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Ab Initio Full-Potential Study of the Structural, Electronic, and Magnetic Properties of the Cubic $Sr_{0.75}Ti_{0.25}X$ (X = S, Se, and Te) Ternary Alloys

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Abstract

Ab initio predictions for strontium chalcogenides such as SrS, SrSe, and SrTe doped with magnetic titanium (Ti) element as the $Sr_{1-x}Ti_xX$ (X = S, Se, and Te) diluted magnetic semiconductor (DMS) compounds in rock-salt ferromagnetic structure have been studied at concentration $x = 0.25$, by using the full-potential linearized augmented plane wave plus local orbital (FP-LAPW+lo) method within the framework of spin-polarized density functional theory (SP-DFT). It has been verified that the ferromagnetic (FM) state of the investigated systems is the most stable phase. The estimated structural parameters of strontium chalcogenides are in good agreement with other available theoretical and experimental values. Predicted band structure and density of states have indicated that $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ compounds have a half-metallic ferromagnetic behaviors with a direct band gap at ($\Gamma - \Gamma$) direction of the spin down case. In addition, the important half-metallic gaps confirm the right ferromagnetic nature of the compounds used. The results obtained from the magnetic moments showed that the Ti impurity element has major contribution compared with nonmagnetic Sr, S, Se, and Te atoms. The value of total magnetic moments has been evaluated to equal to 2 μB per Ti atom. Considering the significance of the obtained results, the suitable half-metallic features of $Sr_{0.75}Ti_{0.25}X$ (X = S, Se, and Te) compounds can play an important role in spintronic applications.

Keywords DFT · Spintronics · Magnetic properties · Band gap · Ferromagnetic materials · Strontium chalcogenides

1 Introduction

Spintronics is a new field of electronics that takes advantage the spin of electrons to create materials with new functionalities in order to support the magnetic data storage industry [1–4]. In this regard, the search for new materials with attractive fundamental features for their exploitations in spintronic applications is still an area of ongoing research work [5–10].

Recently, the motivation for the research of half-metallic ferromagnetic (HMF) materials become important due to their potential applications in the field of spintronics [2]. A number of new half-metallic systems have been performed in which they exhibit a symmetrical energy gap in one spin state [11], whereas the presence of a metallic nature in the other spin-polarized band structure is due to the existence of some bands cross the Fermi level (E_F).

The possibility of introducing magnetic impurities in semiconductors has created an appropriate type of materials called diluted magnetic semiconductors (DMSs) [12]. These materials, whose electronic and magnetic properties are strongly coupled, have attracted much attention because they exhibit half-metallic ferromagnetism and they can be used in the development of spintronics. Sato et al. [13, 14] have investigated

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the origin of the ferromagnetism that has been found in a number of DMSs.

The originality of the both the ferromagnetic and semiconducting behaviors in diluted magnetic semiconductors results from the existence of atoms carrying a magnetic moment leading to a number of exceptional and important fundamental properties. This result is consistent with the prediction of Dietl [15, 16]. Furthermore, a further significant attribute of DMSs is that the different physical characteristics like energy band gap may be monitored by changing the dopant of magnetic ions in these systems [17].

DMSs based on semiconductors II–VI are omnipresent in research on spintronics because of the interesting magnetic properties they have. In this regard, extensive inclusive theoretical researches have been conducted for the purpose of examining the half-metallic ferromagnetic behaviors in the II–VI semiconductors doped with magnetic atoms like Mn-doped BeSe and BeTe [18], $Cd_{1-x}TM_xS$ (TM = Co and V) [19], V-doped BeSe and BeTe [20], Cr-doped ZnS [21], Cr-doped Cd-chalcogenides [22], Cr-doped CaS [23], Cr-doped MgS [24], V-doped CaS [25], $Cd_{1-x}V_xTe$ ($0 \leq x \leq 1$) [26], $Cd_{1-x}Fe_xS$ [27], and Cr-doped BeSe and BeTe [28]. Moreover, the investigations of strontium chalcogenides doped with magnetic atom have been performed to predict the half-metallic ferromagnetic behavior of these semiconductors such as vanadium and chromium-doped rock-salt strontium chalcogenides [29, 30]. This indicates that the ferromagnetism is established in the exchange interaction between host and magnetic elements.

In particular, the appearance of the half-metallic ferromagnetism in Ti-doped II–VI semiconductors such as $Mg_{1-x}Ti_xTe$ ($x = 0.25$, 0.50, and 0.75) [31] and $Be_{1-x}Ti_xSe$ [32] (at concentrations $x = 0.25$, $x = 0.12$, and $x = 0.06$) make it as a favorable systems for spintronic devices. Furthermore, the effect Ti impurity is found to be the original contributor to the ferromagnetism of the doped ZnS [33] and the doped ZnO [34]; the reason for which it was applied in our present paper.

The II–VI strontium chalcogenides (SrS, SrSe, and SrTe) have larger band gap semiconductors, which belong to II–VI elements of the periodic table; they have been studied by many groups [35–51]. These monochalcogenides constitute a group of technologically valuable materials for their promising use in the field of luminescent devices [52–54]. The stable crystal structure of these compounds is the rock-salt (B1) phase at ambient conditions.

The possible use of half-metallic dilute magnetic semiconductors in the spintronic applications and their excellent role in this field encouraged us to investigate $Sr_{0.75}Ti_{0.25}X$ ($X = $ S, Se, and Te) compounds in rock-salt structure. This investigation is carried out by performing first principle calculations of density functional theory (DFT) [55, 56] within the full-potential linearized augmented plane wave (FP-LAPW+lo) method as implemented in the package WIEN2K [57].

2 Computational Approach and Details

The application of first principles computational methods to examine the fundamental characteristics of $Sr_{0.75}Ti_{0.25}X$ ($X = $ S, Se, and Te) compounds. We performed our calculations using the WIEN2k simulation package, which is based on density functional theory.

The full-potential linearized augmented plane wave (FP-LAPW) method [58] is used to solve the Kohn–Sham equations. For the calculation of the exchange-correlation energy, the Perdew–Burk–Ernzerhof generalized gradient approximation (GGA-PBE) [59] was applied.

The II–VI strontium chalcogenides SrX ($X = $ S, Se, and Te) have rock-salt structures with space group 225 (Fm3m), where the Sr element is placed at the location (0,0,0) and X atom at the position (1/2,1/2,1/2), whose experimental lattice constants are 6024 Å [41], 6.236 Å [42], and 6.66 Å [43], respectively.

The structures of the doped binary SrX semiconductors were modeled in ($1 \times 1 \times 1$) supercell consisting of 8 atoms, the supercells of $Sr_{1-x}Ti_xX$ ($X = $ S, Se, and Te) are formed, when Ti was doped in SrS, SrSe, and SrTe lattices at $x = 0.25$ replacing one Sr element at the site (0,0,0). The supercell of ($1 \times 1 \times 2$) was applied to execute antiferromagnetic calculations. We get a systems with 25% concentration, eight-atom cubic structure with space group 221 (Pm-3m).

In these predictions, the electronic configuration for each material has been taken in such a way that the states Sr: Kr ($5s^2$), Ti: Ar ($4s^2 3d^2$), S: Ne ($3s^2 3p^4$), Se: Ar ($3d^{10} 4s^2 4p^4$) and Te: Kr ($5s^2 4d^{10} 5p^4$) are considered as being states of valence, and the rest are considered as core states.

We take the muffin-tin radii (RMT) of Sr, S, Se, Te, and Cr in such a way that the muffin-tin spheres do not overlap. Taking the value of $R_{MT}K_{max} = 8$ determines the plane wave basis functions, where K_{max} is the interstitial plane wave cutoff and R_{MT} is the smallest of all atomic sphere radii. The partial waves used inside the muffin-tin spheres were expanded up to $I_{max} = 10$. The charge density was Fourier expanded up to $G_{max} = 14 \, (a.u)^{-1}$. For B1 phase, the total Brillouin zone was sampled with 1000 k-point. In ferromagnetic calculations, the self-consistent convergence of the total energy of the systems is chosen to equal to 10^{-4} Ry.

3 Results and Discussions

3.1 Structural Properties

The study of the structural properties is essential to determine the parameters of the structure of the material. Above all, for confirming the most stable state from the different magnetic structures, we achieved the structural optimization in the more stable B1 structure by fitting the empirical Murnaghan equation of state [60] for the antiferromagnetic (AFM), ferromagnetic (FM), and

nonmagnetic (NM) states; then, we plot the fluctuation in total energy of $Sr_{0.75}Ti_{0.25}X$ ($X =$ S, Se, and Te) with volume in the three magnetic states. Figure 1 displays the energy-volume curves of the investigated compounds in the FM, AFM, and NM states. It is obvious from the different plots that the lower energies are related to the ferromagnetic states for the three compounds. Also, we found that the sign of total energy differences are positive and are evaluated to equal to 0.0245, 0.0382, and 0.2378 for the predicted values between antiferromagnetic and ferromagnetic states and for the estimated values between nonmagnetic and ferromagnetic states are equal to 0.0360, 0.0342, and 0.0470 for $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ respectively; hence, the most stable phase for these compounds is the ferromagnetic state.

The structural properties such as lattice parameters (a) in Å and bulk modulus B in (GPa) are successfully predicted by calculating the total energy with the unit cell volume of all available alloys in ferromagnetic state. Figure 2 depicts the crystal structures of $Sr_{0.75}Ti_{0.25}S$ (a), $Sr_{0.75}Ti_{0.25}Se$ (b), and $Sr_{0.75}Ti_{0.25}Te$ (c) in which the crystal showed a cubic structure with space group Pm-3m No. 221.

Our evaluated measures are listed in Table 1. In order to validate our results, this table also contains experimental measurements and theoretical work obtained by other methods as well.

It is noticeable that our predicted values of the equilibrium lattice constants of SrX ($X =$ S, Se, Te) semiconductors are somewhat greater than the reported experimental data. The aforementioned difference is essentially a result of the GGA-PBE approximation; generally, our predicted GGA results of the strontium chalcogenides compounds are in very clear accord with the experimental measurements [41–43] and the theoretical calculations [44–46].

In the other hand, it can also be remarked from the results obtained that the studied lattice constant of $Sr_{0.75}Ti_{0.25}Te$ is greater than that of $Sr_{0.75}Ti_{0.25}Se$, whereas the lattice constant of the latter is greater than that of $Sr_{0.75}Ti_{0.25}S$. Hence, the equilibrium lattice parameters increase and the differences in the lattice constant are related to the change in atomic sizes ($V_{Te} > V_{Se} > V_{S}$).

As regards the compressibility, our results obtained for binary compounds reasonably agree with the experimental [41–43] and theoretical works [44, 45], while we can further noticed that the compressibility modulus decreases as the atomic number of the chalcogen element increases going from S to Se to Te atom, which means that the materials become more compressible. Moreover, there are no experimental results of structural parameters for studied compounds to compare them with the calculations of our work.

3.2 Electronic Properties

The significance of the electronic characteristics of a system, which are the band structure and the density of states (DOS), is
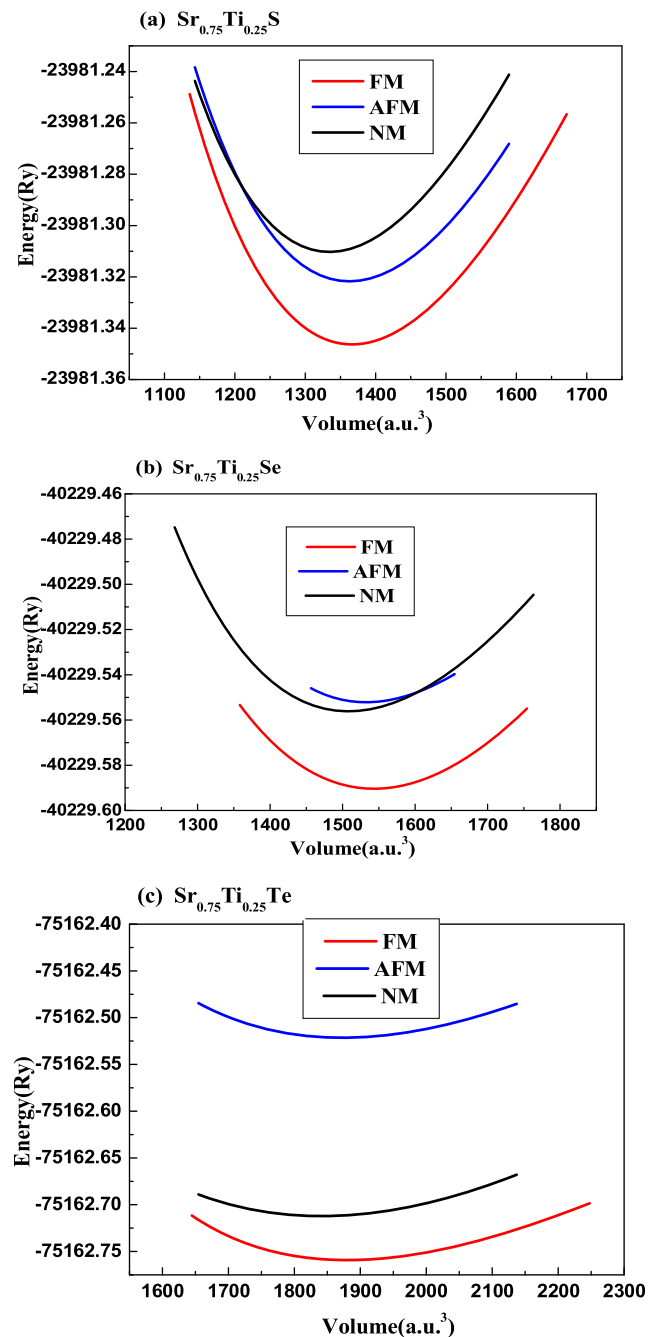

Fig. 1 Total energy of $Sr_{0.75}Ti_{0.25}X$ ($X =$ S, Se, and Te) compounds as a function of volume in the three magnetic states of AFM, FM, and NM state for **a** $Sr_{0.75}Ti_{0.25}S$, **b** $Sr_{0.75}Ti_{0.25}Se$, and **c** $Sr_{0.75}Ti_{0.25}Te$

that they allow us to analyze and understand the nature of the bands that are generated between the different atoms of this material.

The realization of the electronic band structure and the density of states is very important with the aim of elaborating the half-metallicity in $Sr_{0.75}Ti_{0.25}X$ ($X =$ S, Se, and Te) using the GGA-PBE approximation. To this end, we have utilized the predicted lattice parameters presented in this study for investigating the influence of Ti impurity on the electronic

Fig. 2 The crystal structures of $Sr_{0.75}Ti_{0.25}X$ ($X = S$, Se, and Te): **a** $Sr_{0.75}Ti_{0.25}S$, **b** $Sr_{0.75}Ti_{0.25}Se$, and **c** $Sr_{0.75}Ti_{0.25}Te$
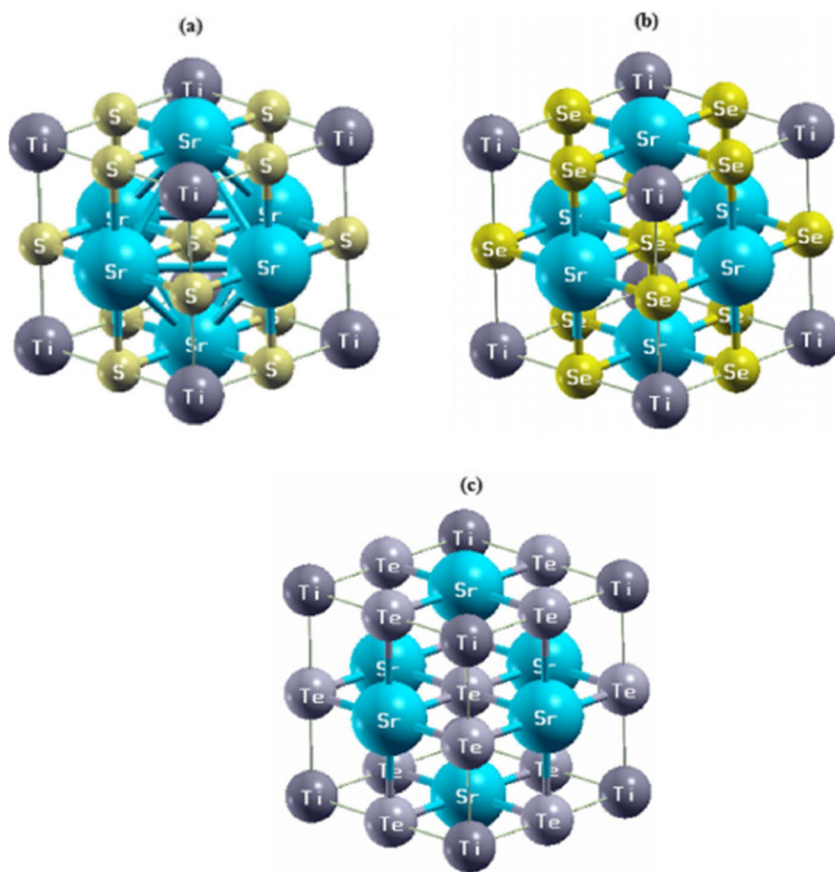
features. For magnetic materials, polarized spin computations are made by using both spin electron (spin up and spin down) individually.

Taking into account the electronic band structures of $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ alloys in both

spin states were studied by using the predicted lattice parameters as displayed in Fig. 3. It can be seen from these plots that for spin up channels of all the compounds studied, some bands exist at the Fermi level, unlike for the spin down channels that show an energy gap around the Fermi level. Consequently, the

Table 1 Calculated bulk parameters of $Sr_{1-x}Ti_xX$ ($X = S$, Se, and Te) compounds with concentration ($x = 0.0$ and 0.25) in rock-salt B_1 phase using the GGA-PBE approximation compared to other theoretical and experimental works: lattice parameters (a) in Å and bulk modulus B (GPa)

Compound	Lattice constant a (Å)			Bulk modulus B (GPa)		
	Our work	Exp	Others	Our work	Exp	Others
SrS	6.061	6.024[a]	6.076[d], 6.05[e], 5.988[f]	47.18	58[a]	47[d], 48.30[e]
SrSe	6.292	6.236[b]	6.32[d], 6.29[e], 6.204[f]	45.82	45[b]	41[d], 40.93[e]
SrTe	6.729	6.660[c]	6.76[d], 6.71[e], 6.621[f]	33.61	39.5[c]	36[d], 32.07[e]
$Sr_{0.75}Ti_{0.25}S$	5.872	–	53.65	–	–	–
$Sr_{0.75}Ti_{0.25}Se$	6.115	–	42.10	–	–	–
$Sr_{0.75}Ti_{0.25}Te$	6.530	–	35.56	–	–	–

[a] Ref. [46]

[b] Ref. [47]

[c] Ref. [48]

[d] Ref. [49]

[e] Ref. [50]

[f] Ref. [51]

alloys, at the Fermi level, demonstrate a half-metallic ferro-magnetic behavior.

According to the band structures calculated with the GGA-PBE method, a difference in the estimate of the width of the energy gap between the valence and conduction bands may be noted. It can also be noted that the rock-salt structures of systems have a direct gap at Γ point.

The latter contributed to the formation of half-metallic fer-romagnetic gaps ($G_{\mathrm{HMF}}(eV)$) and half-metallic gaps ($G_{\mathrm{HM}}(eV)$) in the spin down channels, as shown in Table 2.

The half-metallic ferromagnetic gap for each alloy is direct-ly situated at the Γ point of symmetry between the highest valence bands (VB) and the lowest conduction bands (CB).

It is noticeable as well that 2.12, 1.91, and 1.50 eV dimin-ished from $Sr_{0.75}Ti_{0.25}S$ to $Sr_{0.75}Ti_{0.25}Se$ to $Sr_{0.75}Ti_{0.25}Te$, when approaching the Fermi level, the p (S, Se, and Te) states moved to greater energies.

Additionally, so far as the HM gap is concerned, at the Fermi level, it is a significant determinant for the use of half-metallic materials which is defined as the minimum between the lowest energy of majority (minority) spin conduction bands and the absolute values of the highest energy of major-ity (minority) spin valence bands. For this particular scenario, the half-metallic gaps are situated between the minimum of minority spin conduction bands at Fermi level with the fol-lowing estimations respectively, 0.43, 0.53, and 0.59 eV for $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$. Moreover, the nonzero of HM gaps produces a right half-metallic behavior, which promotes these compounds as viable contestants for spintronic applications. Carrying out the electronic density of states of present alloys was deemed a necessary step to inspect the half-metallic nature and detect the mechanism, which led to generating the ferromagnetism state. Figure 4 presents the total density of states (TDOS) and partial density

Fig. 3 Spin-polarized electronic band structure of majority and minority spin for $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ compounds obtained using the GGA-PBE approximation
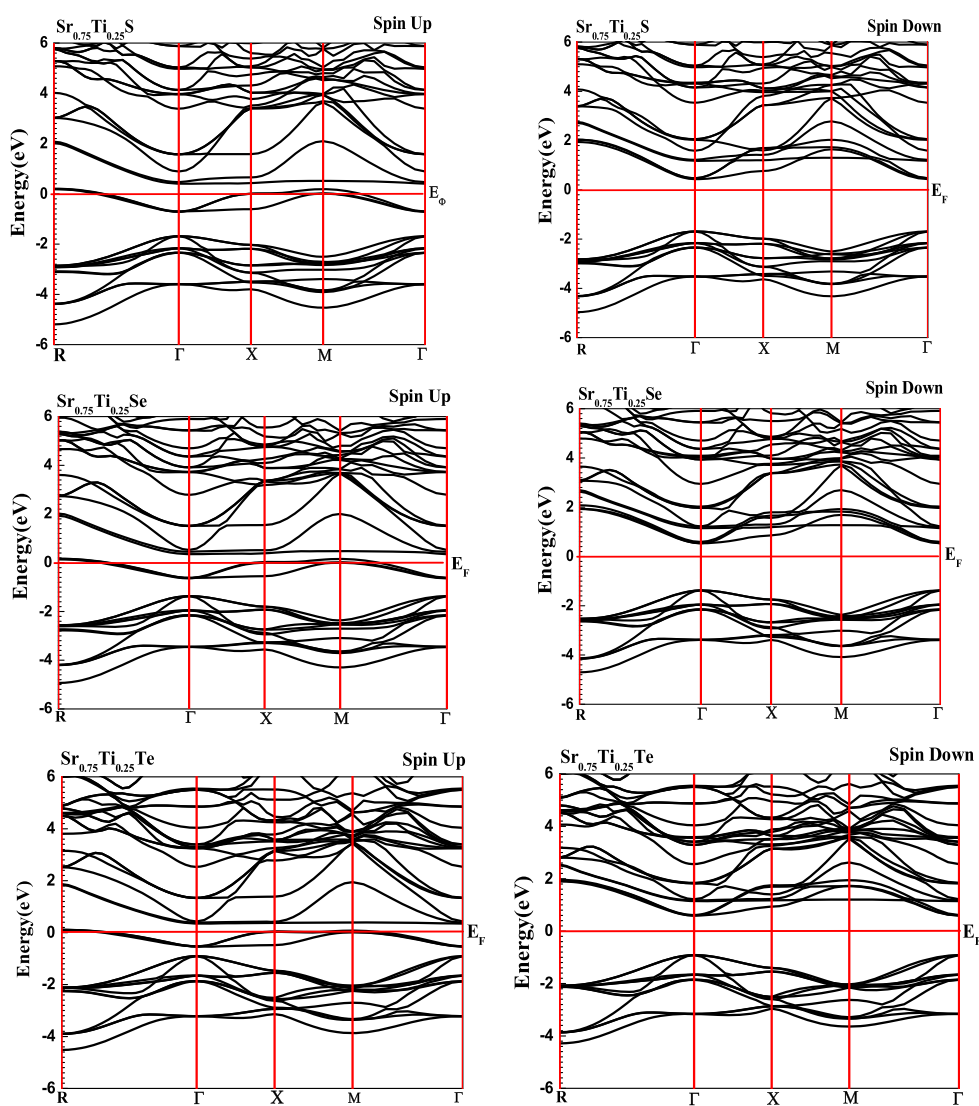
Table 2 The calculated results of half-metallic ferromagnetic gaps G_{HMF}(eV) and the half-metallic G_{HM}(eV) gaps for $Sr_{0.75}Ti_{0.25}X$ (X = S, Se, and Te) alloys calculated using the GGA-PBE approximation

Compound	Behavior	G_{HMF}(eV) Our work	G_{HM}(eV) Our work
$Sr_{0.75}Ti_{0.25}S$	HMF	2.12	0.43
$Sr_{0.75}Ti_{0.25}Se$	HMF	1.91	0.53
$Sr_{0.75}Ti_{0.25}Te$	HMF	1.50	0.59

of state (PDOS) for (a) $Sr_{0.75}Ti_{0.25}S$, (b) $Sr_{0.75}Ti_{0.25}Se$, and (c) $Sr_{0.75}Ti_{0.25}Te$ obtained using the GGA-PBE approximation.

The total and partial DOS of spin up states for all systems are metallic in nature due to the Ti-3d states that are passing through the Fermi level with a small participate of 3p (S), 4p (Se), and 5p (Te) states, while the semiconductor character is preserved in the DOS of spin down channels. We have realized from our results of electronic DOS that studied systems depict a half-metallic ferromagnetic character.

We can also see that the fivefold degenerate 3d states of (Ti) are separated into two parts, the triply degenerate $t_{2g}(d_{xy}, d_{xz}d_{yz})$ and the doubly degenerate $e_g(d_{z^2}, d_{x^2}-d_{z^2})$ states.

From the PDOS, we note that the energies of e_g states are lower than t_{2g} states as a result of reduced Coulomb interactions. Furthermore, the 3d (Ti) majority spin states were investigated close to Fermi level. The outcome of the investigation detected that $3d - e_g$ (Ti) states take place at the bottom part of conduction band top Fermi level and the $3d - t_{2g}$ (Ti) states pass through the Fermi level. The contribution of these two symmetry states intensified completely in the conduction band for spin down channel. Also, the PDOS reveals that the density of states centered in the valence band of both spin up and spin down cases in the energy range -4.33 to -1.68, -4.18 to -1.39, and -3.88 to -0.94 for $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ respectively principally occupied by (S, Se, and Te) p states with small contributions of (Sr) s states.

3.3 Magnetic Properties and Curie Temperature

The first principles calculations are applied for predicting the magnetic moments (MMs) of the mentioned systems in this section of the work. Table 3 illustrates the calculated values of the total and local magnetic moments for $Sr_{0.75}Ti_{0.25}X$ (X = S, Se, and Te) systems. The hybridization between 3d (Ti) and p (S, Se, and Te) states produces the total magnetic moments of (Ti) atom and we observed also the production of a little local magnetic moment on the Sr site and the chalcogen elements (S, Se, and Te). The value of the total magnetic moments has

Fig. 4 Spin-polarized total and partial densities of states of majority and minority spin for **a** $Sr_{0.75}Ti_{0.25}S$, **b** $Sr_{0.75}Ti_{0.25}Se$, and **c** $Sr_{0.75}Ti_{0.25}Te$ obtained using the GGA-PBE approximation
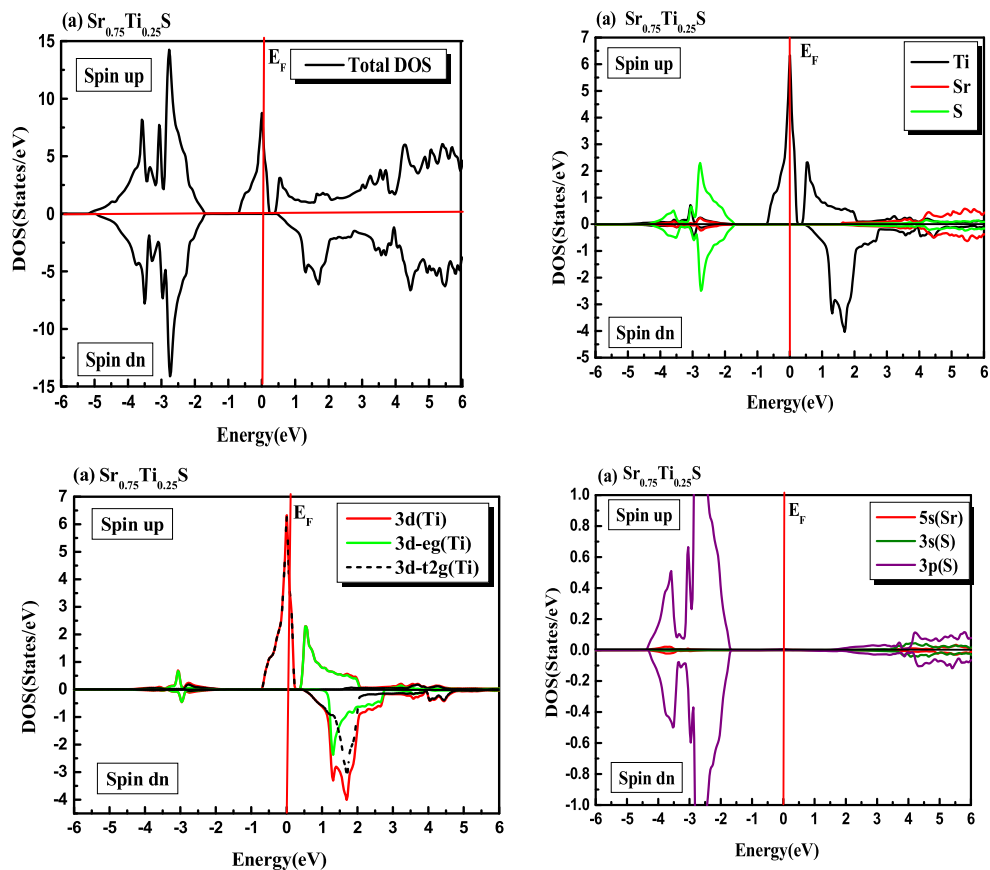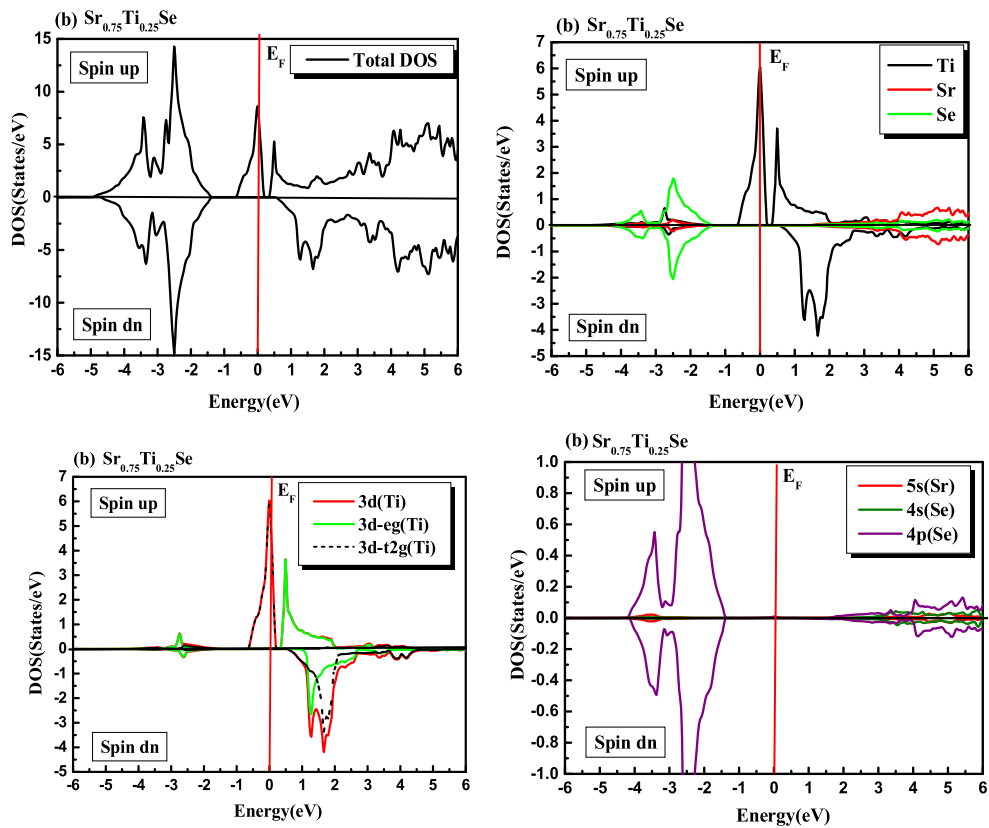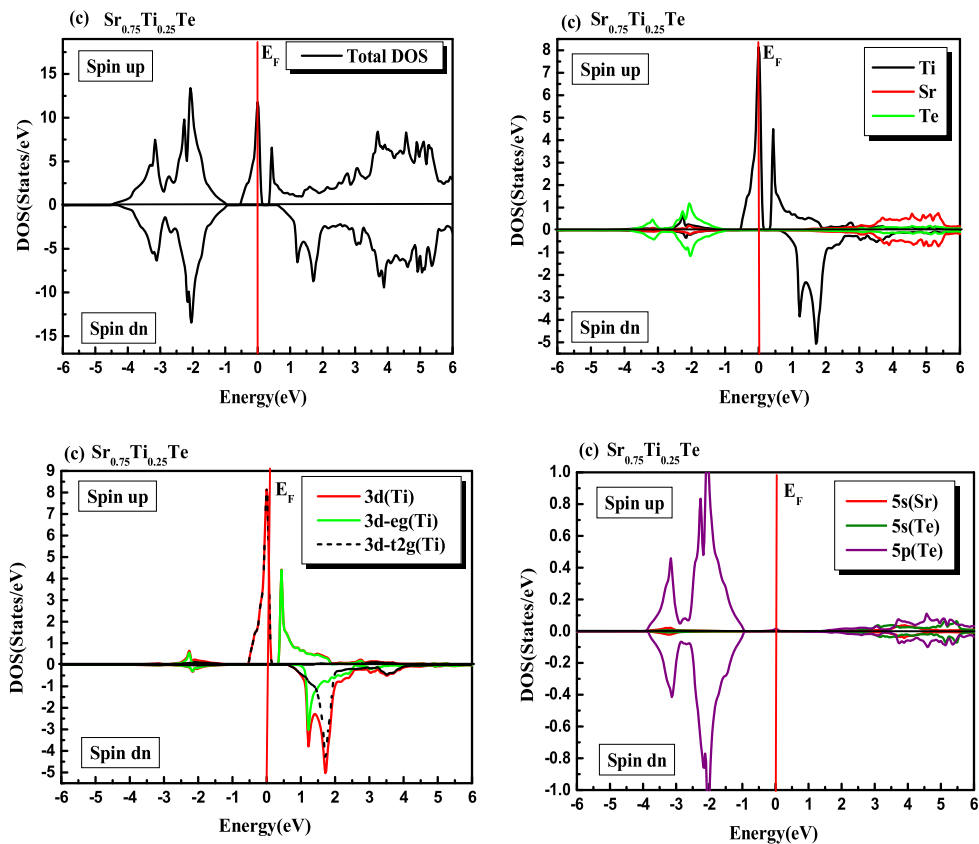
Fig. 4 continued.

Fig. 4 continued.

been evaluated to equal to 2 μ_B per Ti atom where μ_B represents the Bohr magneton, the integral value of Bohr magneton is a characteristic behavior of half-metallic ferromagnetism for all compounds.

The magnetic moments of Ti are behind the emergence of the principle contributions of total magnetic moments. However, the magnetic moments decreased less than the anticipated value of 2 μ_B. The secondary contributions, at a smaller scale, of magnetic moments are generated on the nonmagnetic (Sr, S, Se, and Te) sites, all thanks to the p-d exchange interactions.

Moreover, the negative sign of the value of the local magnetic moments of the chalcogen elements clearly reports that there is an antiferromagnetic interaction between the valence barriers consisting of the p chalcogen element states and Ti valence spins. On the other hand, the ferromagnetic interaction between Sr and Ti magnetic spins is expressed by the positive magnetic moments of Sr elements.

The exchange between Ti local moments and the carriers produced play a fundamental role in the physics of DMSs. This exchange is characterized by two constants: the exchange s-d $N_{0\alpha}$ and the exchange p-d $N_{0\beta}$, which describe the exchange interaction between the Ti-3d states and the electron carries of conduction bands and the holes of valence bands, respectively. Therefore, the exchange constants can be calculated directly from the band-edge spin splitting of the valence and conduction bands at the Γ symmetry point $\left(\Delta E_c = E_c^\downarrow - E_c^\uparrow\right)$ and $\left(\Delta E_v = E_v^\downarrow - E_v^\uparrow\right)$ according to the following expressions [61]:

$$N_{0\alpha} = \frac{\Delta E_c}{x} < S > \tag{1}$$

$$N_{0\beta} = \frac{\Delta E_v}{x} < S > \tag{2}$$

where ΔE_c and ΔE_v are the band-edge spin splitting of the conduction bands and valence bands respectively, and x is the concentration of Ti and $<S>$ is half of the magnetization per Ti atom. Our predicted ΔE_c, ΔE_v, $N_{0\alpha}$, and $N_{0\beta}$ values for $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te) are summarized in Table 4.

Table 3 Total magnetic moment (M^{tot} in μ_B) per Ti doping and atomic magnetic moments for $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te) obtained using the GGA-BPE approximation

Compound	$Sr_{0.75}Ti_{0.25}S$	$Sr_{0.75}Ti_{0.25}Se$	$Sr_{0.75}Ti_{0.25}Te$
M^{tot} (μ_B)	2.00	2.00	2.00
M^{Ti} (μ_B)	1.48	1.45	1.47
M^{Sr} (μ_B)	–	–	–
M^{S} (μ_B)	− 0.01	–	–
M^{Se} (μ_B)	–	− 0.02	–
M^{Te} (μ_B)	–	–	− 0.02

Table 4 The estimated conduction and valence band-edge spin splitting ΔE_c(eV) and ΔE_v(eV) and exchange constants $N_{0\alpha}$ and $N_{0\beta}$ for $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te) alloys obtained using the GGA-PBE approximation

Compound	ΔE_c(eV)	ΔE_v(eV)	$N_{0\alpha}$(eV)	$N_{0\beta}$(eV)
$Sr_{0.75}Ti_{0.25}S$	0.03	− 1.90	0.12	− 7.58
$Sr_{0.75}Ti_{0.25}Se$	0.19	− 1.54	0.74	− 6.16
$Sr_{0.75}Ti_{0.25}Te$	0.24	− 1.02	0.98	− 4.09

These results show that for all compounds, the negative signs of the exchange constants $N_{0\beta}$ and the positive signs of $N_{0\alpha}$ confirm the antiparallel and parallel spins respectively. Furthermore, the values of $N_{0\alpha}$ increase and the predicted results of $N_{0\beta}$ vary from $Sr_{0.75}Ti_{0.25}S$ to $Sr_{0.75}Ti_{0.25}Se$ to $Sr_{0.75}Ti_{0.25}Te$, which affirm the expected magnetic character in these materials.

In materials science, the Curie temperature (T_C) is the temperature at which certain materials lose their permanent magnetic properties to be replaced by induced magnetism. Here, the energy difference ΔE is a significant factor for evaluating magnetic transition temperature in the Heisenberg model. However, the Curie temperature of $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te) was determined in the framework of the mean-field approximation using the following expression:

$$T_C = -\frac{1}{3\,k_B}\left(\Delta E_{AFM-FM}\right) \tag{3}$$

where ΔE_{AFM-FM} is the total energy difference between FM and AFM states, and k_B is the Boltzmann constant [62]. The predicted results of T_C for investigated systems are listed in Table 5. One can notice from the table that, for $Sr_{0.75}Ti_{0.25}S$ and $Sr_{0.75}Ti_{0.25}Se$, the T_C is considerably low, but the Curie temperature of $Sr_{0.75}Ti_{0.25}Te$ has a higher value estimated to equal to 919 K.

4 Conclusion

In a nutshell, the structural, electronic, and magnetic properties of $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te) have been studied by

Table 5 The estimated Curie temperature T_C (K) for $Sr_{0.75}Ti_{0.25}X$ ($X=$ S, Se, and Te)alloys

Compound	ΔE_{FM-AFM} (eV)	T_C (K)
$Sr_{0.75}Ti_{0.25}S$	0.0245	94
$Sr_{0.75}Ti_{0.25}Se$	0.0382	147
$Sr_{0.75}Ti_{0.25}Te$	0.2378	919

first principle density functional calculations using the FP-LAPW+lo method implemented in the WIEN2k package.

We have predicted the structural parameters of in rock-salt crystalline phase using the GGA-PBE approximation. The results obtained for binary semiconductors are in good accord with those determined by experience and those obtained on the basis of other theoretical methods. In addition, the increase of the lattice constants is accompanied by a decrease in compressibility with an increase in the atomic number of the chalcogen element going from S to Se to Te atom. The investigation revealed important facts about the electronic and magnetic features for $Sr_{0.75}Ti_{0.25}S$, $Sr_{0.75}Ti_{0.25}Se$, and $Sr_{0.75}Ti_{0.25}Te$ alloys that represent half-metallic ferromagnetic (HMF) nature. In addition, the results showed that these compounds have a direct gap for the rock-salt phase. The integral Bohr magneton of 2 μ_B confirmed the HMF behavior. Moreover, the HM gaps of the presented compounds appear to be a significant determinant to scrutinize half-metallic ferromagnetism for potential semiconductor spintronic devices. Our research could serve as a reference for further studies in the future.

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