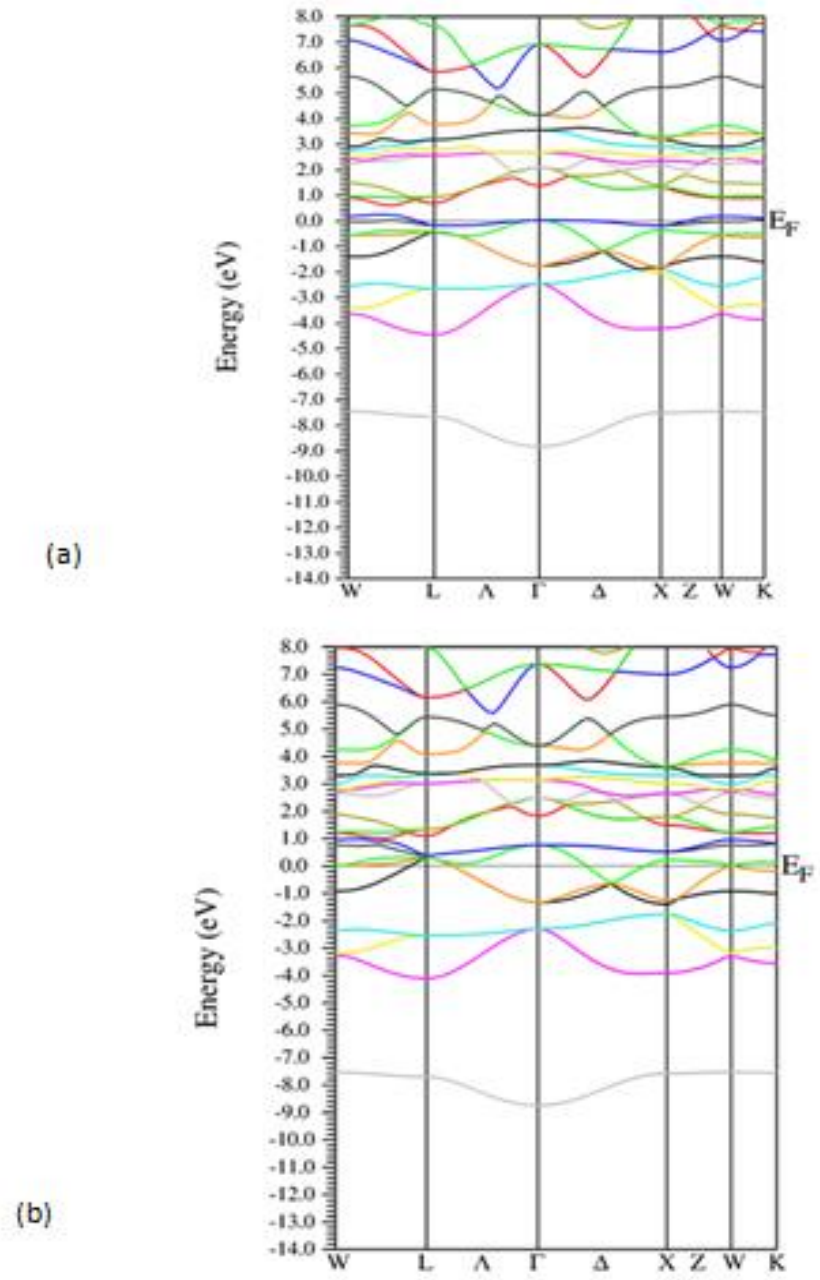
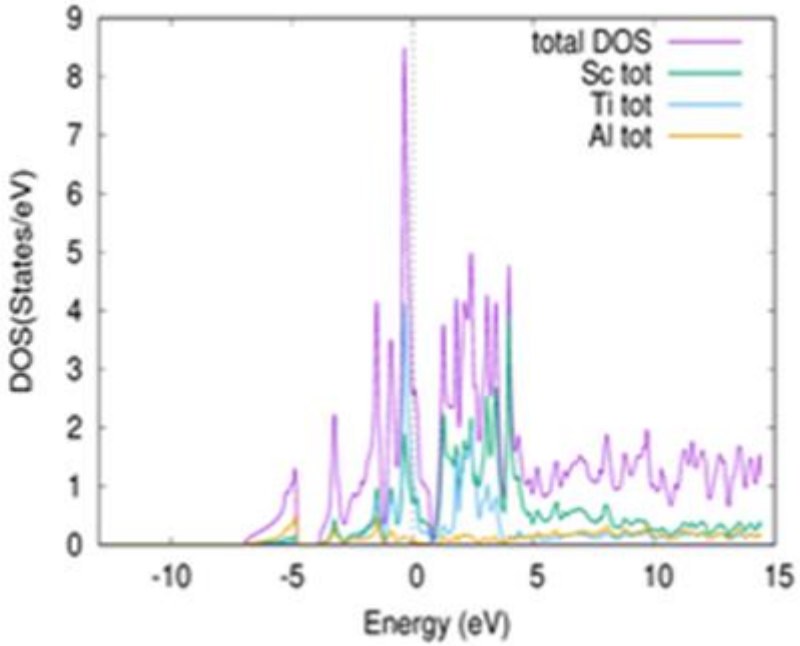


Figure A.2.a

(a) Spin-up total density of states (DOS) for normal Sc_2TiAl and partial density of states(PDOS) of spin-up for (b) Sc atom (c) Ti atom (d) Al atom of normal Sc_2TiAl.

(a)



(b)

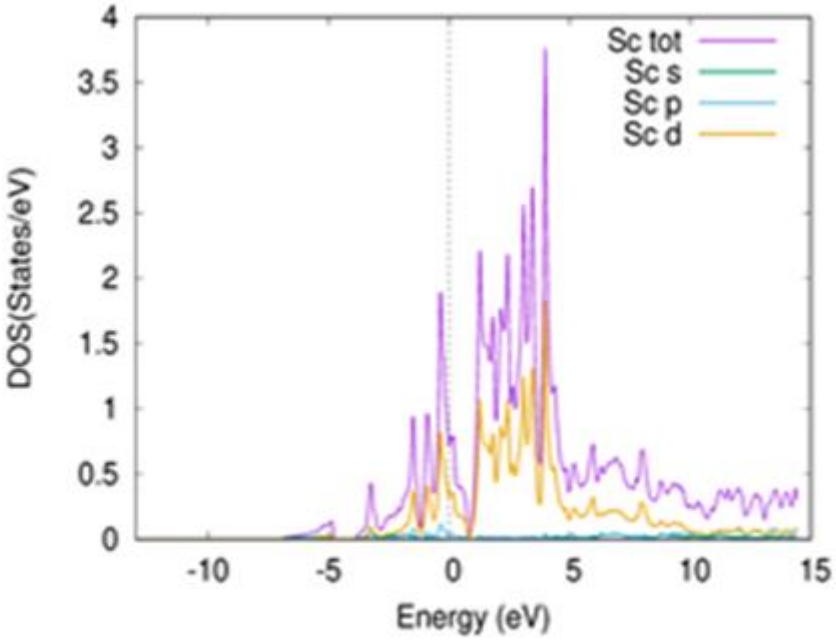


Figure A.2.b

spin-up partial density of states (PDOS) for (c) Ti atom (d) Al atom of normal Sc_2TiAl.

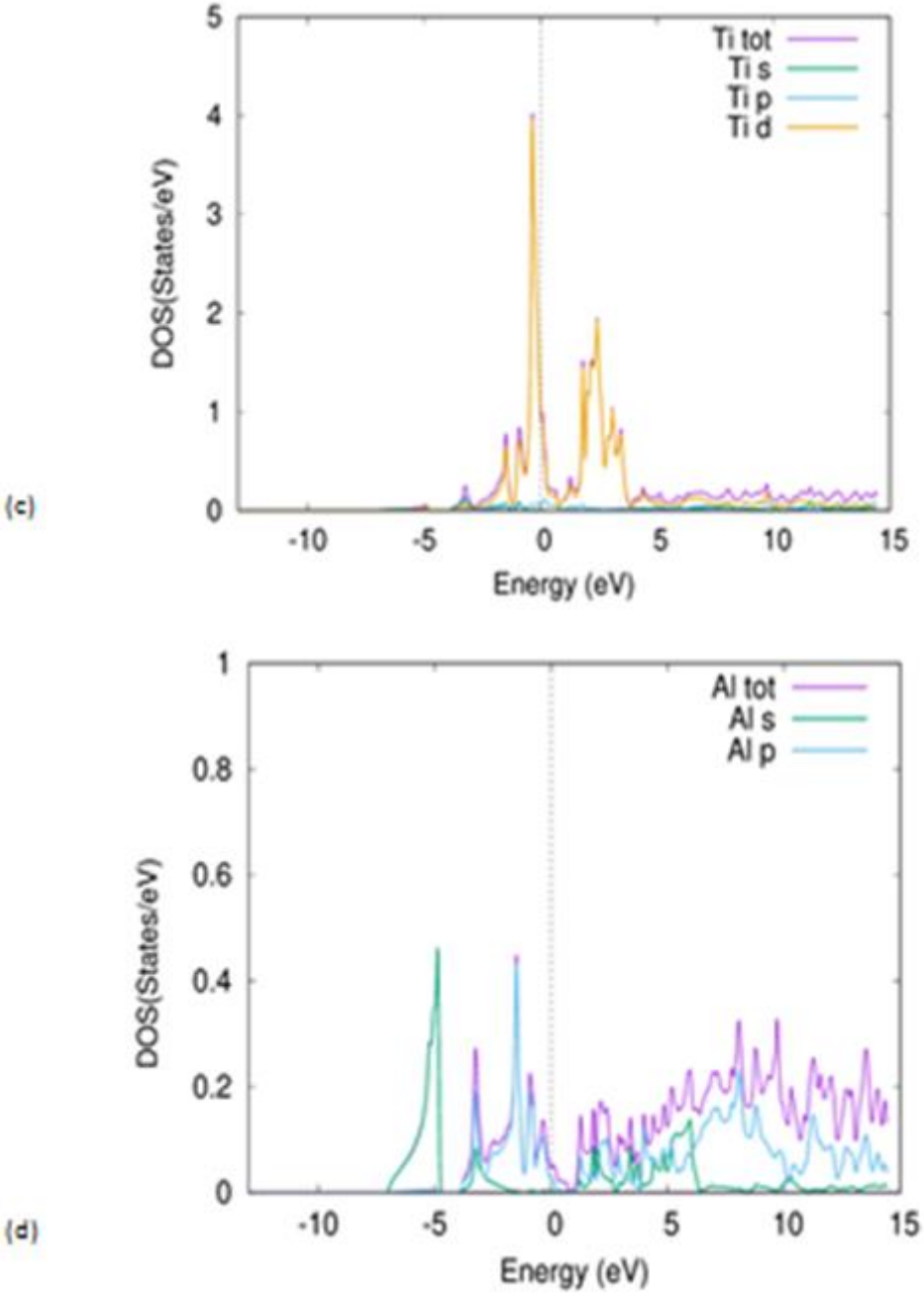
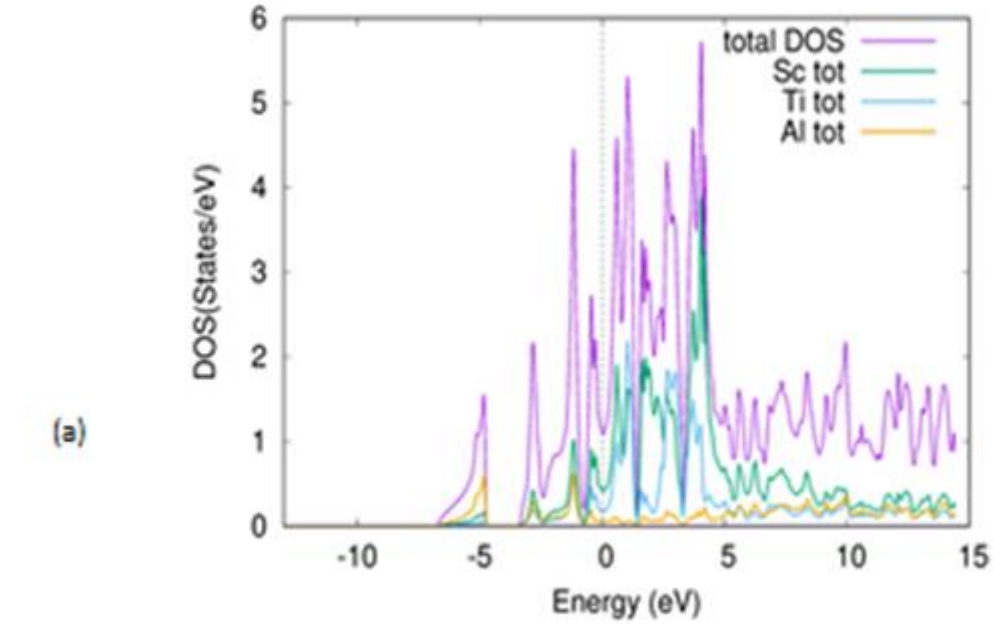


Figure A.3.a

(a) Spin-down total density of states(DOS) for normal Sc_2TiAl and partial density of states(PDOS) of spin down for (b) Sc atom of normal Sc_2TiAl.



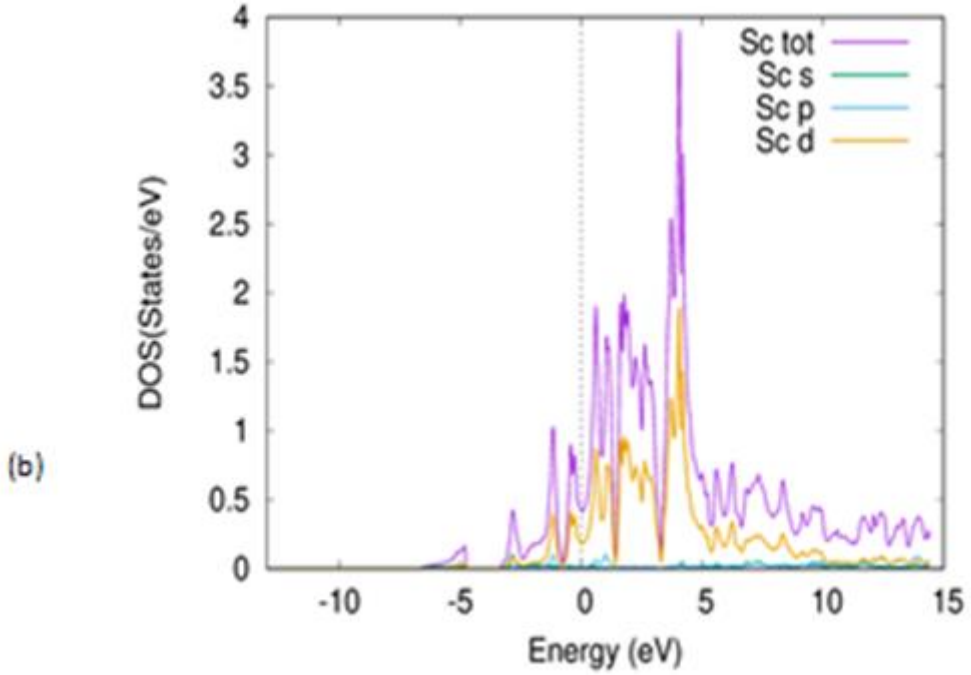


Figure A.3.b

Spin-down partial density of states (PDOS) for (c) Ti atom (d) Al atom of normal Sc_2TiAl.

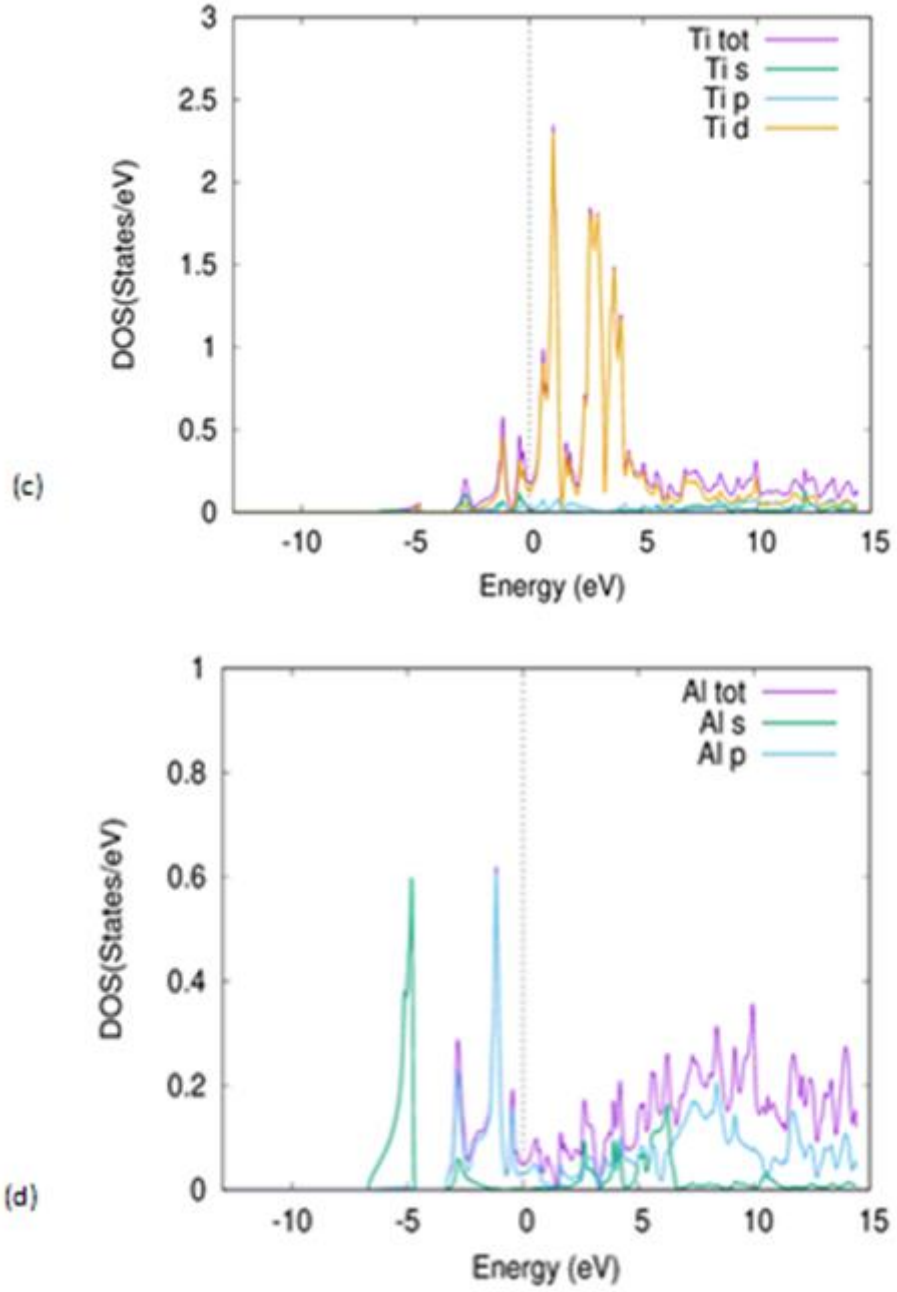


Figure A.4.a

(a) Spin-up total density of states(DOS) for inverse Sc_2TiAl and partial density of states(PDOS) of spin-up for (b) Sc atom number 1 of inverse Sc_2TiAl compound.

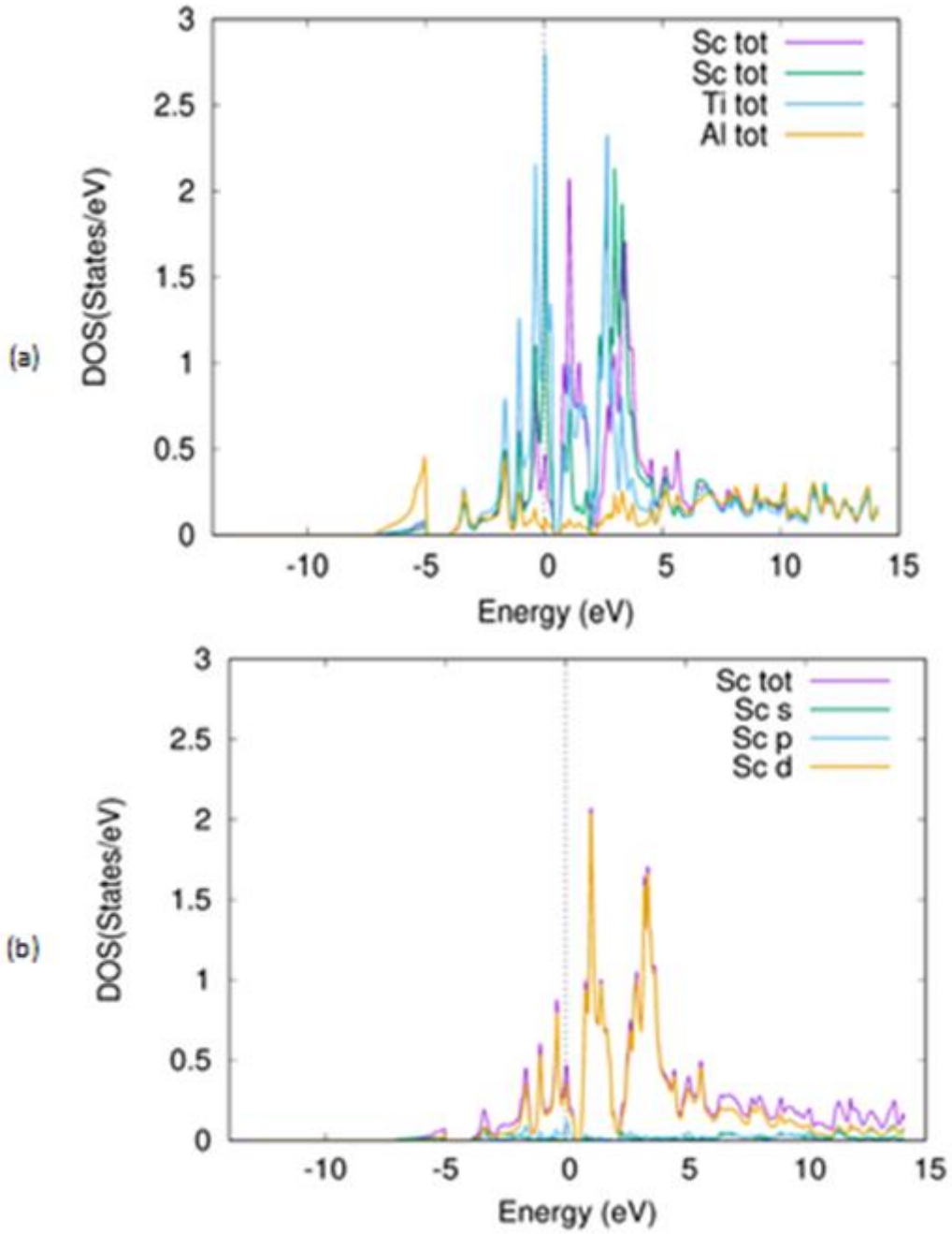


Figure A.4.b

Spin-up partial density of states (PDOS) for (c) Sc atom number 2 (d) Ti atom of inverse Sc_2TiAl compound.

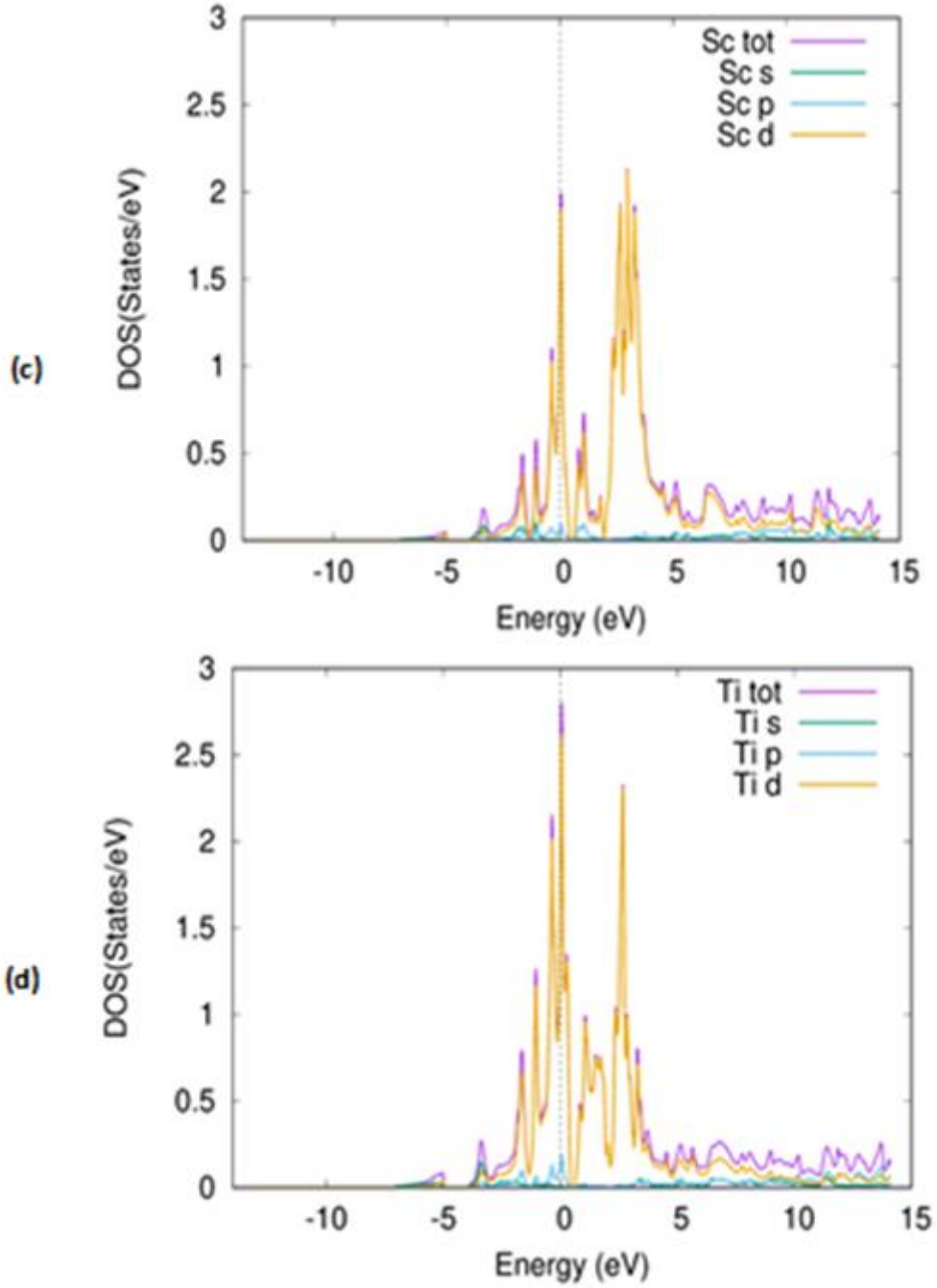


Figure A.4.c

(e) Spin-up partial density of states (PDOS) for Al atom of inverse Sc_2TiAl compound.

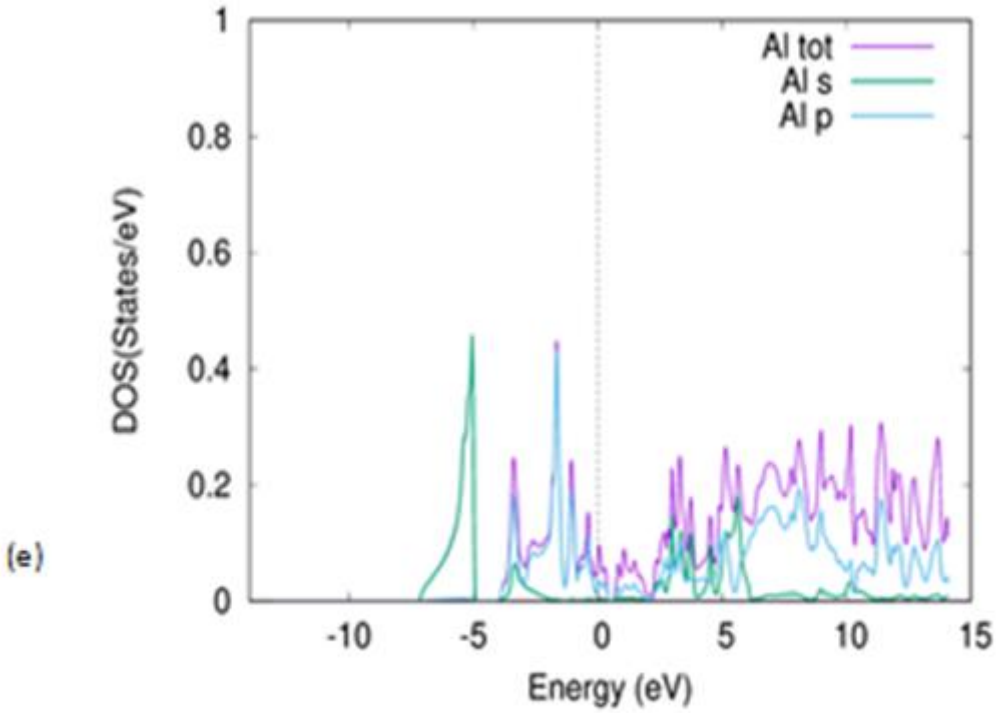


Figure A.5.a

(a) Spin-down total density of states (DOS) for inverse Sc_2TiAl and partial density of states(PDOS) of spin-down for (b) Sc atom number 1 of inverse Sc_2TiAl.

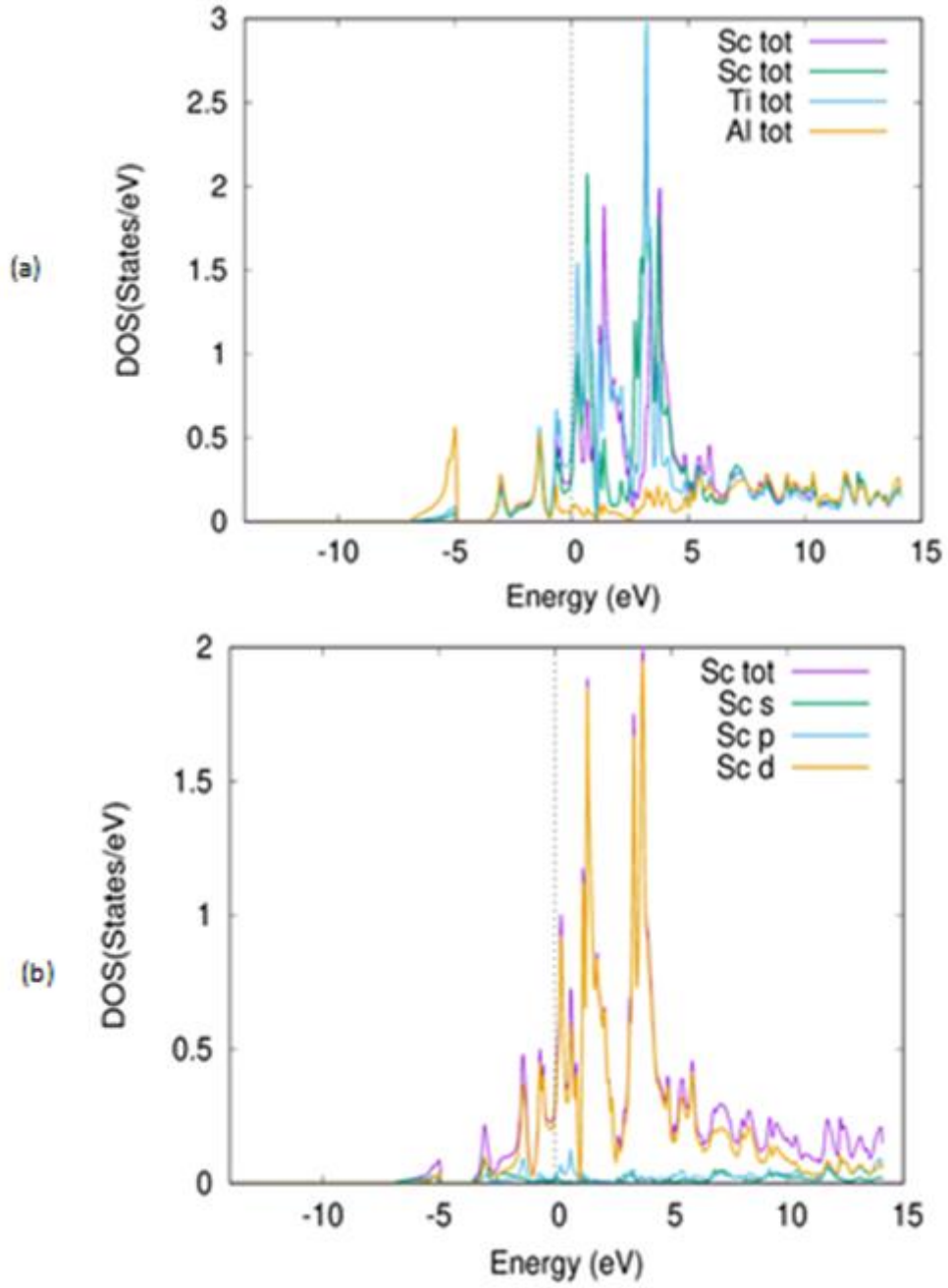


Figure A.5.b

Spin-down partial density of states (PDOS) for (c) Sc atom number 2 (d) Ti atom of inverse Sc_2TiAl.

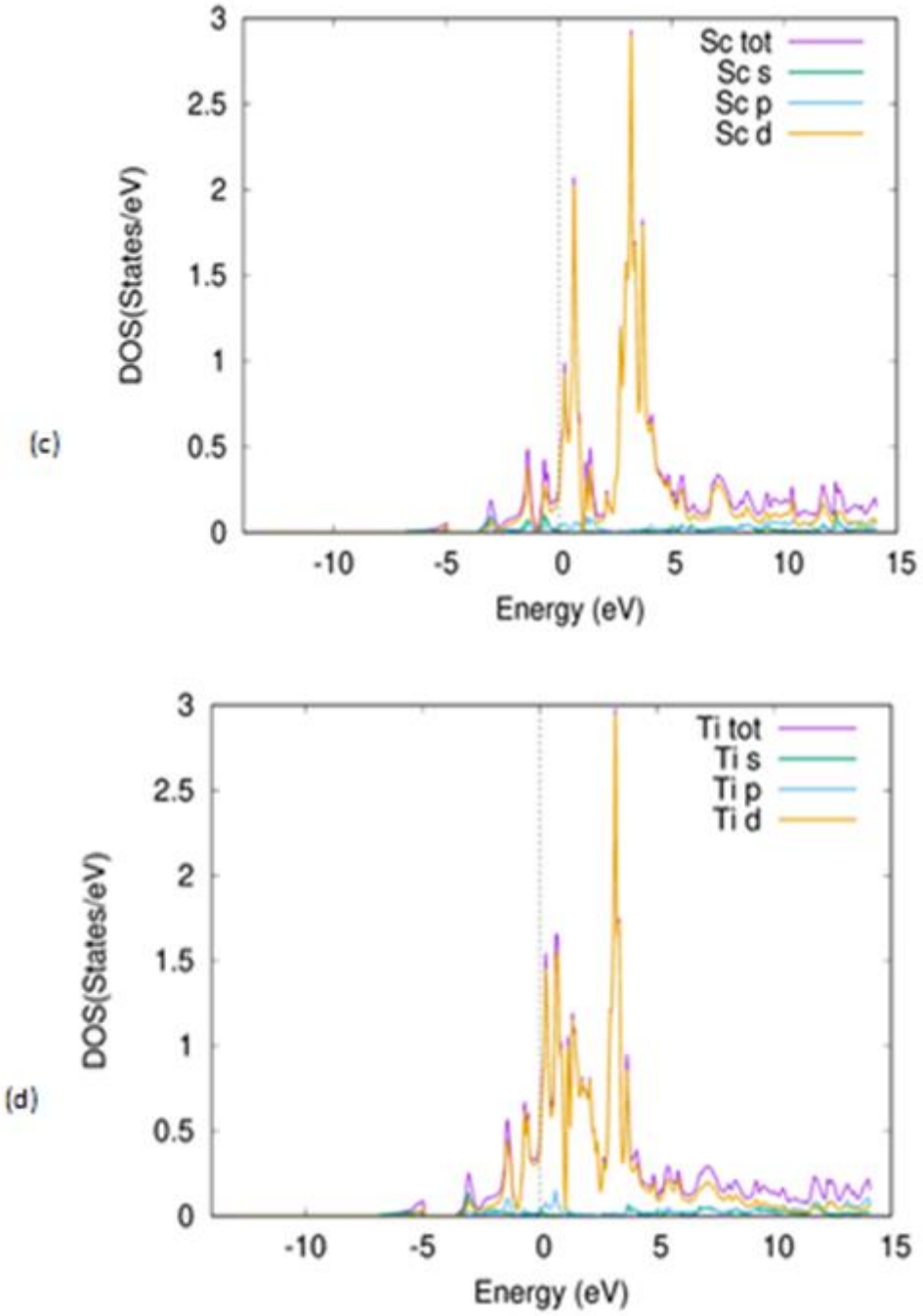


Figure A.5.c

(e) Spin-down partial density of states (PDOS) for Al atom of inverse Sc_2TiAl.

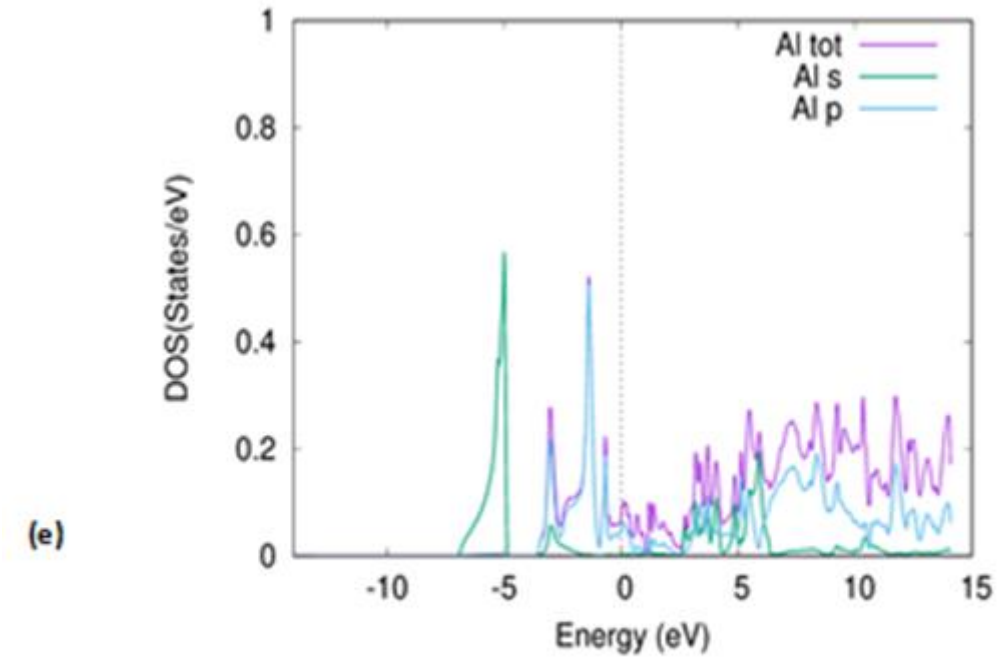
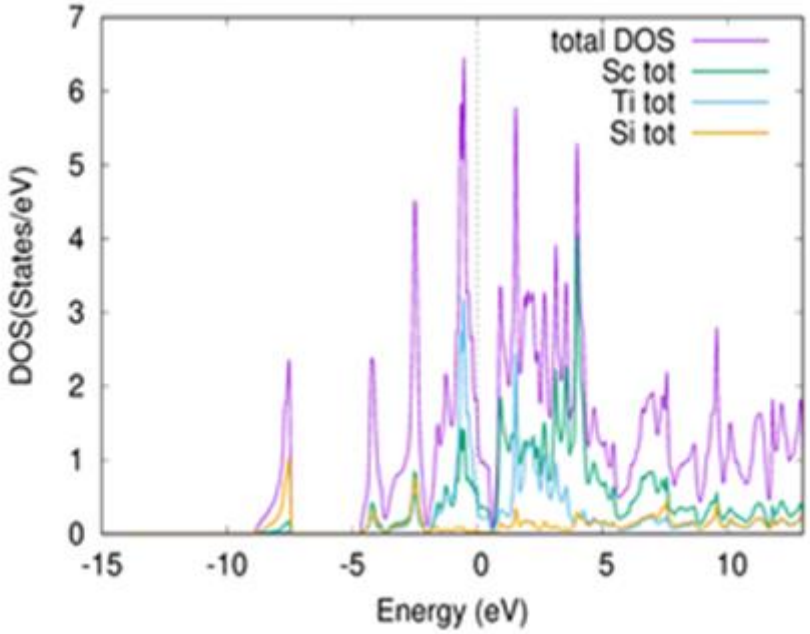


Figure A.6.a

(a) Spin-up total density of states(DOS) for normal Sc_2TiSi and partial density of states(PDOS) of spin-up for (b) Sc atom of normal Sc_2TiSi.

(a)



(b)

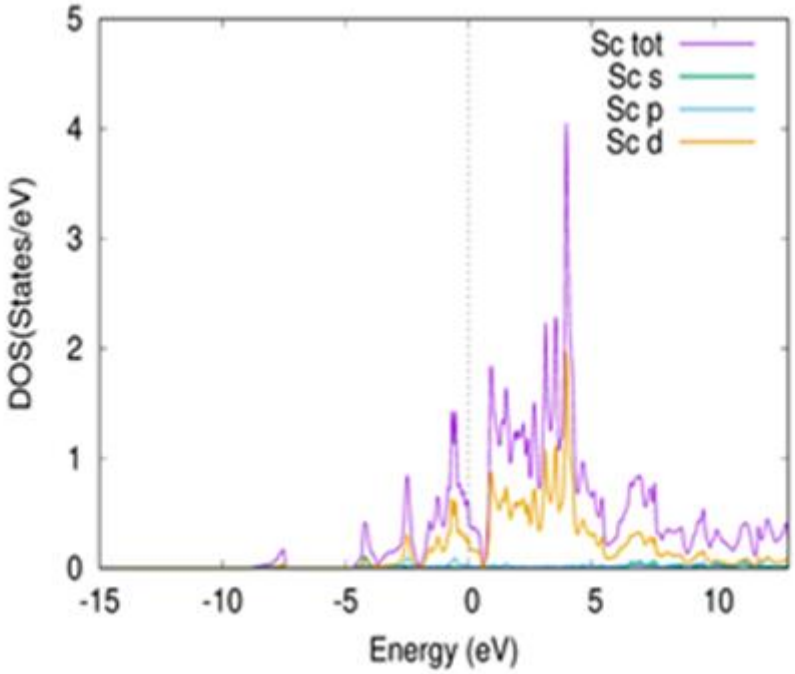


Figure A.6.b

Spin-up partial density of states(PDOS) for (c) Ti atom (d) Si atom of normal Sc_2TiSi.

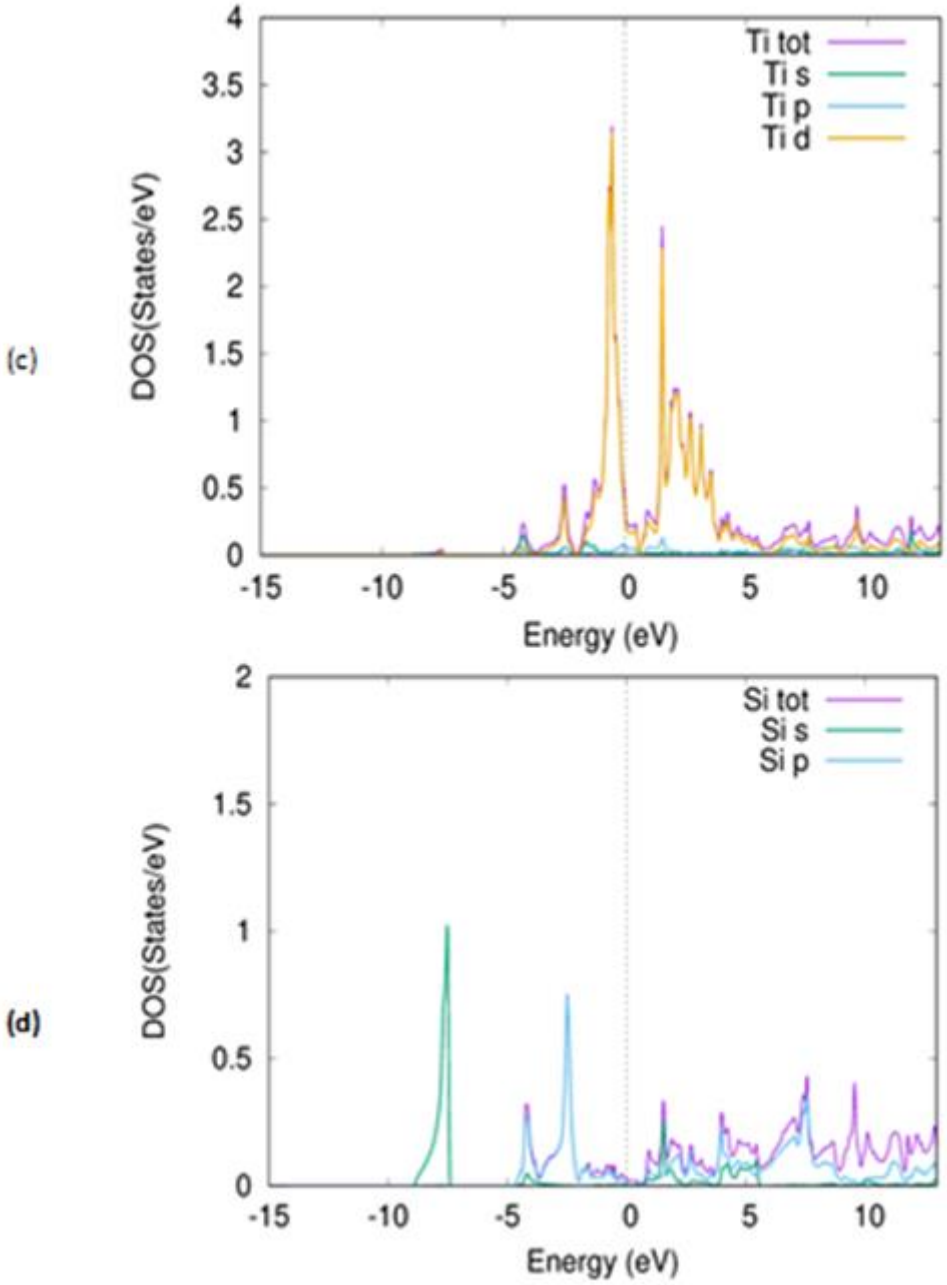


Figure A.7.a

(a) Spin-down total density of states (DOS) for normal Sc_2TiSi and partial density of states(PDOS) of spin-down for (b)Sc atom of normal Sc_2TiSi.

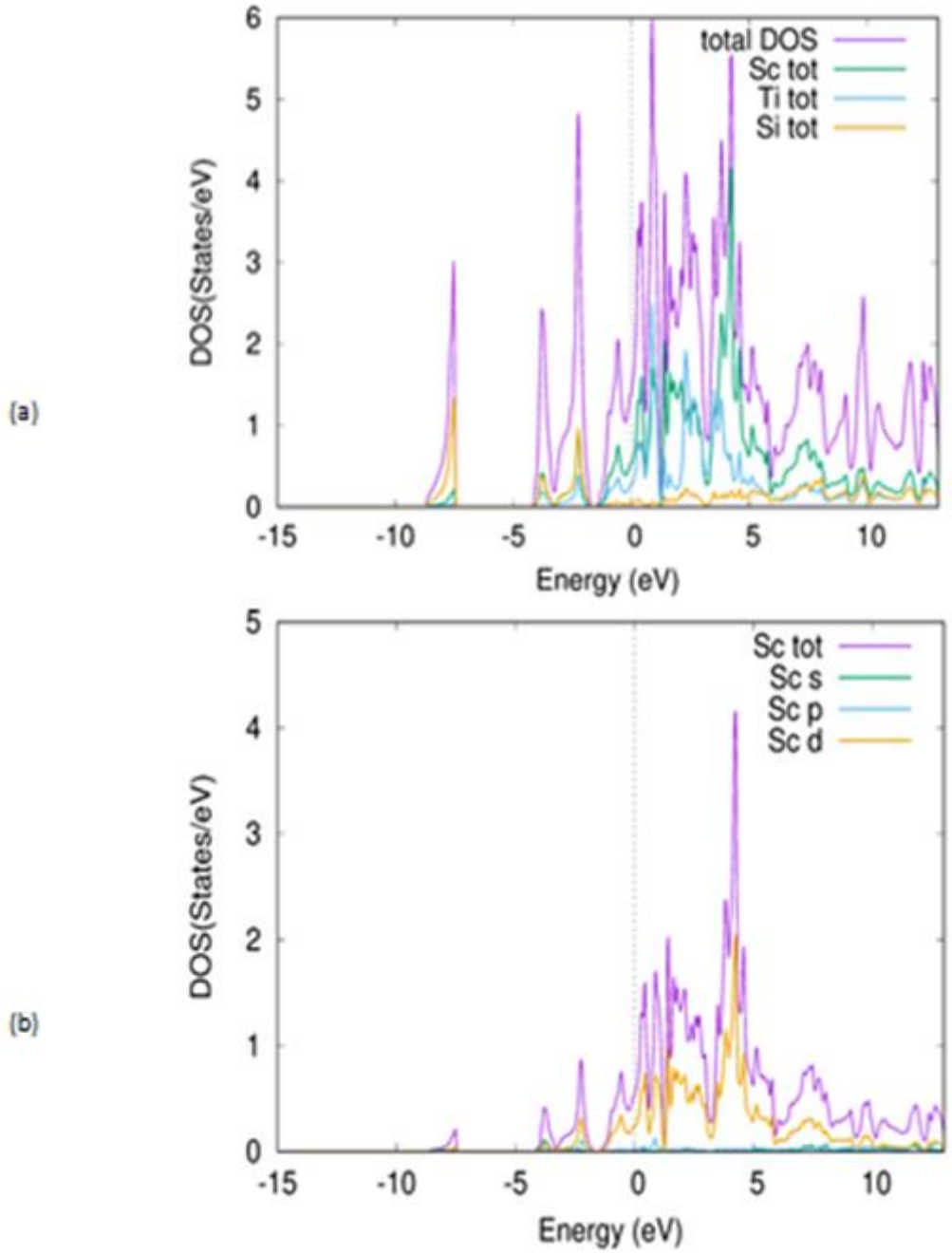


Figure A.7.b

Spin-down partial density of states (PDOS) for (c)Ti atom(d)Si atom of normal Sc_2TiSi.

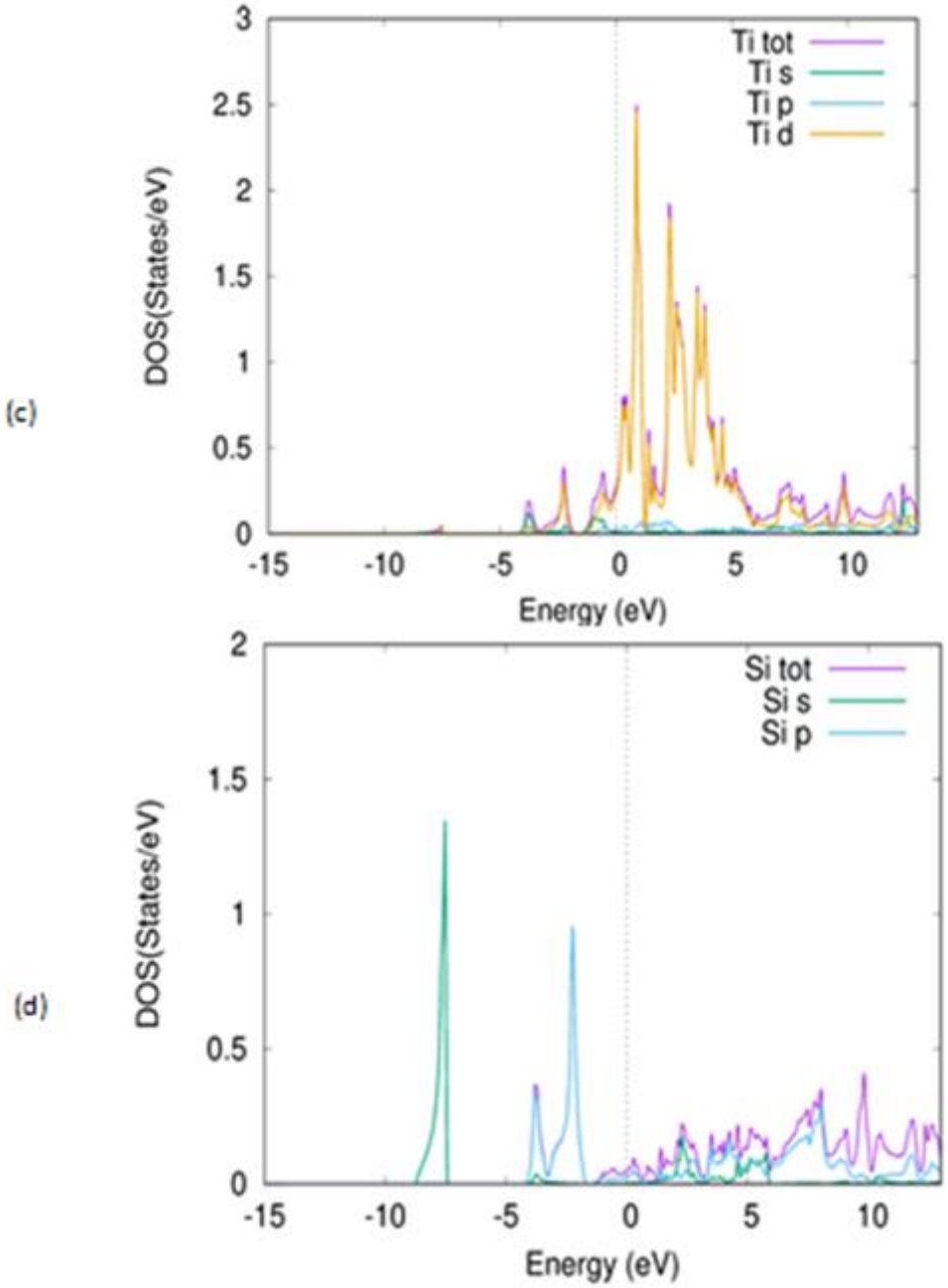


Figure A.8.a

(a) Spin-up total density of states (DOS) for inverse Sc_2TiSi and partial density of states of spin up for (b) Sc atom number 1 of inverse Sc_2TiSi.

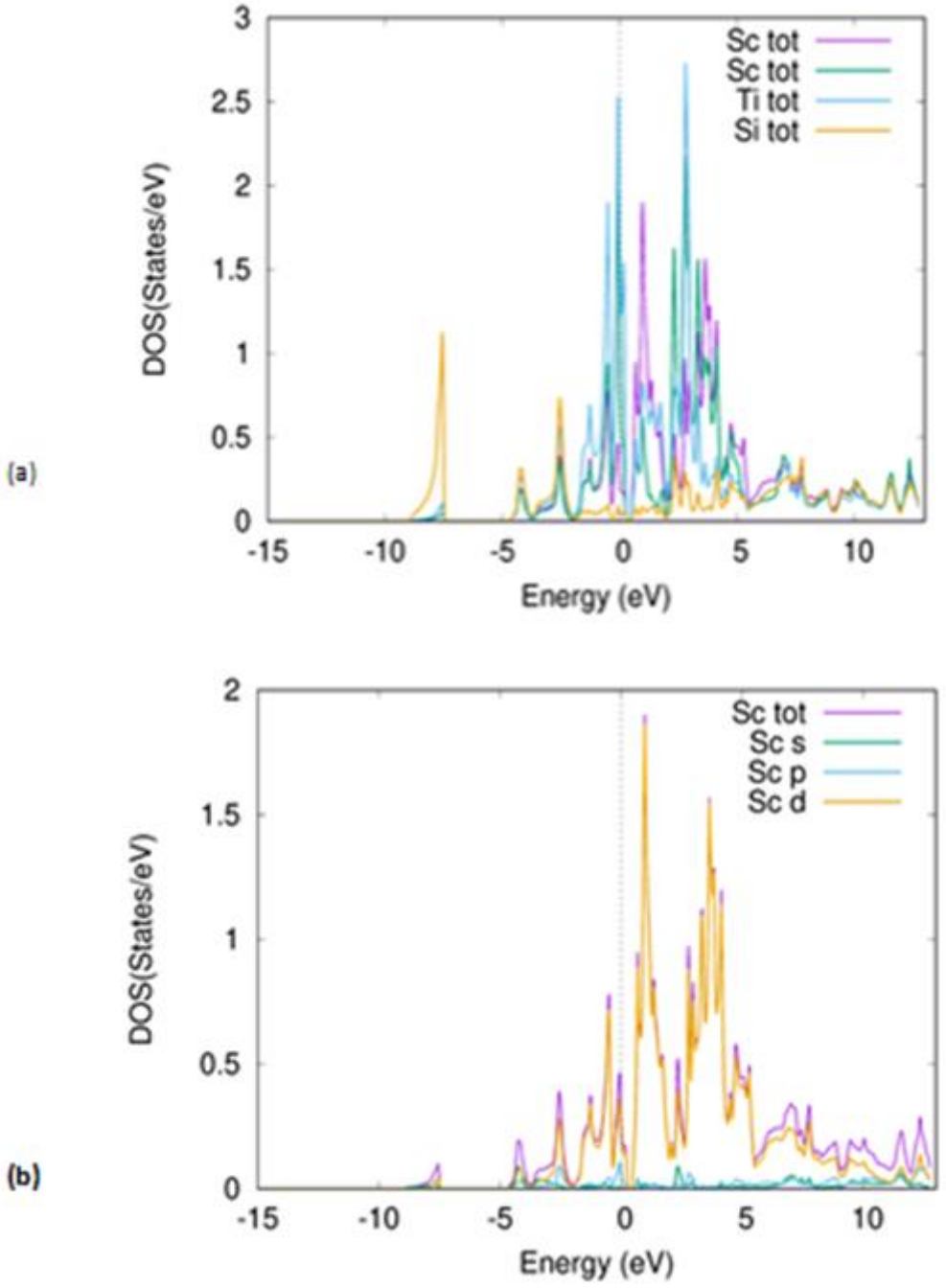
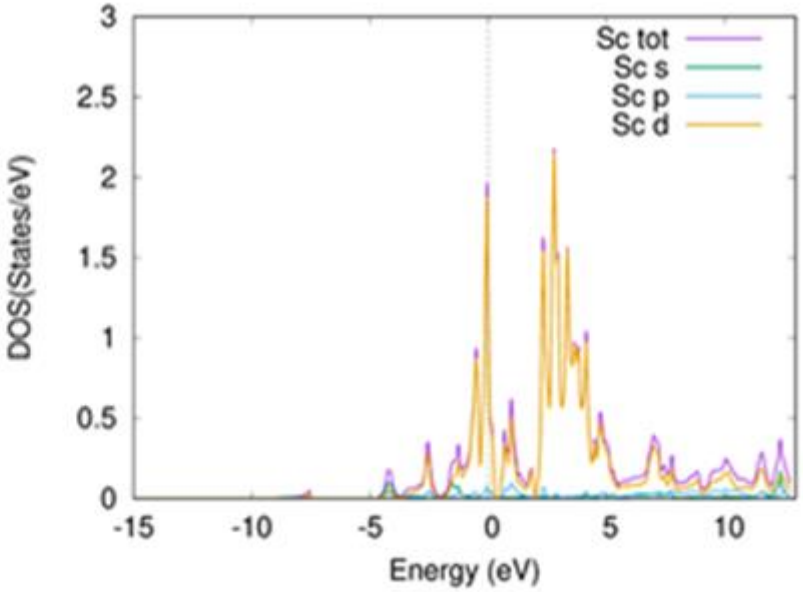


Figure A.8.b

Spin-up partial density of states for (c) Sc atom number 2(d) Ti atom of inverse Sc_2TiSi.

(c)



(d)

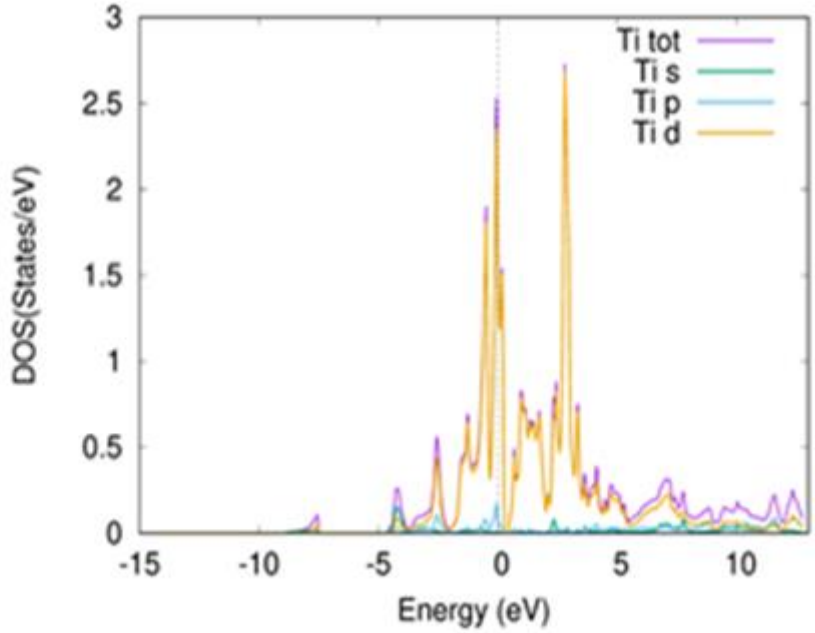


Figure A.8.c

(e) Spin-up partial density of states for Si atom of inverse Sc_2TiSi.

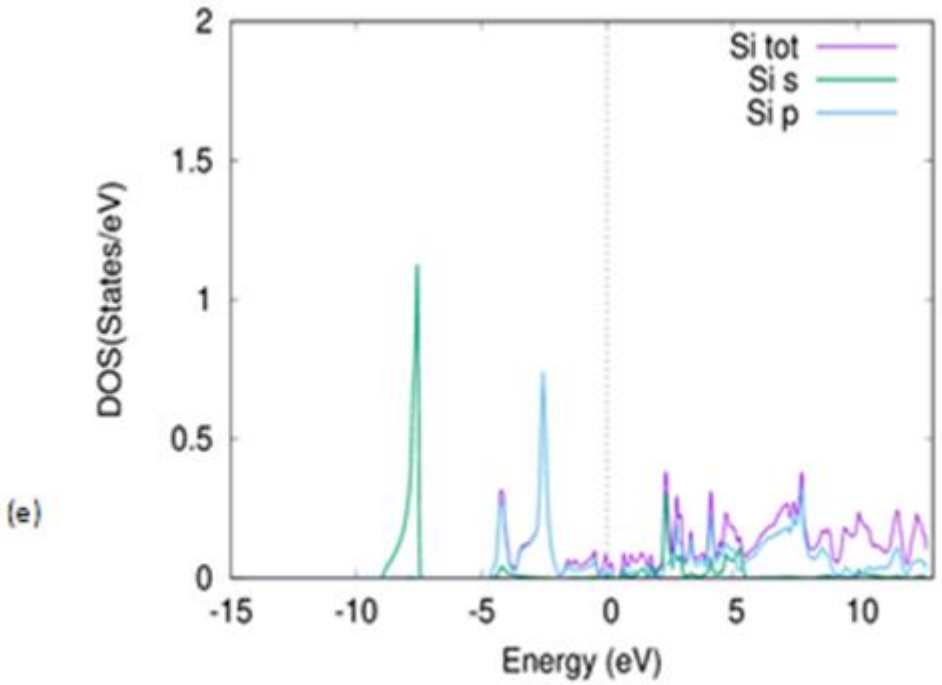


Figure A.9.a

a) Spin-down total density of states(DOS) for inverse Sc_2TiSi and partial density of states(PDOS) of spin down for (b) Sc atom number 1 of inverse Sc_2TiSi.

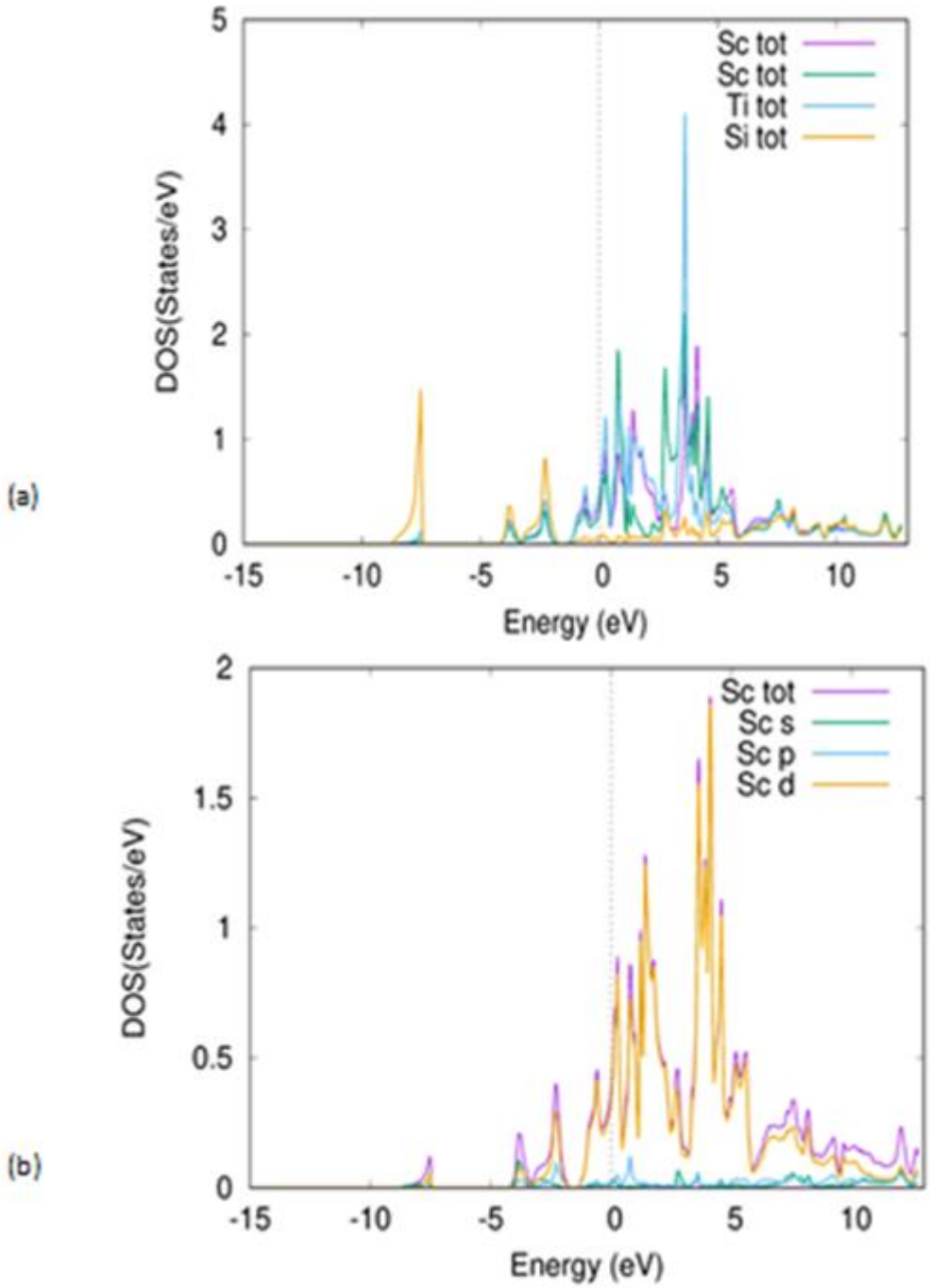


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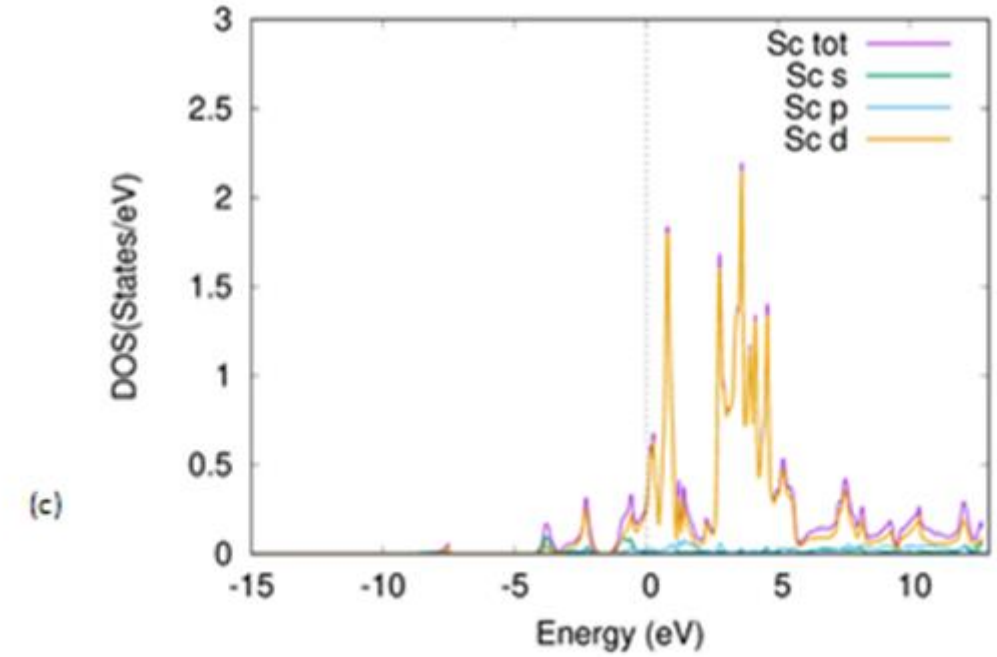
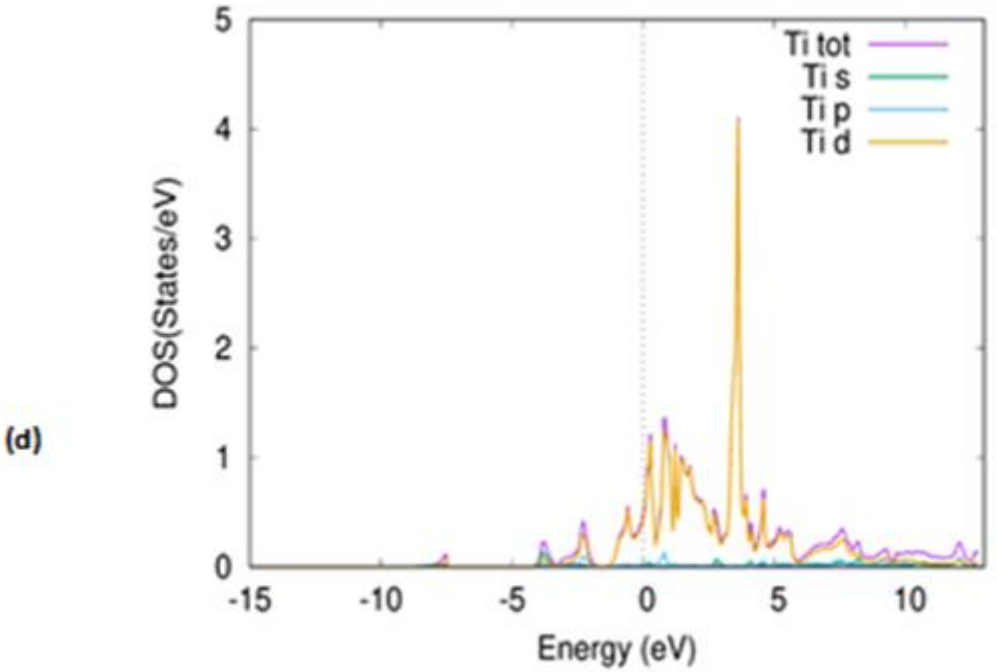
Figure A.9.b

Spin-down partial density of states(PDOS) for (c) Sc atom number 2 (d) Ti atom of inverse Sc_2TiSi.



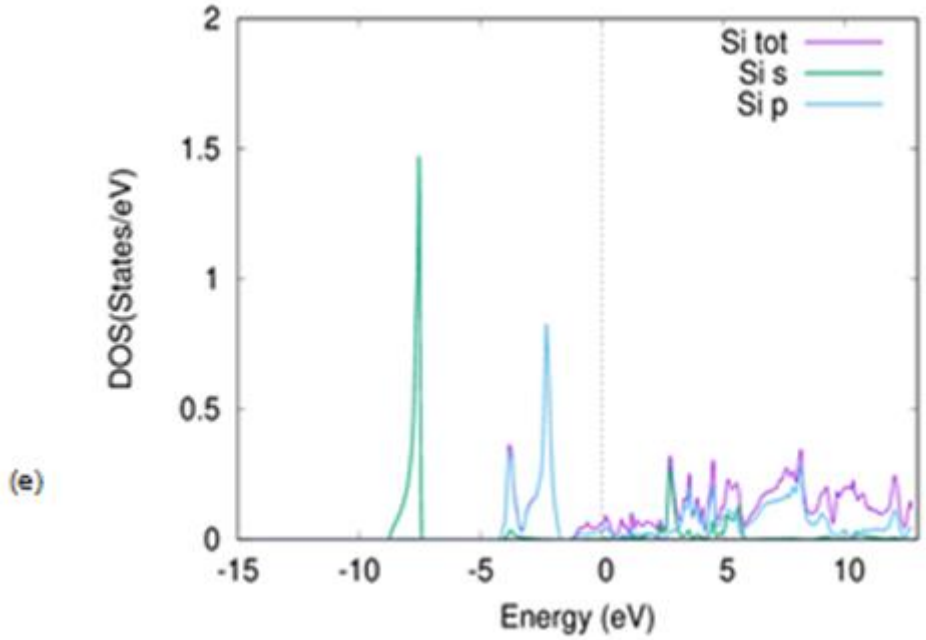
(c)



(d)

Figure A.9.c

(e) Spin-down partial density of states (PDOS) for Si atom of inverse Sc_2TiSi.



جـامعـــة النجاح الوطنية

كليـــة الدراســـات العليـــا

الخصائص التركيبية والالكترونية والمغناطيسية والمرونية لمركبات هزلر الطبيعية والمعكوسة Sc_2TiSi, Sc_2TiAl: باستخدام طريقة الجهد التام

إعداد

خديجة محمود عليان المصري

اشراف

أ. د. محمد أبو جعفر

د. محمود الفاروط

قدمت هذه الرسالة استكمالا لمتطلبات الحصول علي درجه الماجستير في الفيزياء، من كلية الدراسات العليا، في جامعة النجاح الوطنية، نابلس– فلسطين.

2022

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الملخص

تم فحص الخصائص التركيبية والالكترونية والمغناطيسية والمرونية لمركبات هزلر الطبيعية والمعكوسة (**Sc_2TiSi, Sc_2TiAl**) عن طريق استخدام الجهد النظرية الكثافة الوظيفية (**DFT**) والجهد التام المزيد ذو الموجات المستوية الخطية (**FP-LAPW**) والتقريب التدريجي المعمم (**GGA**) ضمن إطار برنامج **.WIEN2k**

تم استخدام التقريب التدريجي المعمم (**GGA**) لحساب ثابت الشبكة (**a**) معامل الصلابة (**B**) ومشتقة معامل الصلابة بالنسبة للضغط (**B´**) وأيضا تم استخدام نظام بيكي جونسون لتحسين فجوة الطاقة (**mBJ-GGA**) وقد وجد أن مركبات هزلر الطبيعية والمعكوسة (**Sc_2TiSi, Sc_2TiAl**) لها خواص معدنية. وقد تم أيضا حساب الخواص المرونية مثل نسبة بوزون $\boldsymbol{\nu}$ ومعامل القص **S** ومعامل يونج **Y** ونسبة **B/S**. وقد تبين أن النتائج التي وجدناها قريبة من النتائج العملية والنظرية الأخرى.