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# FIRST-PRINCIPLES CALCULATION TO INVESTIGATE STRUCTURAL, ELASTIC, ELECTRONIC AND MAGNETIC PROPERTIES OF $Sr_{0.75}Mn_{0.25}X$ (X = S, Se and Te) COMPOUNDS

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**Abstract**

We used the full-potential linearized augmented plane-wave method within the density functional theory framework to investigate the structural, elastic, electronic and magnetic properties of the rock-salt (B1) Sr0.75Mn0.25X (X = S, Se and Te). The Wu-Cohen generalized gradient approximation (WC-GGA) was used to describe the exchange-correlation potential. To get appropriate results about the electronic properties of Sr0.75Mn0.25X (X = S, Se and Te) alloys, the Tran-Blaha modified Becke-Johnson (TB-mBJ) potentials were also used. The experimental, theoretical results and our optimized equilibrium structural parameters are in good accord. Our elastic constants Cij were used to calculate the bulk modulus B, shear modulus S, Young's modulus Y, Poisson's modulus v, Pugh's ratio, acoustic velocities, and Debye temperature. It is confirmed that these compounds have brittleness and mechanical stable. Electronic properties like the spin polarized band structure and electronic density of state, and charge density were carefully examined. The calculated band structures reveal that the analyzed materials are semiconductors ferromagnetic behavior. Moreover, a study of the magnetic properties of Sr 0.75Mn 0.25X (X = S, Se and Te) compounds indicates that the value of the total magnetic moment for each compound is approximately 5μB.

**Keywords**: DFT, Elastic Properties; Electronic Properties. Magnetic Properties, Spintronics.

## 1.Introduction

The alkaline-earth chalcogenides are a class of compounds having the formula AX, where A is a group II element (Be, Mg, Ca, or Sr) and X is a group VI element (O, S, Se, or Te). They are important semiconductors because of their important properties such as high band gaps and valence-band widths. **[1]** At room temperature, these semiconductors crystallize in rock-salt NaCl type (B1) crystals, forming closed-shell ionic systems.

The semiconductors SrY (Y = S, Se, and Te) strontium chalcogenides have been widely investigated in many instrument fabrications. because of its major technological uses in

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sectors such as microelectronics, catalysis, luminous devices, rapid high resolution optically stimulated luminescence imaging **[2,4]**

To incorporate ferromagnetism in nonmagnetic semiconductors, a small fraction of TM elements is doped in the intrinsic host semiconductor **[5-10]**. As a result, ordinary semiconductors doped with a proportion of magnetic element, called to as DMS, in which magnetic ion arrangement monitors energy band gap and other important physical properties **[11–14]**. Because of the utilization of both electron charge and spin,

Because of their higher Curie temperatures and half-metallic ferromagnetic (HMF) behavior, diluted magnetic semiconductors (DMSs) are of particular interest in spintronics devices. **[15]** They show the stability of ferromagnetism at temperatures higher than room temperature. **[16,17]** The HMF character is regarded as an important source of spin injection carriers for spintronics; however, the electronic structure of DMS combines both metallic and semiconductor characteristics, exhibiting a metallic nature in one spin channel and a band gap at the Fermi level in the opposite spin direction and thus exhibiting an HMF feature.

In the last few years, Many magnetic semiconductors, such as Mn doped ZnS [**18]**, Mn doped CdTe **[19],** Be1−xMnxSe and $Be_{1-x}Mn_xTe$ [20], Zn1-x MnxY(Y= S, Se, Te) **[21],** $Ge_{0.94}Mn_{0.06}Te$ **[22],** and Mg1−xMnxTe **[23],** have been investigated in the context of Mn based DMSs and show that manganese (Mn) contributes Strontium sulfide (SrS), a very significant binary semiconductor belonging to the II-IV group, has been investigated theoretically **[23-28]** as well as experimentally **[29,30].**

To the best of our knowledge, Mn doped SrS, SrSe, and SrTe have not yet been comprehensively theoretically and experimentally investigated. As a result, these characterizations are important not just for filling the data gap for these alloys, but also for understanding their essential properties.

In this article, We have contributed to the study of the structural, elastic, electronic, and magnetic properties of Sr1-xMnxX (X = S, Se, and Te) x = 0.25 in the rock-salt phase, using first-principles calculations of density functional theory based Wein2K code within the full-potential linearized augmented plane-wave method (FP-LAPW) with generalized gradient approximation functional was used in the calculations of the structural and elastic properties whereas The modified Becke-Johnson potential(TB-mBJ) was used to determine the electronic and magnetic properties .

## 2. COMPUTATIONAL METHODS

The first-principles simulation is carried out by employing the full-potential linearized augmented plane-wave (FP-LAPW) approach based on density functional theory (DFT) for the calculation of the Kohn–Sham equations **[31,32],** as implemented in the WIEN2k code **[33],** which is based on density functional theory [**34-35].** The main advantages of this approach are the ease with which forces and stresses can be computed; good convergence control with respect to all computational parameters used; favorable scaling with the number of atoms in the system; and the ability to make simpler calculations by

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ignoring core electrons. The structural and elastic properties were estimated using the generalized gradient approximation (WC-GGA) [36] to simulate the correlation and exchange effects of electrons, while the electronic and magnetic properties were calculated using the modified Becke-Johnson potential (TB-mBJ) [**37]**.

To obtain a good convergence, the fundamental functions were enlarged up to RMT * KM = 8, where RMT is the lowest muffin-tin radius and KM is the highest value of the k vector utilized for plane-wave expansion. Similarly, the highest value of the $l_{max}$ = 12 was utilized inside the atomic sphere, whereas the Fourier expansion vector of charge density was fixed at Gmax = 14. When the total energy of the system is stabilized within $10^{-4}$ Ry, the self-consistent convergence conditions of total energy calculations are met. The approach was utilized to integrate across the Brillioun zone by using a dense k-points mesh of 11*11*11 for the cubic structures. The simulated unit cell was optimized for total energy as a function of volume, and the system's ground state was assured to be at zero strain.

## 3. RESULTS AND DISCUSSION

### 3.1. Structural parameters

We assumed in our studies that SrX (X= S, Se, and Te) semiconductors had a rock-salt (B1) structure with a space group of 225 Fm-3m. To get the ground-state values, the total energy was computed with respect to volume, and the atomic positions were relaxed for each volume using the Wien2k packages to minimize both the force.

The equilibrium optimization structural parameters have been computed [**38**] by fitting the results of the total energies as function of volume by the empirical equation of states the Birch-Murnaghan. The lattice constants, the bulk moduli and the first pressure derivative along with the theoretical results where available **[39-41],** and the results are summarized in Table 1.

**Table 1: Lattice parameter (*a*), bulk modulus (*B*), and its pressure derivative (*B'*) for SrS, SrSe, SrTe and Sr0.75Mn0.25X (X = S, Se and Te) semiconductor and other available theoretical and experimental results**

| Compound | a (A) | B (GPa) | B' |
|---|---|---|---|
| SrS | 6.043, 6.05**a**, 5.988**b**, 6.024**c** | 47.184 52.83, 58**c** | 4.109 4.34 |
| SrSe | 6.204, 6.29**a**, 6.204**b**, 6.234**d** | 43.23, 45**d** | 4.22, 4.5**d** |
| SrTe | 6.624, 6.71**a**, 6.621**b**, 6.659**e** | 34.77, 39.5**e** | 4.40, 5**e** |
| Sr0.75Mn0.25S | 5.881<br>5.895**f** | 49.553<br>51.258f | 3.933<br>4.219f |
| Sr0.75Mn0.25Se | 6.072<br>- | 36.892<br>- | 3.254<br>- |
| Sr0.75Mn0.25Te | 6.551<br>**-** | 33.622<br>**-** | 4.031<br>**-** |

**a** Ref.42 **b** Ref.43 **c** Ref.39 **d** Ref.40 **e** Ref.41 **f**Ref.44

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Table 1 shows that the computed lattice parameter (*a*) using the WC-GGA approximation, which are 5.881, 6.072 and 6.551, for Sr0.75Mn0.25S, Sr0.75Mn0.25S, and Sr0.75Mn0.25S, respectively, vary with the atomic size of the chalcogen involved in the compound. The calculated equilibrium lattice constant of binary semiconductors SrY (Y= S, Se and Te) are very close to theoretical calculations with the same GGA-WC and our results are in good agreement with the available theoretical results

The lattice parameters of Sr0.75Mn0.25X (X = S, Se and Te) systems are smaller than that of binary compounds because the ionic radius of Mn atom may be a smaller than that of Sr. As consequence, the bulk modules of Sr0.75Mn0.25X (X = S, Se and Te) are higher than that of SrY (Y = S, Se and Te) lower one, and hence the SrY (Y = S, Se and Te) are easily compressible compared to the Sr0.75Mn0.25X (X = S, Se and Te) alloys.

The a(Å) and B (GPa) of studied compounds Sr0.75Mn0.25S, Sr0.75Mn0.25Se and Sr0.75Mn0.25Te increases by the replacement of S with Se and Te because of greater atomic size of Te, Se than S. Therefore, the system becomes less compact and more ordered with increasing lattice constant and decreasing the bulk modulus (*B*).

### 3.2. Elastic properties

In this section, the elastic constants are important quantities to describe the mechanical properties of materials.  explain how a crystal response to external stresses. They are used to obtain the elastic modules, especially: the bulk modulus, the shear modulus, the Young modulus, the Poisson ratio, the acoustic wave velocity, the Debye temperature,

In accordance with the cubic crystal structure symmetry, the elastic tensor contains only three independent elastic constants (C11, C12, C44) are required. The elastic constants of the compounds under consideration were computed using the WIEN2k package **[33].** To estimate these three elastic constants, three different selected deformations are applied to the lattice parameter of the cubic unit cell to compute the corresponding total energy changes. These constants are studied with the same parameters used in the study of structural and electronic properties (radius $R_{MT}$, angular momentum lmax, cut-off radius $R_{MT}$Kmax and total energy, number of points in the Brillouin zone, etc.) with the WC-GGA approximation.

The computed WC-GGA elastic constants Cij for Sr0.75Mn0.25X (X = S, Se and Te) are presented in Table 2. Mechanical stability of a cubic crystals requires that its independent elastic constants should obey the following Born's stability criteria **[45–47]:**

$$C11>, C12 > 0, C44 > 0, C11 + 2C12 > 0, C11 > B > C12$$

**Table 2: Calculated elastic constants (Cij, in GPa) of the Sr0.75Mn0.25X (X = S, Se and Te) compound in cubic (RS structure) at ambient pressure by using WC- GGA approximation**

| Cij (GPa) | Sr0.75Mn0.25S | Sr0.75Mn0.25Se | Sr0.75Mn0.25Te |
|---|---|---|---|
| C11 | 160.7842 | 100.5517 | 71.6523 |
| C12 | 20.0632 | 20.9449 | 12.8675 |
| C44 | 28.7555 | 23.323 | 16.3608 |

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From Table 2, the Born criteria for elastic stability are clearly satisfied, indicating that cubic Sr0.75Mn0.25X (X = S, Se and Te) compound phases of interest are mechanically stable.

The estimated elastic constants are observed to decrease progressively from Sr0.75Mn0.25S to Sr0.75Mn0.25Te. It is worth mentioning that no experimental or theoretical data for the elastic constants of Sr0.75Mn0.25X (X = S, Se and Te) compounds are currently available in the literature; hence, our results serve as the first prediction of these characteristics for future reference.

From the calculations of the elastic constants, one can determine the parameters Bulk moduli (B), Shear moduli (S), Young moduli (Y), the anisotropic ratio (A), Poisson's ratio (r), as well as compressibility (b) of the Sr0.75Mn0.25X (X = S, Se and Te) (Table 3).

For this purpose, we utilize the Voigt-Reuss-Hill (VRH) approximation **[48-50]** for evaluate the polycrystalline bulk and shear moduli. In this approach, two main approximations: the Voigt (V) approximation [**49]**, uniform strain is assumed in the structure, whereas the Reuss (R) approximation **[50]** assumes a uniform distribution of the strain corresponding to the external strain. In turn, in Reuss's model the bulk and shear modules (BR and GR) are calculated. The following Hill expressions, in terms of the arithmetic mean, for Bulk and Shear's moduli are used to calculate the effective moduli findings for isotropic polycrystalline materials:

$$B_H = 1/2\,(B_v + B_R) \text{ and } S_H = 1/2\,(S_v + S_R)$$

where the averaged compressibility is given by: β=1/B.

For this system, the Hill Bulk modulus (BH) and Hill shear modulus (SH), which are related to the elastic constants, are given by respectively,

$$B_H = \frac{1}{3}(C_{11} + 2C_{12})$$

$$S_H = \frac{S_v + S_R}{2}$$

where $S_v = \frac{C_{11} - C_{12} + 3C_{44}}{5}$ is the Voigt shear modulus and $S_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$ is termed as the Reuss shear modulus?

To determine the Young's modulus (Y) and Poisson's ratio (υ), the following equations are used, respectively

$$Y = \frac{9BS_H}{3B + S_H}$$

$$\sigma = \frac{3B - 2S_H}{2(3B + S_H)}$$

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**Table 3: Calculated bulk (BV, BR, and BH) and shear moduli (SV, SR, and SH) in Voigt, Reuss and Voigt-Reuss-Hill approximations (in GPa), Young modulus (Y, in GPa), Poisson 's ratio (υ), B/SH ratio, for the Sr0.75Mn0.25X (X = S, Se and Te) compound**

| | Sr0.75Mn0.25S | Sr0.75Mn0.25Se | Sr0.75Mn0.25Te |
|---|---|---|---|
| BV | 66.970 | 47.480 | 32.462 |
| BR | 66.970 | 47.480 | 32.462 |
| BH | 66.970 | 47.480 | 32.462 |
| SV | 45.397 | 29.915 | 21.572 |
| SR | 37.663 | 27.953 | 19.887 |
| SH | 41.530 | 28.934 | 20.729 |
| YV | 111.089 | 74.168 | 52.980 |
| YR | 95.151 | 70.101 | 49.543 |
| YH | 51.273 | 72.146 | 51.273 |
| υ V | .223 | .239 | .227 |
| υ R | .263 | .253 | .245 |
| υ H | .243 | . 246 | . 236 |
| B/SH | 1.61 | 1.64 | 1.56 |

Table 3 shows our estimated bulk, Young's, and shear moduli for Sr0.75Mn0.25X (X = S, Se and Te). It is found that the bulk modulus B decreases when going from Sr0.75Mn0.25S to Sr0.75Mn0.25Se to Sr0.75Mn0.25Te, which is consistent with the fact that B is inversely proportional with the volume (V) of the unit cell (B ~ 1/ V) **[51],** B value decreases with increasing volume of the unit cell. As presented in Table 3,

In our case, the Young's moduli were found Sr0.75Mn0.25S is stiffer than Sr0.75Mn0.25Se and Sr0.75Mn0.25Te

According to Pugh **[52],** A high B/SH value indicates ductility, whereas a low B/SH value indicates brittleness. 1.75 has been found as the key number that distinguishes the two behaviors. The results listed in Table 3 shows that the Sr0.75Mn0.25X (X = S, Se and Te) alloys have B/SH ratios lower than the critical value of 1.75, which classifies this composition as brittle materials

We also used the Poisson's ratio rule of Frantsevich et al. **[53]** to determine if the composition were ductile or brittle. This rule states that if the Poisson's ratio (υ) is less than0.26, the compound is brittle; otherwise, the material is ductile. As listed in Table 3, all the calculated Poisson's ratios (υ) are less than 0.26, indicating that the compounds Sr0.75Mn0.25X (X = S, Se and Te) are brittle in nature. These results exactly agree with the results of the B/SH ratio values.

Parameter elastic Poison's ratio is used to get information about the properties of bonding forces. Poisson's ratios (υ) for covalent materials are very small (υ ̰0.1), but average values of υ for ionic materials are around 0.25 **[54]**. In our situation, the values of υ for all three compounds investigated, as shown in Table 3, are more than 0.25. As a result, we may estimate that ionic bonds contribute considerably to the overall interatomic interactions in these cubic crystals. Moreover, the average bulk-shear modulus ratios for covalent and ionic materials are 1.1 and 0.6, respectively **[55].** In our situation, the ratio'is

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almost equal to 0.61, indicating that the interatomic bonding in all three alloys is mostly ionic in character.

Debye temperature ($\Theta_D$), an essential parameter, is strongly correlated with a variety of physical properties such as elastic constants, melting temperature, specific heat, and so on. Furthermore, thermal loss processes, often known as a material's temperature dependency, are appropriately described in terms of $\Theta_D$. One typical method for calculating the Debye temperature is to utilize elastic constant values, because $\Theta_D$ is predicted from vm using the following equation **[56].**

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3} v_m$$

where h is Plank's constant, $k_B$ is Boltzmann's constant, $N_A$ is Avogadro's number, n is the number of atoms per formula unit, ρ is the density, M is the molecular weight and vm is average sound velocity. The average sound velocity is average sound velocity $u_m$ can be calculated as follows **[57]:**

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\right]^{-1/3}$$

where $u_l$is the longitudinal velocity and $u_t$ is the transverse sound velocity, which are obtained from Navier's equation [**58]:**

$$v_l = \left(\frac{B+\frac{4S}{3}}{\rho}\right)^{1/2} \text{ and } v_t = \left(\frac{S}{\rho}\right)^{1/2}$$

where ρ is the mass density per unit volume.

Using the computed results of the elastic constants in Table 2, we estimated ut, ul, um, $\Theta_D$, and density for Sr0.75Mn0.25X(X = S, Se and Te), as shown in Table 4. It is worth noting that the sound velocities are mostly affected by the elastic moduli (Bulk modulus (B) and shear modulus (S)) of a material. This indicates that if a material has a high elastic modulus, it will have a high sound velocity. To the best of our knowledge, no measurable data is available in the literature for comparison.

In general, a higher Debye temperature $\Theta_D$ indicates a higher thermal conductivity. As listed in Table 4, the highest $\Theta_D$ value for Sr0.75Mn0.25S is 374.445K, while the lowest is attributed to Sr0.75Mn0.25Te (207.412K). Sr0.75Mn0.25S has the highest thermal conductivity among the materials tested, according to our findings. The decrease of the elastic constants Cij from Sr0.75Mn0.25S to Sr0.75Mn0.25Te can be explained by the decrease of ΘD from Sr0.75Mn0.25S to Sr0.75Mn0.25Te. It should also be observed that the hardness and ΘD demonstrate similar patterns for this material series. Because of the scarcity of previous experimental data and theoretical conclusions, our results can be

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used as a reference for future research. From Table 4, it can be further seen that the results of the longitudinal sound velocity ul are much higher than that of the transversal sound velocity ut for each alloy.

**Table 4: The calculated values of density (ρ in g/cm3), the sound velocity of transverse ut , longitudinal ul, and average sound elastic wave velocities um, Debye Temperature ((ϴD) in K) of Sr0.75Mn0.25X(X = S, Se and Te) compound**

| | Sr0.75Mn0.25S | Sr0.75Mn0.25Se | Sr0.75Mn0.25Te |
|---|---|---|---|
| ρ(g/cm3) | 3.9336 | 4.6986 | 4.8908 |
| | - | - | - |
| υl (m/s) | 5576.93 | 4279.7 | 3505.48 |
| | - | - | - |
| υt (m/s) | 3249.27 | 2481.53 | 2058.72 |
| | - | - | - |
| υm(m/s) | 3604.39 | 2753.93 | 2282.07 |
| | - | - | - |
| ϴD(K) | 374.445 | 270.034 | 207.412 |
| | - | - | - |

## 4. ELECTRONICS PROPERTIES

To determine the nature of the materials $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te), the electronic band structure, total density of states (TDOS), and partial density of states (PDOS) were utilized. The electronic band structures of ferromagnetic $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) compounds along high symmetry directions of the first Brillouin zone, each for spin-up and for spin-down are plotted in **Fig. 5**, respectively. We used TB-mBJ potential for calculating their electronic properties.

The result of band structure indicates that the spin polarized band structures investigation for these compounds show a semiconducting nature in spin up and down. For further clarification, we can see that in the case of the majority spin states, the upper valence bands are closer to Fermi level than the minimum of the conduction bands, which is moving toward higher energies, whereas the minority spin states show a semiconducting nature in spin up and down channels. At this point, it is evident from these plots that the spin down states exhibit direct band gaps at high symmetry points for the specified alloys since the top of the valence bands and the minimum of the conduction bands are both positioned at the gamma (Γ) point of the Brillouin zone. But for spin up channels of all the compounds studied show an energy gap around the Fermi level. The top of the valence band (VB) is positioned at the Γ point, while the bottom of the conduction band (CB) is located at the point, suggesting that these compounds indicate semiconductor nature behavior with an indirect band gap (Γ-M). Table 5 shows the estimated indirect (Γ-M) band gap values,

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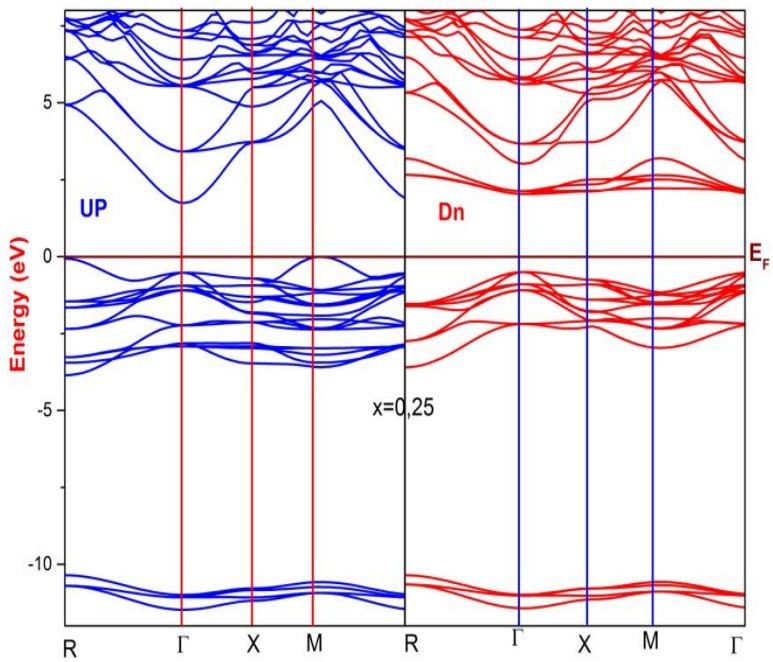
**Table 5: The computed results of energy band gaps Eg [Γ- M] (eV) in $Sr_{0.75}Mn_{0.25}X$(X=S, Se, and Te) alloys calculated using the (TB-mBJ) approximation**

| Compound | Eg (eV) |
|---|---|
| $Sr_{0.75}Mn_{0.25}S$ | 1.74 |
| | - |
| $Sr_{0.75}Mn_{0.25}Se$ | 1.1 |
| | - |
| $Sr_{0.75}Mn_{0.25}Te$ | 0.31 |
| | - |

Table 5 shows that for all three materials, the fundamental indirect band gap values increase with decreasing chalcogen atomic number, with the order of the band gaps is Eg($Sr_{0.75}Mn_{0.25}XS$) >Eg($Sr_{0.75}Mn_{0.25}Se$) > Eg($Sr_{0.75}Mn_{0.25}Te$).




**$Sr_{0.75}Mn_{0.25}S$**

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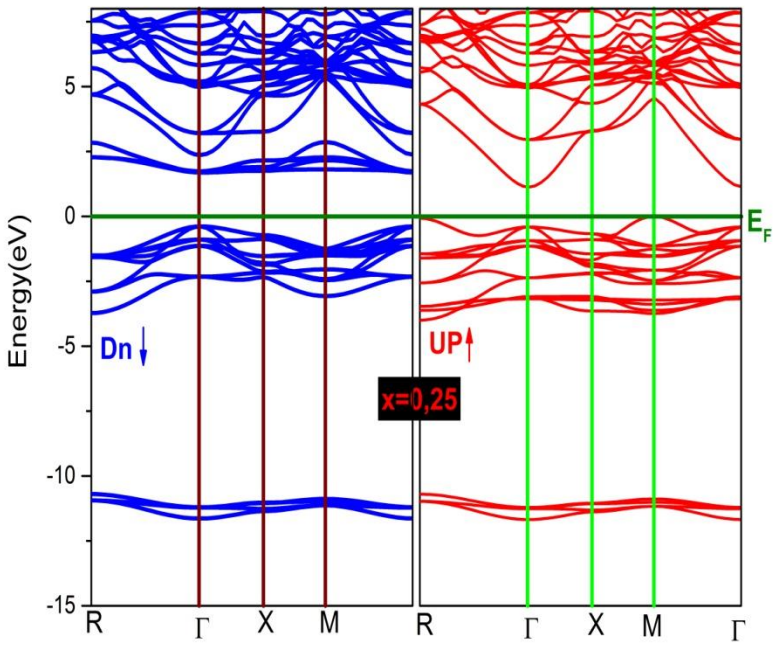
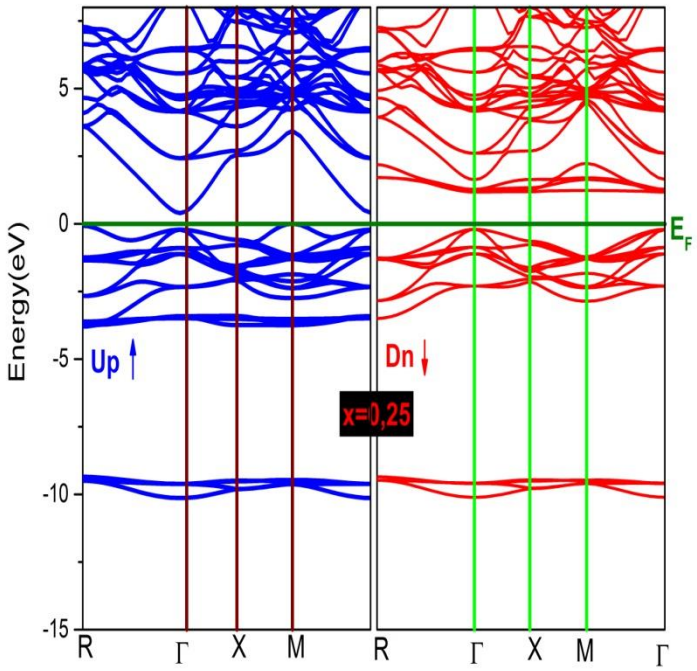



**$Sr_{0.75}Mn_{0.25}Se$**




**$Sr_{0.75}Mn_{0.25}Te$**

**Fig 5: Spin polarized electronic band structure of majority spin (up) and minority spin(down) for $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) compounds calculated using the (TB-mBJ) approximation**

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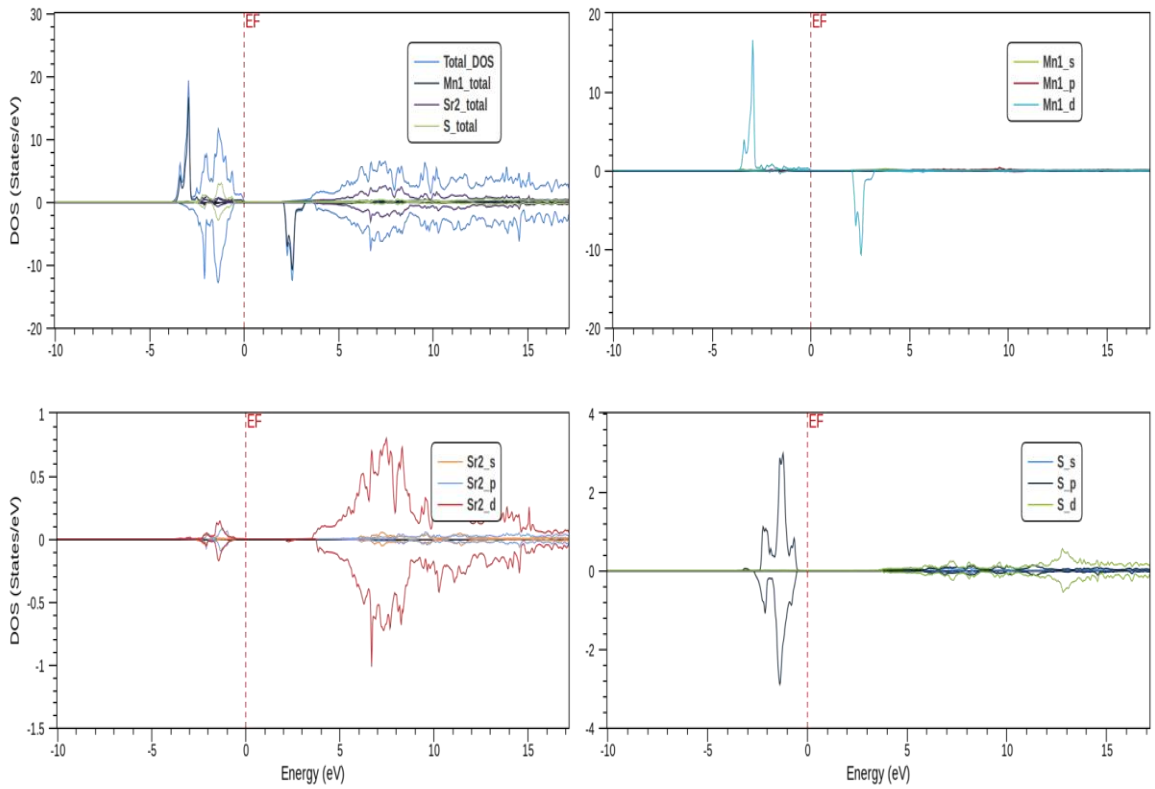
Figure 6 shows the (TDOS) and (PDOS) of Sr0.75Mn0.25X (X=S, Se, and Te) using the TB-mBJ potential. The total and partial DOS of spin up and down states for all systems are semiconductors in nature due to the the negative p_d exchange interaction between X-3p and Mn-3d there is some states are raised to the Fermi level (EF) in the case of the majority spin. The majority-spin states are s, The highest and lowest parts of the valence and conduction band respectively, are constructed by 3d orbitals of Mn atoms with a small participate of 3p (V) and 5s(Sr) states for all compounds, unlike the minority-spin states, it can see that the densities of states disappeared at Fermi level, consequently it mirrors the semiconductor attributes.



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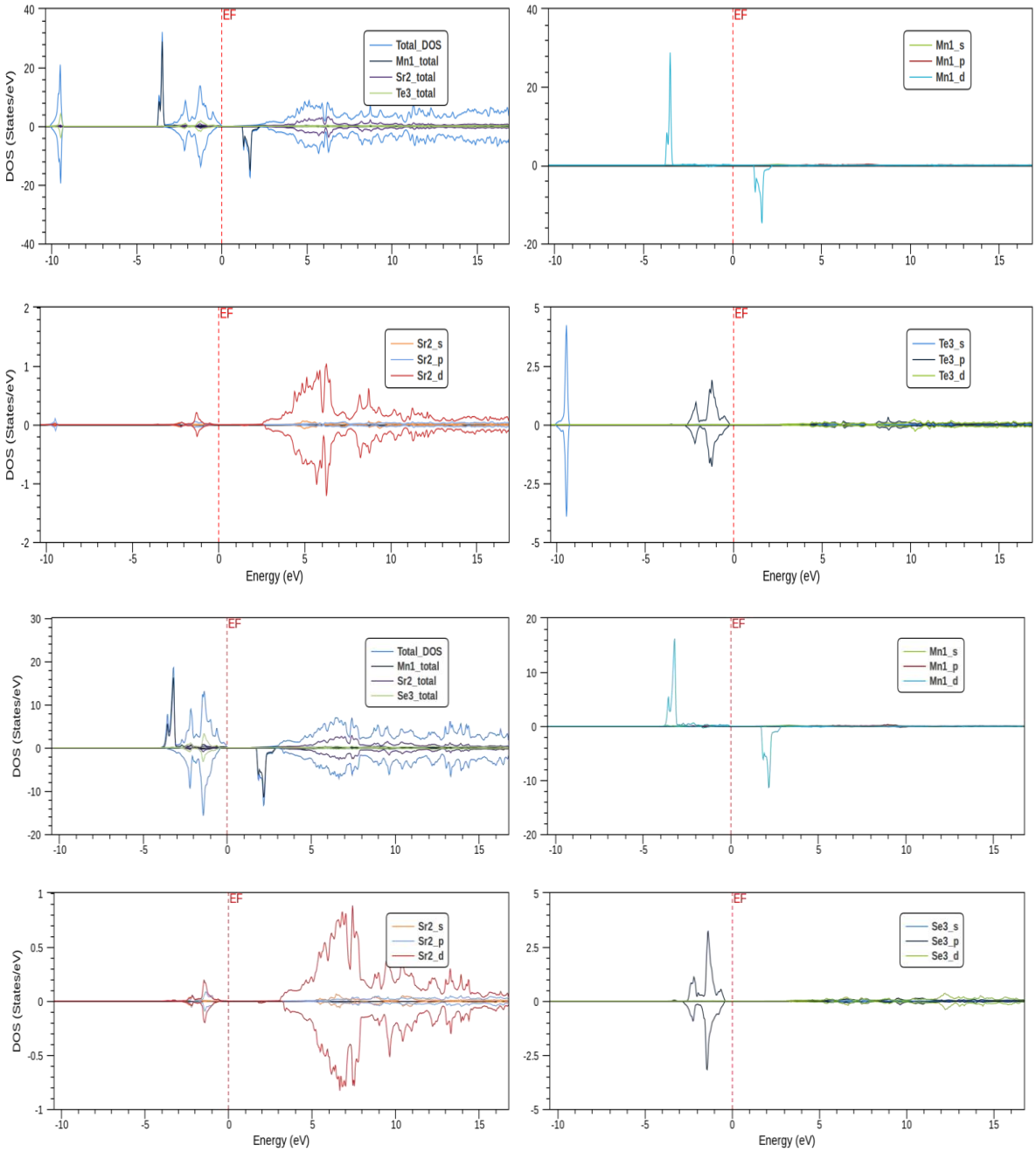


**Fig 7: Spin polarized total and partial densities of states of spin up and minority spin down for $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) calculated using (TB-mBJ) approximation**

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## 5. MAGNETIC PROPERTIES

In this section of the work, Magnetic moments can also be used to investigate the magnetic characteristics of the alloys under investigation. The computed total and local MMs within the muffin-tin spheres of the relevant atoms and at the interstitial sites for $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) compounds are listed in Table 3.

The Pauli Exclusion Principle shows how electrons with the same spin in 3d states contribute to the magnetic moment. As a result, the 3d electron of Mn possesses two unpaired electrons, which contribute to the total magnetic moment 5B. The p-d hybridization of S/Se (p-states) and Mn (d-states) decreases the magnetic magnet from the Mn side and induces it to the nonmagnetic sites Sr and S/Se Te. Furthermore, as shown in the electronic version of the paper, the integer value of TM verifies 100 percent spin polarization.

**Table 6: Total magnetic moment (Mtot in μB) per Mn doping and local magnetic moments $M_{Mn/Sr/x}$ for $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) obtained using (TB-mBJ) approximation**

| Compound | $Sr_{0.75}Mn_{0.25}S$ | $Sr_{0.75}Mn_{0.25}Se$ | $Sr_{0.75}Mn_{0.25}Te$ |
|---|---|---|---|
| Mtot | 5.00008 | 5.00008 | 5.00010 |
| MMn | 4.67815 | 4.65452 | 4.62612 |
| MSr | 0.00006 | 0.00063 | 0.00114 |
| MX | 0.04427 | 0.04218 | 0.03342 |

## 6. CONCLUSION

In summary, we studied the structural, elastic, electronic and magnetic characteristics of rock-salt (B1) $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) utilizing first principle calculations within density functional theory (DFT) employing the full potential linearized augmented plane wave (FP-LAPW) within the TB-mBJ approximations. For our result of structural properties, it can be said that the ground-state properties, including lattice parameters, bulk moduli, and their pressure derivatives. Our results are very compatible with the current experimental results. In addition, the increase of the lattice parameters a is accompanied by a decrease in compressibility B with an increase in the atomic number of the chalcogen element going from S to Se to Te atom.

The elastic constants calculated for the investigated compounds using the total energy-strain method obey the stability criteria. These compounds are classified as brittle materials by the calculated 'ratios and Poisson's ratios, and their brittle decreases in the following order. Sr0.75Mn0.25S→ Sr0.75Mn0.25Se and Sr0.75Mn0.25Te the calculated Vickers hardness and Debye temperature also show the same trend.

The electronic properties were investigated utilizing the TB-mBJ potentials. All of the potentials employed indicate that these materials are indirect band gap semiconductors (Γ-M) for spin up and direct band gap of spin down. The predicted band gaps for $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) level are 1.74eV, 1.1 eV, and 0.31 eV respectively, which are predicted to be more similar to the ones seen When X in the Sr0.75Mn0.25X series

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is changed from S to Te, the band gaps decrease, as seen by the calculated Poisson's ratios, 'ratios, and band structures. According to the analysis of magnetic properties for Sr0.75Mn0.25S, Sr0.50Mn0.50Se and Sr0.25Mn0.75Te show a semiconducting ferromagnetic behavior, the investigated alloys' magnetism is attributable to Mn-3d states, in which the ferromagnetic semiconductor character of these alloys is harmonic with total magnetic moments ($M_{tot}$ = 5μB). These observations will aid in the development of relevant theoretical guidance for the use of $Sr_{0.75}Mn_{0.25}X$ (X=S, Se, and Te) in semiconductor spintronics.

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