



Theoretical Investigation of Structural, Electronic, Magnetic, and Mechanical Properties of Quaternary Heusler Alloys CoVTiX ($X = \text{As, Si}$)

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Abstract

The structural, electronic, magnetic, and mechanical properties of CoVTiAs and CoVTiSi quaternary Heusler alloys are studied using the full-potential linearized augmented plane-wave (FP-LAPW) method in the framework of the density functional theory (DFT). The generalized gradient approximation (GGA) is chosen for the exchange-correlation energy, whereas the modified Becke-Johnson (mBJ) formalism is applied for the electronic properties. Both CoVTiAs and CoVTiSi are stable in the type 2 (FM) structure. The mechanical properties of CoVTiX ($X = \text{As, Si}$) are predicted from the calculated elastic constants. Results identify that these compounds are mechanically stable. Our results with the mBJ approximation predict that CoVTiAs and CoVTiSi alloys are half-metallic ferromagnets with band gaps of 0.450 and 0.424 eV, respectively.

Keywords Quaternary Heusler compound · AFM · Elastic constants · Half metallic · Magnetic properties

1 Introduction

In recent years, Heusler alloys have attracted the attention of many researchers due to their uses in spintronic applications such as tunneling magnetoresistance (TMR) and giant magnetoresistance (GMR) [1]. There are two classes of Heusler alloys that include full- (FHA) and half-Heusler alloys (HHA). The FHA have L_{21} structure with X_2YZ chemical composition forming four interpenetrating face-centered cubic (fcc) lattices, where X and Y are transition metals and Z is a main group element. However, the HHA has the $C1_b$ structure with the XYZ chemical composition forming three interpenetrating fcc lat-

tices and one vacant lattice. Most of these alloys exhibit half-metallic electronic property with a semiconducting structure in only one spin direction, whereas the other spin channel is strongly metallic. Another category of Heusler compounds known as quaternary Heusler alloys with the chemical formula $XX'YZ$ with LiMgPdSb-type crystal structure and $F\bar{4}3m$ space group [2, 3] have attracted a great deal of interest. Galanakis [4] predicted that $\text{Co}_2[\text{Cr}_{1-x}\text{Mn}_x]\text{Al}$, $\text{Co}_2\text{Mn}[\text{Al}_{1-x}\text{Sn}_x]$, and $[\text{Fe}_{1-x}\text{Co}_x]_2\text{MnAl}$ are typically half-metallic ferromagnets with total spin magnetic moments that vary linearly between 2 and 4 μ_B for Fe_2MnAl and Co_2MnAl compounds, respectively. The substitutional series of the quaternary Heusler compound $\text{Co}_2\text{Mn}_{1-x}\text{Fe}_x\text{Si}$ [5] was synthesized and investigated both experimentally and theoretically. For example, Alijani et al. have performed theoretical and experimental investigations of NiFeMnGa, NiCoMnGa, and CuCoMnGa [6]. They found that NiFeMnGa and NiCoMnGa exhibit excellent half-metallic ferromagnetism, while CuCoMnGa was found to be a metallic ferromagnet. In addition, Goa et al. studied the electronic, structural, and magnetic properties of CoFeCrZ ($Z = \text{Al, Si, Ga, and Ge}$) [7] using full-potential linearized augmented plane-wave (FP-LAPW) method. They found that both CoFeCrGa and CoFeCrGe quaternary Heusler alloys are nearly half

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metals, while CoFeCrAl and CoFeCrSi are excellent half-metallic (HM) ferromagnets with gaps of 0.16 and 0.28 eV, respectively. Nehra et al. [8] also showed that CoFeCrAl exhibits a HM ferromagnetic structure with a band gap of 0.41 eV around the Fermi level in the minority spin channel. Experimentally, the quaternary equiatomic Heusler alloy (CoFeMnGe) was found to have the cubic Heusler structure of LiMgPdSn type with a considerable amount of DO₃ disorder at Curie temperature of 750 K [9]. Using FP-LAPW method, Berri et al. [10] predicted a ferromagnetic half-metallic behavior of ZrFeTiAl, ZrFeTiSi, ZrFeTiGe, and ZrNiTiAl alloys with total magnetic moments of 1, 2, 2, and 3 $\mu_B/f.u.$, respectively, and large gap values between 0.56 and 0.92 eV. Furthermore, Wei et al. predicted half-metallic ferromagnetic structure of NiCoCrAl, NiCoCrGa, and NiFeCrGa alloys [11]. Moreover, FeMnScZ ($Z = Al, Ga, \text{ and } In$) alloys were predicted to be half-metallic ferromagnets with total magnetic moments of 3 $\mu_B/f.u.$ [12]. Another series of CoFeMnZ ($Z = Si, As, \text{ and } Sb$) quaternary Heusler alloys were predicted to have ferromagnetic half-metallic behavior with high magnetic moment and Curie temperature [13]. Recently, Mohamedi et al. [14] reported a theoretical study of the elastic, electronic, and thermal properties of CoMnCrZ ($Z = Al, As, Si, \text{ and } Ge$) compound using FP-LAPW method. The authors pointed out that the type 1 structure with the FM configuration is energetically more favorable than types 2 and 3 structures. It has been found that the CoMnCrGe, CoMnCrAl, CoMnCrSi, and CoMnCrAs quaternary Heusler compounds are half-metallic ferromagnets with half-metallic gaps of 0.03, 0.19, 0.34, and 0.50 eV, respectively.

Motivated by the promising properties of the quaternary Heusler compounds specially those containing Co, V, and Ti elements, we performed computational investigation by first-principle calculations to study the structural, mechanical, electronic, and magnetic properties of CoVTiX ($X = As, Si$) alloys. To our knowledge, there is no comprehensive theoretical or experimental study on these compounds. The rest of the paper is organized as follows: Section 2 outlines the computational methods used in our study. The results discussed in this paper are obtained using density functional theory (DFT) and are presented in Section 3, and Section 4 summarizes our main results.

2 Computational Details

First-principle calculations were performed using the FP-LAPW method as implemented in the Wien2K [15] code to study the structural, mechanical, and magnetic properties of CoVTiX ($X = As, Si$) compounds. The electron-electron interaction was treated within the generalized gradient

approximation (GGA) by Perdew, Burke, and Ernzerhof (PBE) exchange correlation potential [16] in the case of the structural and mechanical properties. However, the modified Becke-Johnson potential (mBJ) [17] was adopted to obtain the electronic structure. The expansion of the valence wave functions inside the non-overlapping muffin-tin spheres were confined to $l_{\max} = 10$, while the charge density was Fourier expanded up to $G_{\max} = 14$. In order to achieve energy convergence, the wave functions in the interstitial region were expanded in plane waves with a cutoff of $K_{\max} = 8/R_{MT}$ where R_{MT} denotes the smallest atomic sphere radius and K_{\max} gives the magnitude of the largest K vector in the plane-wave expansion. The R_{MT} are taken to be in the range 1.8–2.15 atomic units (a.u.) for Co, V, Ti, As, and Si atoms for all types. Brillouin zone (BZ) integrations within the self-consistency cycles were performed via the tetrahedron method [18, 19] using 47k points for CoVTiX ($X = As, Si$) in their irreducible BZ (IBZ). The energy convergence was obtained when the difference is less than 0.1 mRy.

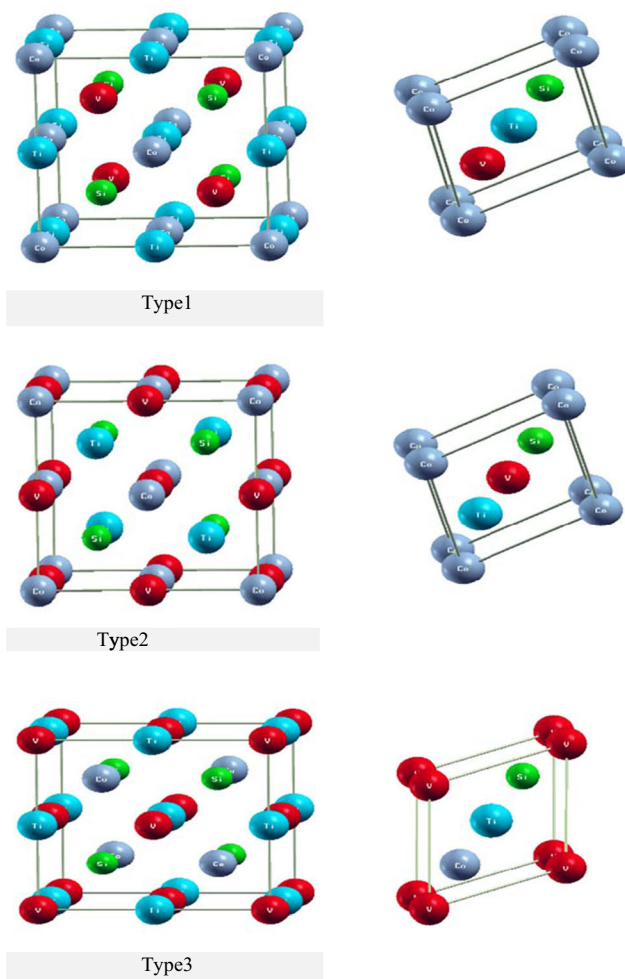


Fig. 1 Crystal structure of CoVTiX ($X = As, Si$) at different types

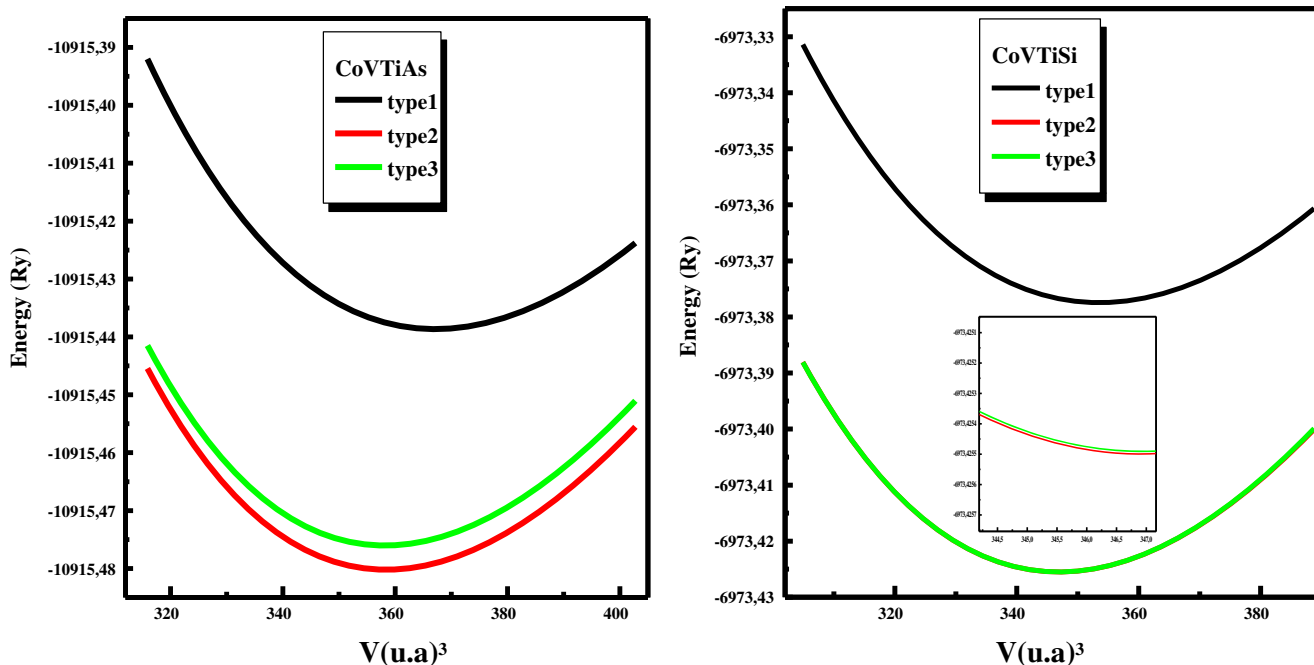


Fig. 2 Variation of total energies as a function of volume of unit cell using GGA for CoVTiX ($X = \text{As, Si}$) at different types

3 Results and Discussions

In this section, we present the structural, mechanical, and electronic properties of CoVTiX ($X = \text{As, Si}$) alloys.

3.1 Structural Properties

The quaternary Heusler alloys have $XX'YZ$ chemical structure with 1:1:1:1 stoichiometry, where $X, X',$ and Y

are transition metals and Z is a main group element. These compounds crystallize in the LiMgPdSn crystal structure with a space group $F\bar{4}3m$. In general, in LiMgPdSn-type quaternary Heusler alloys can have three different types as shown in Fig. 1. These types are as follows: (i) type 1: $X (0, 0, 0), X' (1/4, 1/4, 1/4), Y (1/2, 1/2, 1/2),$ and $Z (3/4, 3/4, 3/4),$ (ii) type 2: $X (0, 0, 0), X' (1/2, 1/2, 1/2), Y (1/4, 1/4, 1/4),$ and $Z (3/4, 3/4, 3/4),$ and (iii) type 3: $X (0, 0, 0), X' (1/4, 1/4, 1/4), Y (1/2, 1/2, 1/2),$ and Z

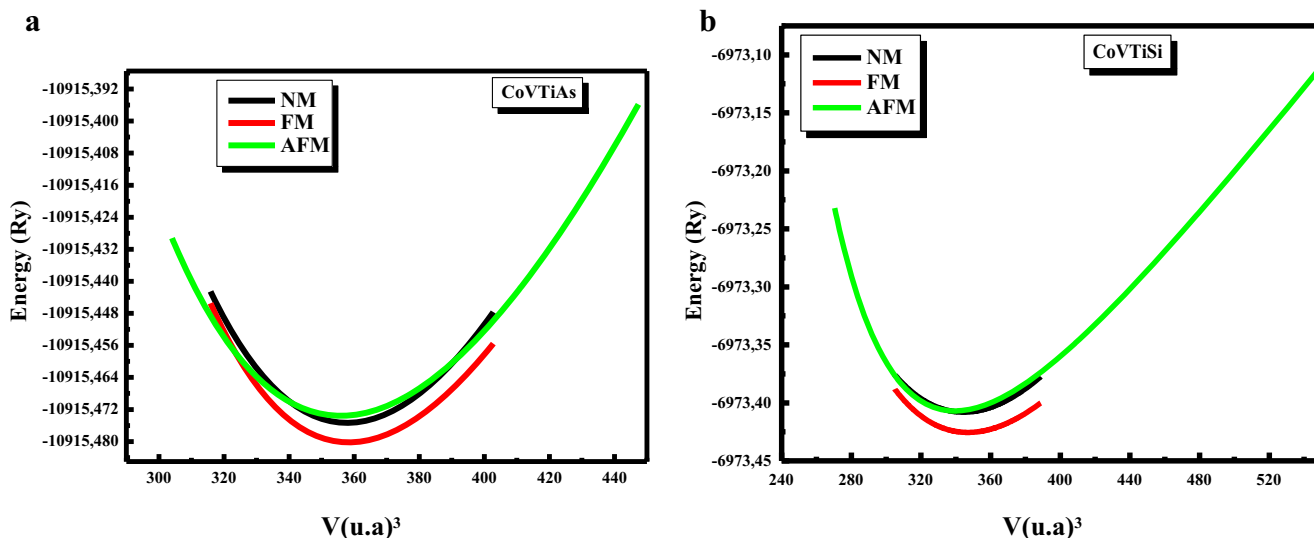


Fig. 3 Variation of total energies as a function of volume of unit cell using GGA for CoVTiX ($X = \text{As, Si}$) in the three magnetic states FM, AFM, and NM

(3/4, 3/4, 3/4). In order to obtain the ground state structure of each alloy and find the favorable magnetic state, we performed total energy calculations as a function of volume for the three different possible site occupations for non-magnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM) states. The structures of all quaternary Heusler alloys were optimized by calculating the total energy as a function of volume, which was followed by fitting the data with Murnaghan equation of state [20]. The site occupation preference is obtained by comparing the total energy versus volume of the three types of CoVTiX ($X = \text{As, Si}$) compounds as shown in Fig. 2. From this figure, one can see that CoVTiAs and CoVTiSi prefer to crystallize in the type

Table 1 Calculated lattice constants (a (Å), bulk modulus (B (GPa), and pressure derivative (B') at equilibrium volume using GGA compared with the available theoretical data of CoVTiX ($X = \text{As, Si}$) compounds

Physical parameter	FM	Other works
CoVTiAs		
Type 1		5.97 [21]
a (Å)	6.0147	
B (GPa)	148.0966	
B'	4.1970	
E_{\min} (Ry)	- 10,915.438657	
Type 2		
a (Å)	5.9669	
B (GPa)	162.0954	
B'	4.2653	
E_{\min} (Ry)	- 10,915.480207	
Type 3		
a (Å)	5.9611	
B (GPa)	162.1599	
B'	4.4719	
E_{\min} (Ry)	- 10,915.476781	
CoVTiSi		
Type 1		5.90 [21]
a (Å)	5.9396	
B (GPa)	162.2271	
B'	3.5447	
E_{\min} (Ry)	- 6973.377449	
Type 2		
a (Å)	5.9024	
B (GPa)	176.9564	
B'	3.6978	
E_{\min} (Ry)	- 6973.425508	
Type 3		
a (Å)	5.9024	
B (GPa)	177.5436	
B'	3.6019	
E_{\min} (Ry)	- 6973.425499	

2 structure. Our calculations show that the energy difference of the two types (2 and 3) is only about $\Delta E = 10^{-4}$ Ry. The most stable magnetic structure is found to be the FM structure as compared with the AFM and NM states for CoVTiX ($X = \text{As, Si}$) compounds in all types (1, 2, and 3), see Fig. 3. In Fig. 3a, b, type 2 of both compounds CoVTiAs and CoVTiSi has the lowest energy curve. Therefore, it is clear that the most stable phase at ambient pressure is type 2 structure. Similar compounds such as CoMnCrZ ($Z = \text{Al, As, Si, and Ge}$) alloys were found to prefer type 1 (FM) structure [14]. In Table 1, we report our calculated equilibrium lattice constants, along with bulk modulus, pressure derivatives (B'), and the total energy in their different types compared with previous works [21]. From this table, one can see that the lattice constant decreases, whereas the bulk modulus increases when the Z element decreases.

3.2 Elastic Properties and Mechanical Stability

The knowledge of elastic constants of a solid provides valuable information on their dynamical and mechanical properties. The elastic constants C_{ij} for these quaternary Heusler alloys are calculated to determine their mechanical behavior. It is well known that a cubic crystal has only three independent elastic constants, C_{11} , C_{12} , and C_{44} . There are three conditions that should be satisfied in order to have mechanical stability in a cubic structure [22]: $C_{11} + 2C_{12} > 0$; $C_{11} - C_{12} > 0$; and $C_{44} > 0$. Accordingly, we found that the compounds are elastically stable in the cubic structure except for the case of CoVTiAs in the type 1 structure, see Table 2.

The shear (C_S), Voigt (C_V), and Reuss (C_R) moduli can be expressed as follows [23–25]:

$$C_S = (C_{11} - C_{12})/2 \quad (1)$$

Table 2 Calculated elastic constants (C_{ij} (GPa)), calculated bulk modulus (B), Young's modulus (E (GPa)), Poisson's ratio (ν (GPa)), and Debye temperature (Θ_D (K)) for CoVTiX ($X = \text{As, Si}$) compounds

	CoVTiAs compounds			CoVTiSi compounds		
	Type 1	Type 2	Type 3	Type 1	Type 2	Type 3
C_{11}	100.3	182.5	183.1	126.3	246.9	236.7
C_{12}	157.71	167.3	167.1	115.6	170.06	160.6
C_{44}	17.5	30.2	29.9	82.3	88.1	87.8
B	138.6	172.4	172.4	119.1	195.7	185.9
E	68.31	50.87	51.44	87.82	171.09	169.36
ν	0.417	0.45	0.45	0.377	0.354	0.348
Θ_D	260.7	222.5	223.7	335.8	463.8	468.2
A	- 0.6	3.9	3.7	15.4	2.3	2.3

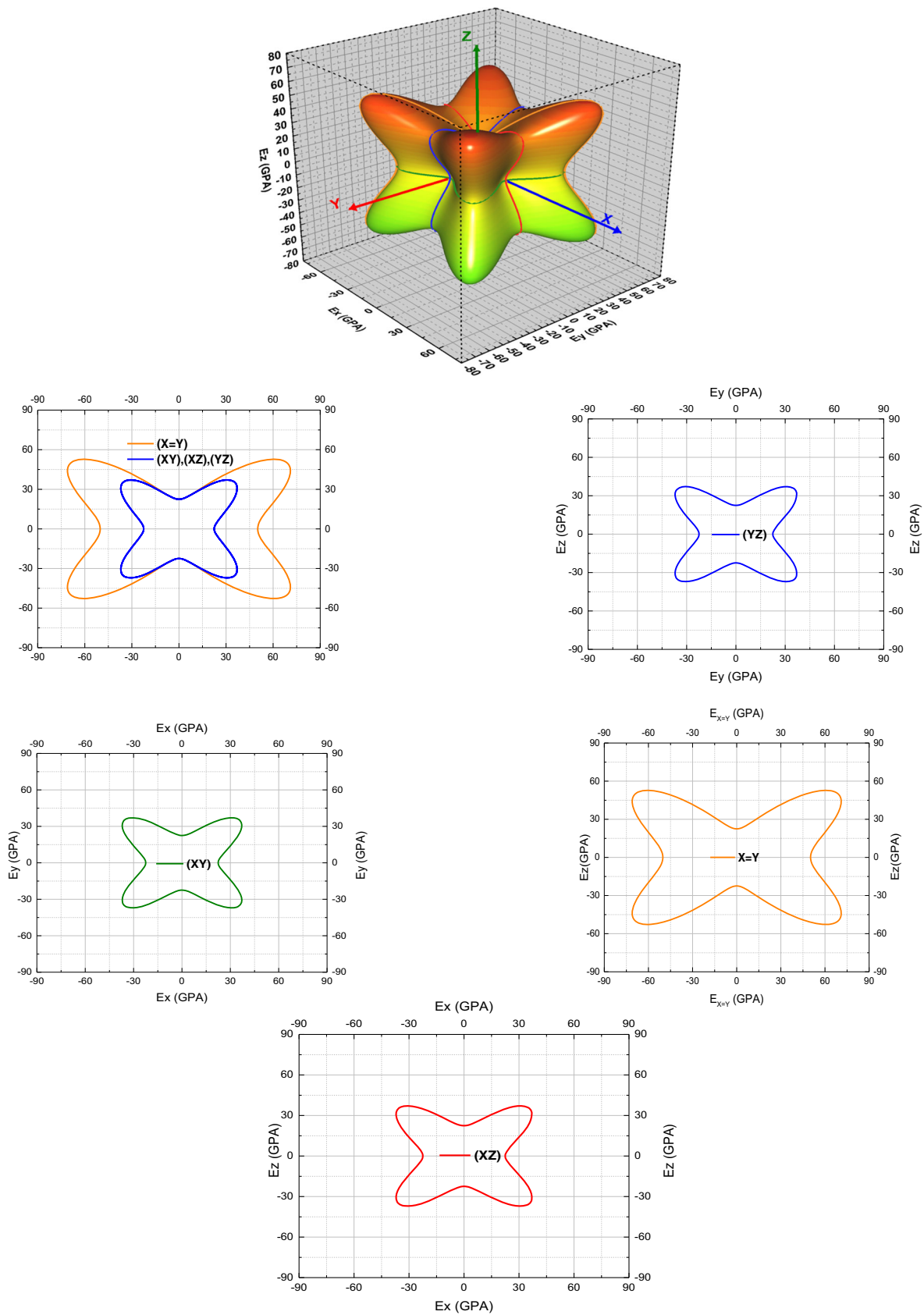


Fig. 4 3D representation of directional dependence of Young’s modulus and cross-section in some reticular planes of 3D representation of CoVTiAs type 2

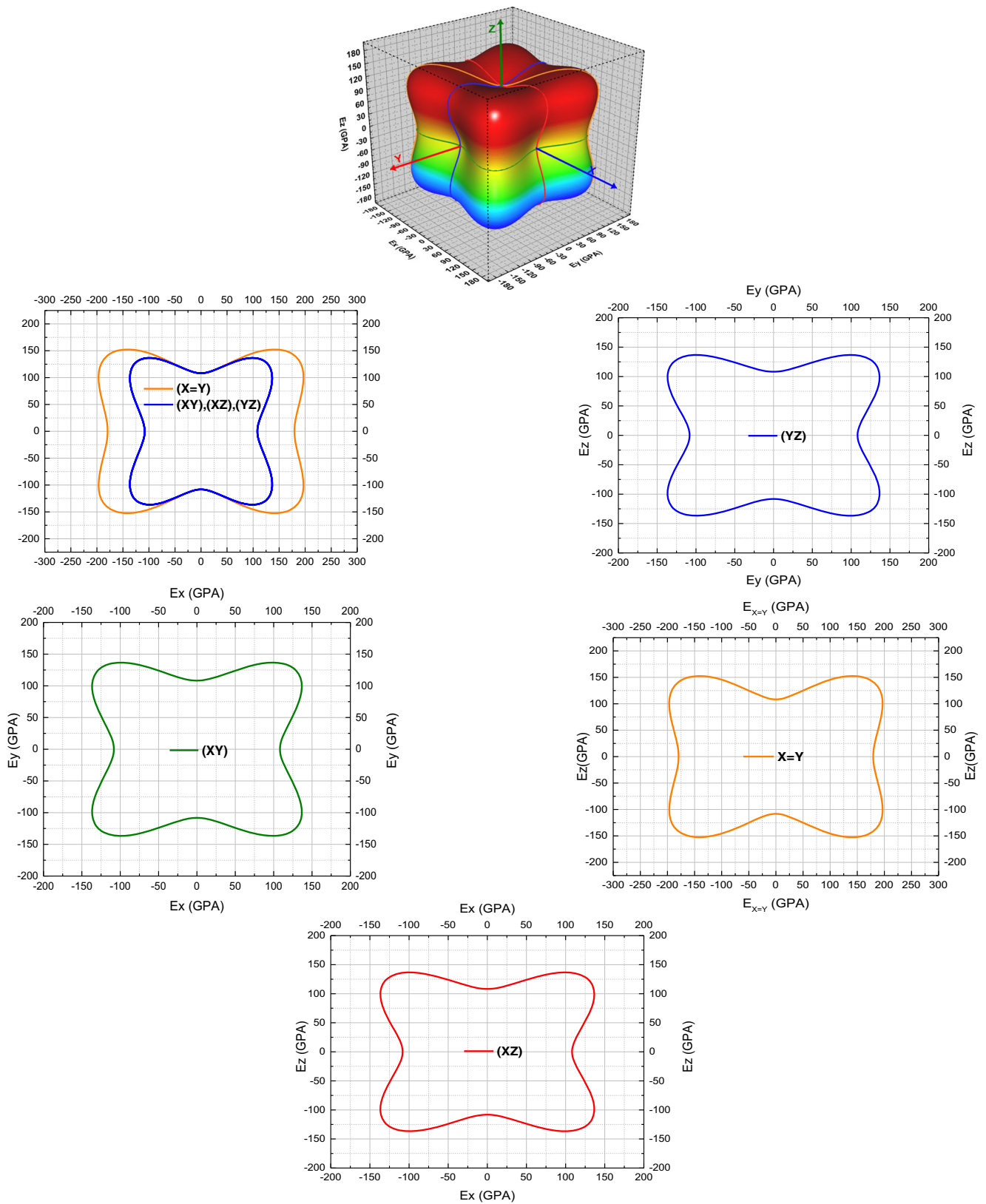


Fig. 5 3D representation of directional dependence of Young’s modulus and cross-section in some reticular planes of 3D representation of CoVTiSi type 2

$$G_V = \frac{1}{5} (C_{11} - C_{12} + 3C_{44}) \tag{2}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{4C_{44} + 3(C_{11} - C_{12})} \tag{3}$$

The Voigt-Reuss-Hill approximation [26, 27] could be approximated by the arithmetic mean of the two well-known limits for mono-crystals according to Voigt [28] and Reuss [29] and is given by the following expression [27, 30]:

$$G_H = \frac{1}{2}(G_V + G_R) \tag{4}$$

For the cubic system, the modulus of rigidity B can be expressed as a linear combination of the two elastic constants C_{11} and C_{12} given by [25]:

$$B = \frac{C_{11} + 2C_{12}}{3} \tag{5}$$

The elastic constants are found to increase when As is replaced by Si in type 2. The elastic constant values of C_{44} for all compounds are found to be far less than the values of C_{11} , which suggests that these quaternary Heusler alloys show weaker resistance to bulk strains. To the best of our knowledge, there are no experimental or theoretical results for the elastic constants of these compounds reported yet; hence, our results serve as a prediction for future

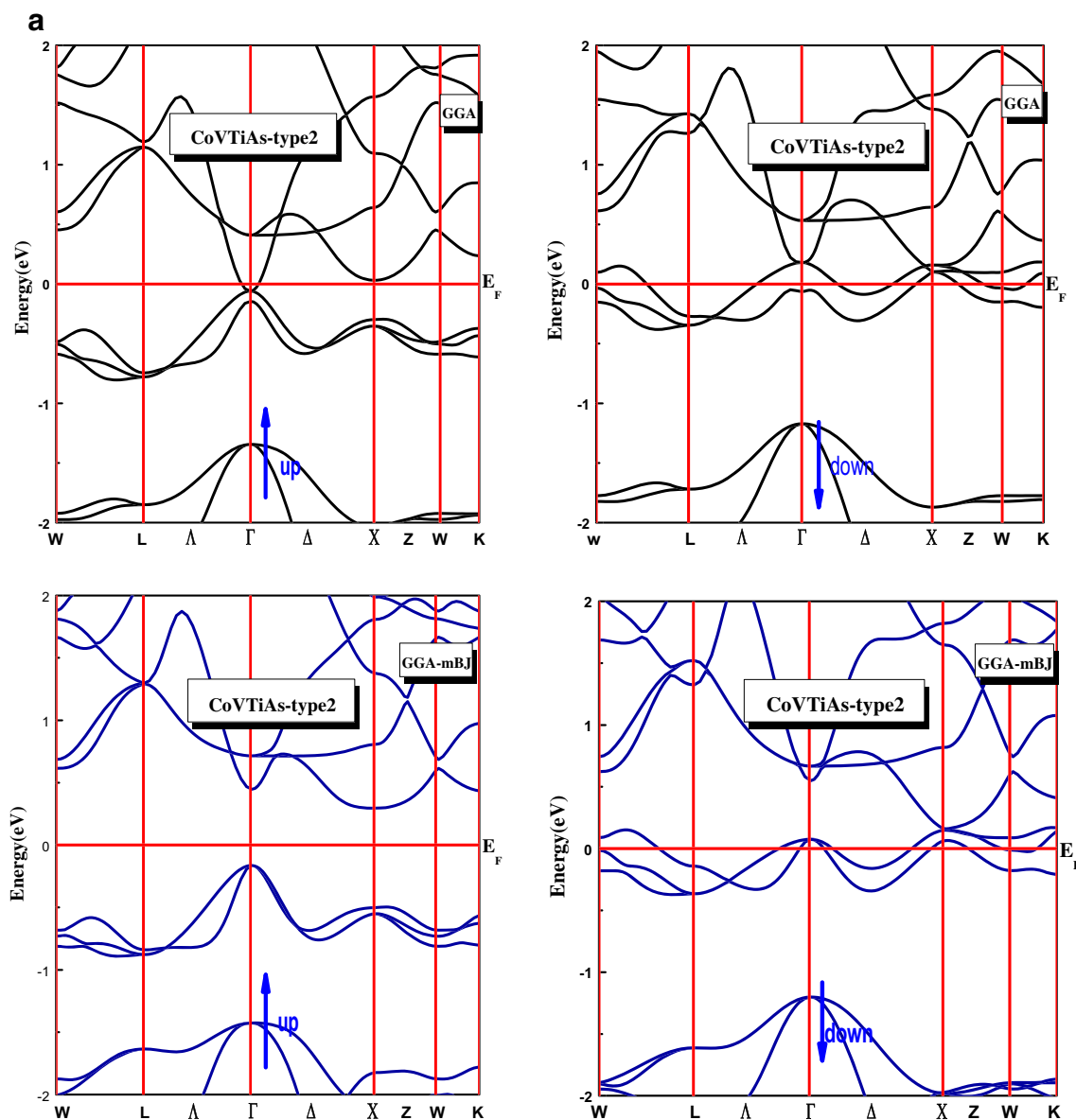


Fig. 6 Band structures for CoVTiX ($X = \text{As, Si}$) in type 2 structure calculated using GGA and GGA-mBJ approximations

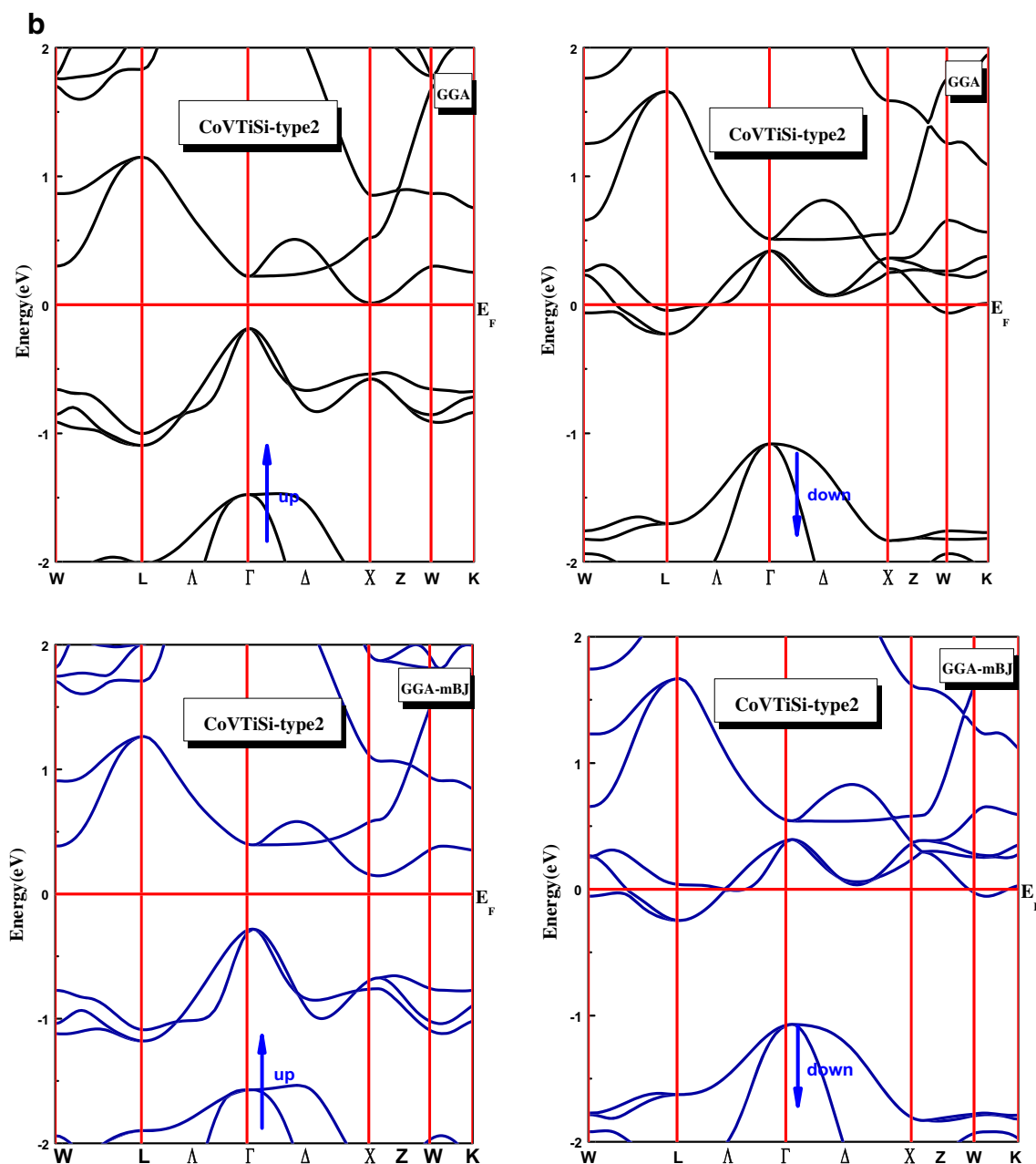


Fig. 6 (continued)

investigations. The calculated values of the bulk modulus (B), Young's modulus (E), and Poisson's ratio (ν) of the title materials using VRH approximations in GGA are listed in Table 2. The higher calculated bulk moduli for CoVTiX ($X = \text{As}, \text{Si}$) in type 2 confirm the stability of this structure. It is noted that the higher bulk and Young's moduli suggest a strong incompressibility for these compounds. The Young's modulus is the property of a material, which is used to characterize stiffness. The higher the value of E , the stiffer is the material. Young's modulus is found to increase when replacing As by Si, which means that CoVTiAs is stiffer than CoVTiSi. In addition, Poisson's

ratio for CoVTiX ($X = \text{As}, \text{Si}$) is found to fall in this limit, which indicates that the interatomic forces in this compounds are central forces. This is ascribed to the fact that Poisson's ratio provides more information about the characteristics of the bonding forces than any of the other elastic constants [31]. It has been proven that $\sigma = 0.25$ is the lower limit for central force and 0.5 is the upper limit [31]. Therefore, the high σ values of CoVTiAs ($\sigma = 0.4$) and CoVTiSi ($\sigma = 0.3$) indicate that the interatomic forces in the title compound are central. Moreover, the Debye temperature of CoVTiAs is found to be lower than that of CoVTiSi.

Table 3 Calculated band gap (E_g (eV)) of CoVTiX ($X = \text{As, Si}$) compounds using GGA and GGA-mBJ

Approximation		CoVTiAs		CoVTiSi	
		Type 2	Type 3	Type 2	Type 3
Gap	GGA	–	–	0.197	0.196
E_g (eV)	GGA-mBJ	0.45	0.49	0.427	0.424

The anisotropy factors (A) of the alloys can be expressed as follows:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{6}$$

It is found that A is higher than 1 in all types of both alloys except for CoVTiAs in type 1, which means that the crystals are harder in the $\langle 111 \rangle$ direction. To complete the

study of the mechanical properties, we obtained a three-dimensional (3D) surface, representing the dependence of the Young’s modulus on crystallographic directions, which is an effective method to visualize the elastic anisotropy of a material. The 3D closed surfaces that represent the dependence of E on the crystallographic directions of a cubic crystal is defined as follows [23]:

$$\frac{1}{E} = S_{11} - 2 \left(S_{11} - S_{12} - \frac{1}{2} S_{44} \right) (l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2) \tag{7}$$

where $S_{ij} = C_{ij}^{-1}$
 $l_1 = \sin \theta \cos \varphi$, $l_2 = \sin \theta \sin \varphi$, and $l_3 = \cos \theta$ are the directional cosines with respect to the x , y , and z axes, respectively. The obtained 3D closed surfaces of the Young’s modulus of type 2 CoVTiAs and CoVTiSi are depicted in Figs. 4 and 5, respectively. It is found that the shapes of these surfaces are clearly different from the

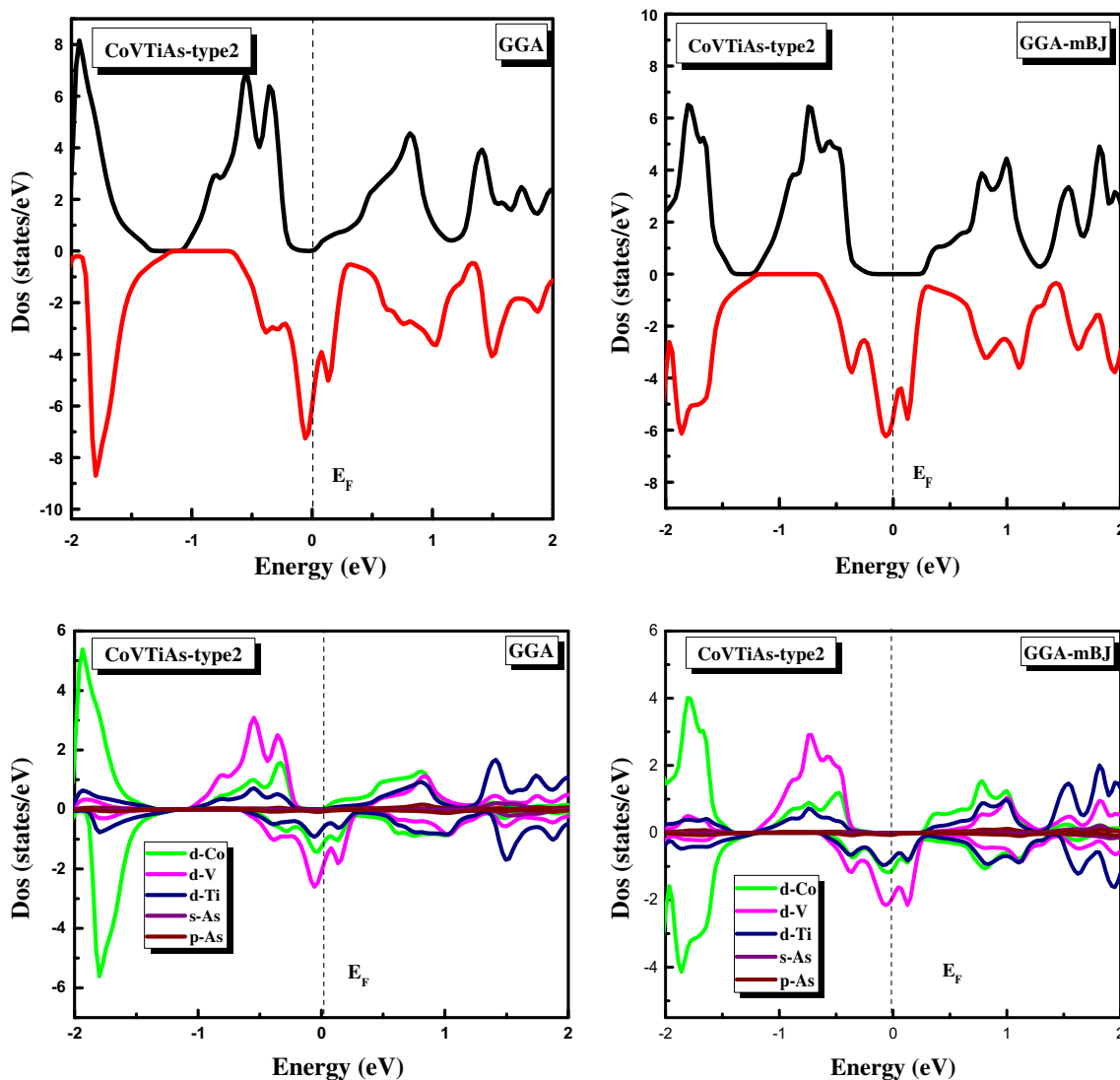


Fig. 7 Partial and total density (DOS) CoVTiX ($X = \text{As, Si}$) with GGA and GGA-mBJ approximations in type 2 structure

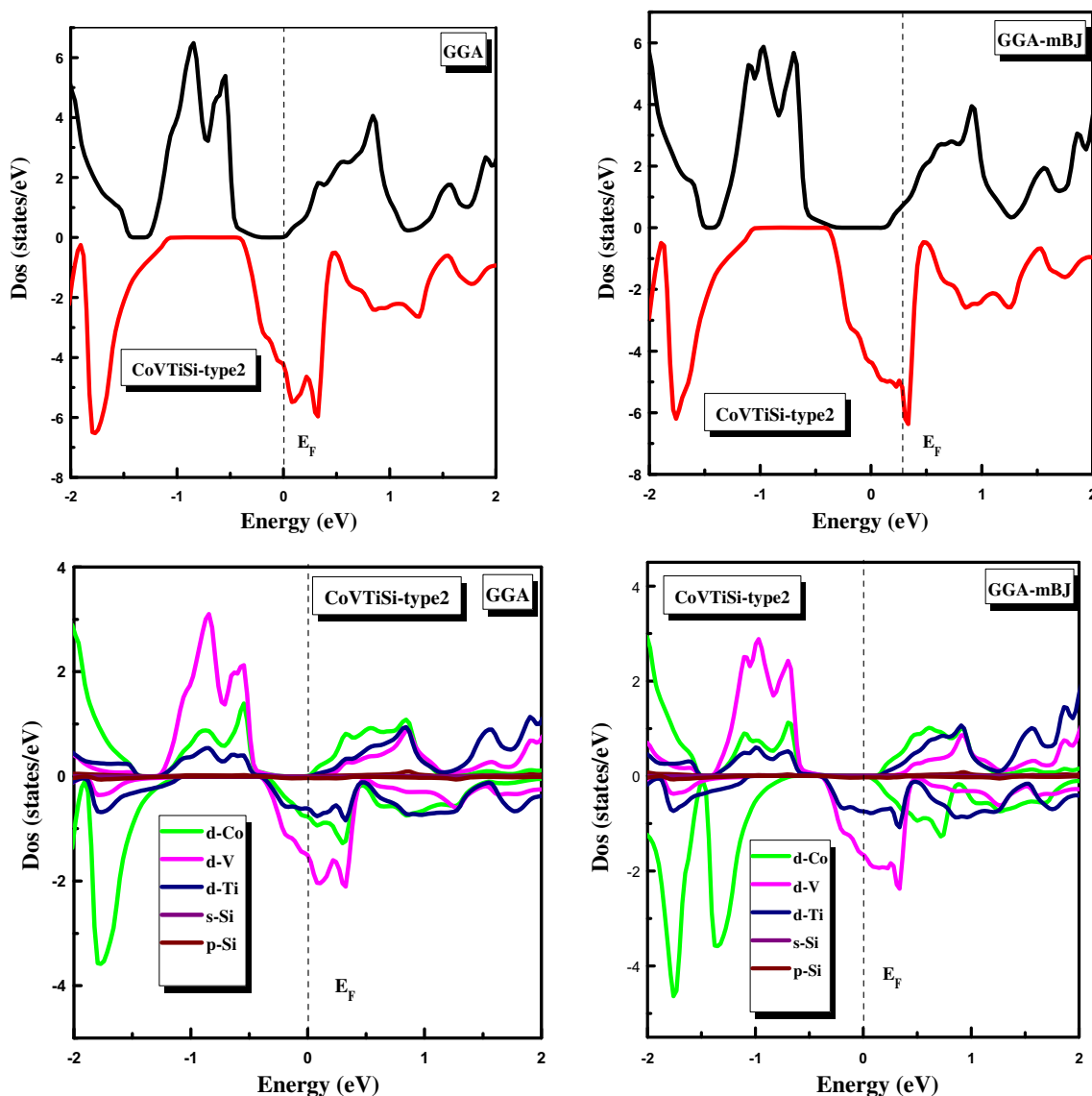


Fig. 7 (continued)

spherical shape, which indicates the presence of a strong elastic anisotropy in the studied quaternary Heusler alloys. We also plotted the cross-sections of these surfaces in different planes. From the 2D plane projections, one can see that the Young's modulus at different planes has a large anisotropic character.

3.3 Electronic and Magnetic Properties

In this subsection, we present the electronic and magnetic properties of these quaternary Heusler alloys using GGA and mBJ functionals. The band structures of CoVTiX ($X = \text{As, Si}$) alloys were calculated using the theoretical equilibrium lattice constants along high symmetry directions of the first Brillouin zone, see Fig. 6. Both CoVTiAs and CoVTiSi are found to exhibit a metallic behavior in the case of type 1

structure using GGA and mBJ approximations. For the case of type 2 CoVTiAs , GGA calculations predict a metallic behavior in the spin-up and spin-down channels, see Fig. 6a. However, using the GGA-mBJ approximation, the minority spin remains metallic, whereas the majority spin exhibits a metallic behavior due to the downward and upward shifts of the valence band maximum (VBM) and conduction band minimum (CBM), respectively. The majority spin band of the type 2 CoVTiAs alloy is found to be 0.45 eV, which extends from the Γ high symmetry point at the VBM to the X high symmetry point at the CBM that leads to a 100% spin polarization at the Fermi level. Similarly, CoVTiAs and CoVTiSi alloys of type 3 show half metallicity due to the semiconducting and metallic characters of the majority and minority spin channels, respectively, in agreement with CoMnCrZ ($Z = \text{Al, Si, Ge, and As}$) alloys [14]. The results

of GGA-mBJ approximation are believed to present good predictions for the band structures. It has been found that the band gaps of 15 out of 27 semiconductors are in agreement with experiment within a 5% error or less for both GW and the mBJ potentials [32]. However, the computations using GGA-mBJ functional is less time consuming with reasonable results as compared with GW. Previous electronic structure calculations of Fe₂VAl alloy, using GGA-mBJ functional, predicted a band gap of 0.22 eV [33], which is in a good agreement with the experimental values in the range of 0.1–0.2 eV [34]. A half-metallic behavior is also predicted for the case of CoVTiSi, where the minority band structure exhibits a metallic structure, whereas the majority spin channel is semiconducting. It is obvious that the band gap decreases when replacing As by Si. The band gap values are listed in Table 3. To confirm the nature of band structure of the studied compounds, the total and partial densities of states are depicted in Fig. 7. From this figure, one can see that the region between –13 and –11.5 eV of CoVTiAs shows the contribution of 4s orbitals of As atom for both majority and minority spin channels and two bands between –6 and –3 belong to p states with small contributions from the Co d states. The region extending from –4 eV to the Fermi energy is mainly formed by Co, V, and Ti d states. The d states of Co, V, and Ti transition metals are found to be the main contribution of the conduction band. For CoVTiSi compound, in both the majority and minority spin channels, significant contributions to the total density of states in the energy range between –9 and –7 eV, come from s states of Si atom. The second region of the valence band from –6 to –3 eV contains the small contributions of Si p orbitals and Co d orbitals. The remaining region between –3 and 5 eV shows a strong hybridization of Co, V, and Ti 3d orbitals. The density of states also confirms that these quaternary Heusler alloys are half-metallic ferromagnets using mBJ functional, which suggests these compounds as candidate materials for future spintronic applications. In Table 4, we present the calculated spin total and partial magnetic moments per formula unit for the studied quaternary Heusler compounds. The total moments of type 2 CoVTiAs and CoVTiSi alloys are found to be 1 and 2 μ_B, respectively. The main contribution of the total magnetic moment comes from Co and V local magnetic moments, which are found to be ferromagnetically coupled. However, Ti and As, and Si exhibit very small local magnetic moments. The magnetic moment is defined as the difference between the integral of the spin-up and spin-down densities of states. This explains the higher total and local magnetic moments in the case of CoVTiSi than those of CoVTiAs, which is attributed to the shift of the d states in the valence band of the minority spin channel to higher energy levels in the case of CoVTiSi as compared with CoVTiAs, see Fig. 7. To the best of our knowledge, there are neither experimental nor theoretical

Table 4 Total magnetic moment (μ_{tot}(μ_B)), local magnetic moment per atom (Co, V, Ti, As, Si), and magnetic moment in the interstitial region (μ_{int}) in CoVTiX (X = As, Si) compounds

Approximation	GGA					
	CoVTiAs compounds			CoVTiSi compounds		
	Type 1	Type 2	Type 3	Type 1	Type 2	Type 3
μ _{int}	0.21	0.24	0.24	0.61	0.40	0.40
μ _{Co}	0.66	0.11	0.11	1.23	0.27	0.27
μ _V	0.12	0.65	0.65	1.11	1.27	1.27
μ _{Ti}	0.31	0.02	0.02	0.82	0.076	0.075
μ _X	0.009	–0.018	–0.018	–0.010	–0.009	–0.009
μ _{tot}	1.31	1.00	0.99	3.76	2.00	2.00

magnetic moments obtained for these quaternary Heusler compounds in the literature.

4 Conclusions

The structural, electronic, magnetic, and mechanical properties of CoVTiX (X = As, Si) quaternary Heusler alloys were investigated using DFT calculations. Three possible different types were investigated for these alloys, where the type 2 ferromagnetic structure was found to be energetically more favorable than types 1 and 3. The mechanical properties reveal that the studied compounds are mechanically stable in their energetically stable phase. This study shows that these quaternary Heusler compounds possess a gap in the majority spin channel with a half-metallic ferromagnetic behavior, which is suitable for spintronic applications. The results in this work appear promising for future experimental investigations.

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