

Systematic Study of Structural and Magneto-Electronic Properties of $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ Alloys for Spintronic Applications

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Abstract – In this work, the structural and the magneto-electronic properties of the $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ compounds at dopant concentration $x=0.25, 0.50,$ and 0.75 in the rock-salt ferromagnetic phase are studied using first-principles calculations based on density functional theory. The structural properties of the three compounds calculated indicate promising findings. The electronic band profiles, the density of states plots, and the integral magnetic moment validate the half-metallic feature only at $x=0.25$. As a result, the $\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$ compound is the most promising spintronic material in the series.

Keywords – Structural properties, magneto-electronic properties, strontium chalcogenide, DFT, spintronic applications.

I. INTRODUCTION

In recent years, the diluted magnetic semiconductors (DMSs) obtained by doping classical semiconductors with small fraction of transition metal atoms have attracted both scientific and technological interest, because, they exhibit half-metallic ferromagnetism which is a key ingredients for the future high-performance spintronic devices [1]. The semiconductor SrS from group II-IV elements has attracted more attention due to its wide band gap and its excellent properties. Because pure semiconductors are not appropriate for producing operational devices, these elements are doped with impurity atoms to improve their operating qualities. Diluted magnetic semiconductor (DMS) compounds based on II-IV are the perfect material for producing all spin-based semiconductor devices. There have been various efforts over recent decades towards ferromagnetic semiconductor synthesis [2-4]. In diluted magnetic semiconductors, the uniqueness of ferromagnetic and semiconducting behaviors is the consequence of a number of extraordinary and significant basic characteristics of atoms that carry an extra-magnetic moment. This result is consistent with that of Dietl [5]. A further essential element of DMSs is the tracking of the different physical characteristics, including the energy band gap, by changing the dopant of magnetic ions [6]. In this respect, we have computed, for three distinct concentrations $x=0.25, 0.50$ and 0.75 , the structural, electronic and magnetic characteristics of the Ti-doped SrS compound. Our purpose is to monitor the compound's half-metallic conduct by changing

the dopant concentration and to perform profound studies using the first-principle full-potential linearized augmented plane-waves (FP-LAPW) method with the generalized gradient approximation of Perdew-Burk- Ernzerhof for solids (GGA-PBESol) [7]. It is worth to mention that there is no theoretical or experimental evidence on the three compounds with this approximation are available, thus our results are only predictions.

II. METHOD OF CALCULATION

The calculations of the structural, electronic and magnetic properties of $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ Compounds were carried out following density functional theory as implemented in Wien2k code [8]. In order to generate the three 25%, 50%, and 75% concentrations of Ti, a standard cubic supercell of $(1 \times 1 \times 1)$ which containing eight atoms in the rock-salt phase was constructed. The Brillouin zone was sampled in $8 \times 8 \times 8$ Monk horst-Pack grid. The wave functions in the interstitial region were expanded up to $R_{\text{mt}}K_{\text{max}} = 8.0$ (where K_{max} is the magnitude of the largest K vector in the plane wave and R_{mt} is the average radius of the muffin-tin spheres). The partial waves inside the atomic sphere had a maximum value of $l_{\text{max}} = 10$. The charge density, on the other hand, was set at $G_{\text{max}} = 14 \text{ a.u.}^{-1}$.

III. RESULTS AND DISCUSSION

3.1 Structural parameters

The structural optimization of $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ compounds with $x=0.25, 0.50,$ and 0.75 was carried out in the neighborhood of the parent SrS semiconductor's lattice parameter. In the rock-salt structure, one, two, and three Sr cation atoms are substituted by one, two, and three Ti dopant atoms in $1 \times 1 \times 1$ supercell to reach 0.25, 0.50, and 0.75 concentrations, respectively. The obtained structures are optimized through calculating their total energies as a function of the reduced volume. The results are fitted into Birch-Murnaghan equation of state [9] to define the lattice parameter and the bulk modulus for the doped systems. The simulated results are listed in Table 1.

Table 1

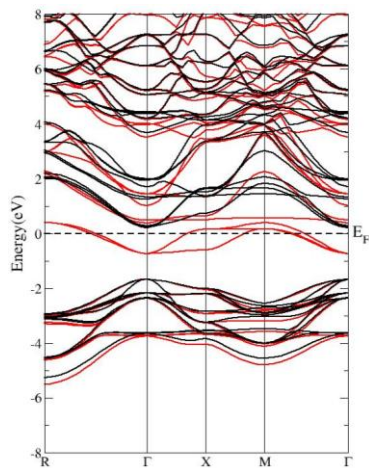
Computed values of lattice parameter a (Å) and bulk modulus B (GPa) for $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ ($x=0.25, 0.50, \text{ and } 0.75$)

Compound	a (Å)	B (GPa)
$\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$	5.763	59.306
$\text{Sr}_{0.50}\text{Ti}_{0.50}\text{S}$	5.537	71.909
$\text{Sr}_{0.25}\text{Ti}_{0.75}\text{S}$	5.227	82.073

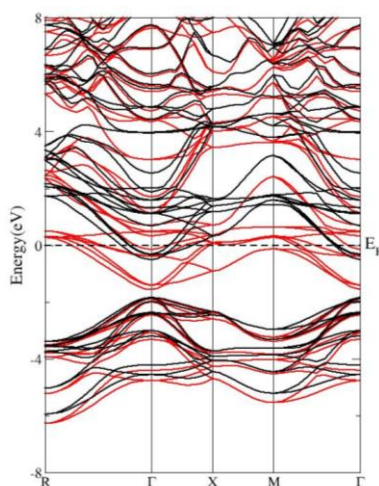
It can be seen from Table 1 that the lattice constant of the doped systems decreases and the bulk modulus increases with increasing Ti content. This is due to the fact that the ionic radius of Ti is smaller than that of Sr atom.

3.2 Electronic band structures and densities of states

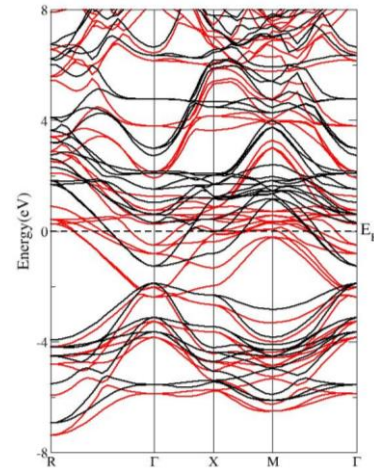
We have utilized the optimized lattice parameters of the compounds to study the electronic band structures and densities of states. Spin resolved energy band gap structures for the two-spin channels direction along with high symmetry points in first Brillouin zone for $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ at different concentrations 0.25, 0.50 and 0.75 are illustrated in the Fig. 1, respectively.



a)



b)



c)

Fig. 1 Electronic band structures of $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ at a) $x=0.25$, b) $x=0.50$, and c) $x=0.75$ (Red color: spin up, Black color: spin down).

From the profiles of band structures, it is evident for the $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ at $x=0.25$ that in majority spin channel, the band gap crosses the Fermi level (E_F) and therefore exhibits metallic character, but the minority spin channel does not pass the Fermi level and hence shows semiconductor feature. This indicates that this material is half-metallic ferromagnetic. On increasing the concentration over 25%, the HMF character disappear and the nature turn to be metallic for both the compounds $\text{Sr}_{0.50}\text{Ti}_{0.50}\text{S}$ and $\text{Sr}_{0.25}\text{Ti}_{0.75}\text{S}$.

The energy band gap E_g exists in minority spin channel has the direct nature, in which the valence band maxima (MVB) and the conduction band minima (MCB) occur at Γ point. Recalling that the occurrence of the half-metallic G_{HM} gap is a remarkable feature of the investigated DMS compounds. The estimations of minority spin channel E_g (eV) and G_{HM} (eV) for $\text{Sr}_{1-x}\text{Ti}_x\text{S}$ are listed in Table 2.

Table 2
Calculated band gap E_g (eV) and half-metallic band gap G_{HM} (eV) for $\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$ compound.

Compound	E_g (eV)	G_{HM} (eV)
$\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$	1.892	0.215
$\text{Sr}_{0.50}\text{Ti}_{0.50}\text{S}$	-	-
$\text{Sr}_{0.25}\text{Ti}_{0.75}\text{S}$	-	-

We may deduce from this table that only the $\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$ compound is capable of generating completely spin-polarized current owing to feasible excitation and is thus responsible for improving the efficiency of spin-based devices.

The plots of spin-polarized total (TDOS) and partial (PDOS) densities of states for the $\text{Sr}_{0.75}\text{Ti}_{0.25}\text{S}$, $\text{Sr}_{0.50}\text{Ti}_{0.50}\text{S}$, and $\text{Sr}_{0.25}\text{Ti}_{0.75}\text{S}$ ferromagnetic compounds are displayed in Fig.2.

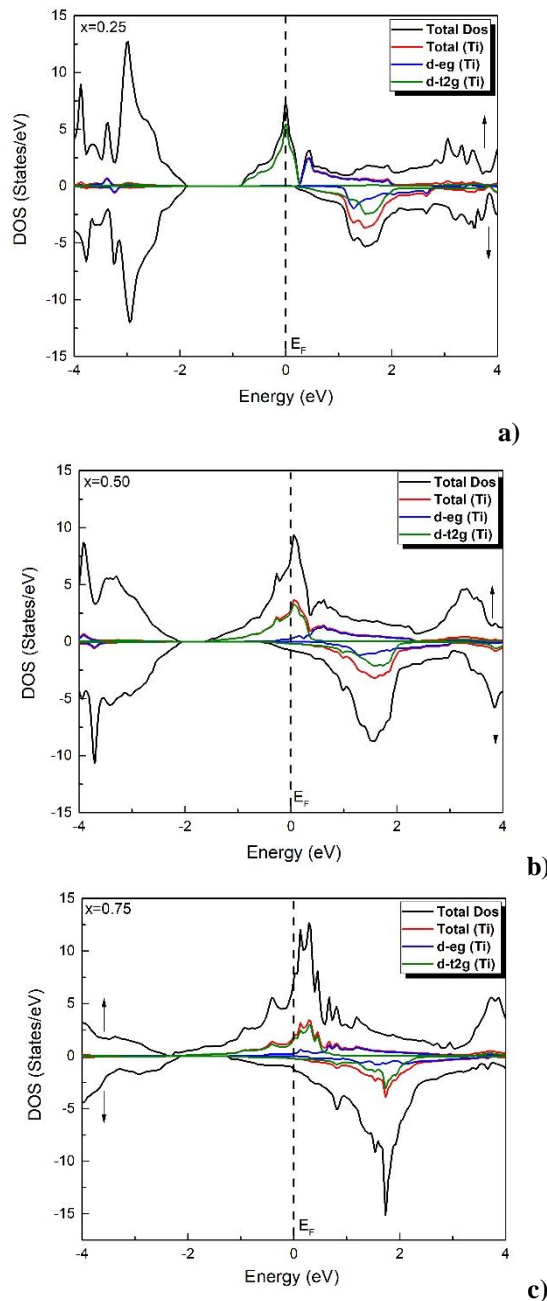


Fig. 2 Total and partial densities of states of $Sr_{1-x}Ti_xS$ at a) $x=0.25$, b) $x=0.50$, and c) $x=0.75$

For the $Sr_{0.75}Ti_{0.25}S$, the observed total and partial densities of states (DOS) reveal the half-metallic behavior, which is produced by metallic majority spin and semiconducting minority spin, culminating in 100% spin polarization at Fermi level. Both $Sr_{0.50}Ti_{0.50}S$ and $Sr_{0.25}Ti_{0.75}S$ have a metallic character due to the existence of 3d-Ti and 3p-S states at the Fermi level E_F . The findings of the band structures are confirmed by these studies.

The e_g states have a greater energy than the t_{2g} states, indicating that the Ti ions are located in an octahedral environment.

3.3 Magnetic properties

The computed values of total and local magnetic moments per Ti atom for $Sr_{1-x}Ti_xS$ ($x=0.25, 0.50$, and 0.75) are collected in Table 3.

Table 3
Computed total and local magnetic moments (μ_B) per Ti atom for $Sr_{1-x}Ti_xS$ ($x=0.25, 0.50$, and 0.75)

Compound	Total	Sr	S	Ti
$Sr_{0.75}Ti_{0.25}S$	2	0.006	-0.012	1.583
$Sr_{0.50}Ti_{0.50}S$	1.93	0.019	-0.005	1.527
$Sr_{0.25}Ti_{0.75}S$	1.87	0.050	0.042	1.455

The p-d hybridization (between 3d-Ti and p-S) creates the overall magnetic momentum of (Ti) atoms. A small locally-based magnetic moment was previously produced on the site Sr and the chalcogenide element S. A typical behavior of half-metallic ferromagnetism is the integral value of $2 \mu_B$ on $Sr_{0.75}Ti_{0.25}S$. The positive and negative signs of the local magnetic moment values demonstrate the ferromagnetic and the antiferromagnetic interaction between Sr-Ti and S-Ti, respectively.

IV. CONCLUSION

In this paper, we have studied the structural, electronic and magnetic properties of $Sr_{1-x}Ti_xS$ compound at $x=0.25, 0.50$ and 0.75 concentrations by means of first principles calculations. Our calculated electronic structures predict the half metallicity with direct band gap for the Ti doped SrS at $x=0.25$. We expect the metallic nature for both concentrations $x=0.50$ and 0.75 . We have found that the ferromagnetism is stabilized by the p-d hybridization. The negative sign in local magnetic moment of S atoms demonstrates that induced magnetic polarizations of S atoms are anti parallel to Ti atom. As a result of these findings, the $Sr_{0.75}Ti_{0.25}S$ is the ideal material for spintronic applications.

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