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Study of the electronic, magnetic, and thermoelectric aspects of spinel chalcogenides SrCe_2Z_4 ($\text{Z} = \text{Te, Se, S}$) for spintronic and energy applications

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Spinel chalcogenides are promising candidates for the advancement of spintronic and thermoelectric devices. Therefore, this article presents the structural, electronic, and magnetic characteristics of SrCe_2Z_4 ($\text{Z} = \text{S, Se, Te}$) spinels employing WIEN2k in the context of density functional theory. The expansion of the unit cell is witnessed with the incorporation of larger anions and lattice parameters, including 12.01 Å for SrCe_2S_4 , 12.52 Å for SrCe_2Se_4 , and 13.42 Å for SrCe_2Te_4 . The maximum release of energy in the FM states (rather than AFM states) and the negative enthalpy of formation (−2.20 eV, −2.05 eV, and −1.94 eV) confirm their dominant ferromagnetic nature and the thermodynamic stability of the system. The spin-polarized band structure exhibits the ferromagnetic semiconducting nature of SrCe_2S_4 and SrCe_2Te_4 , as well as the half-metallic ferromagnetic behavior of SrCe_2Se_4 . The analysis of the total density of states also endorses the exact nature predicted during the band structure investigation. The magnetic properties are explored by calculating the direct exchange energy $\Delta_x(f)$, indirect exchange energy $\Delta_x(pf)$, along with the exchange constants $N_o\alpha$ and $N_o\beta$ to analyze the magnetic behavior. The significant hybridization of chalcogenide's 2p states and the f states from the Ce atom located at the Fermi level results in the total magnetic moments. All these compositions reveal that the Curie temperature is near or above room temperature. The thermoelectric characteristics of the spinels are examined utilizing the BoltzTrap code to inspect the parameters including power factors and the figure of merit as a function of temperature. The *ZT* value of 0.90 for SrCe_2Te_4 indicates its higher thermoelectric efficiency and potential for future thermoelectric devices.

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1. Introduction

The high energy consumption, low processing speed, and large size of traditional electronic devices make them outdated, emphasizing the need for novel nanoscale chips that are more effective, faster, and more appropriate for cutting-edge

technologies.¹ Nowadays, spintronics is one of the emerging fields that uses both the spin and charge of electrons, offering significant potential for next-generation electronic devices.² Electrons exist in two spin channels, *i.e.*, spin-up ($S\uparrow$) and spin-down ($S\downarrow$).³ Understanding spintronics is essential to harness the full potential of electron spin to revolutionize the electronics industry, as it enables a wide range of innovative applications in data processing and storage.² The identification of giant magnetoresistance (GMR) in 1988 illustrated that under an applied magnetic field, the resistance of a thin magnetic layer significantly changes and can improve the performance of data storage devices. This internal response of electron spin has led to the development of memory devices that offer both rapid access and non-volatility.⁴ High spin-polarization is a key to improving the quality, faster data processing, and data storage aptitude of spintronics devices.^{5,6} Ferromagnetic (FM) semiconductor materials have the highest spin polarization because of the different semiconducting and insulation properties in the spin majority ($S\uparrow$) and spin minority ($S\downarrow$) orientations.⁷ For

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potential spintronic devices, the Curie temperature (T_c) must be higher than RT.^{8,9} GMR applications mostly involve spin filtering,¹⁰ including spin valves and magnetic field sensors used to form hard disks.¹¹ Double perovskites, Heusler alloys, and spinels have potential applications in spintronics, but the FM spinels, which have anions from chalcogens, have gained special interest for the newly discovered spintronic applications.¹²

In spintronics, spinel chalcogenides are recognized for their unique structural, electrical, magnetic, and transport characteristics. The empirical formula of spinel is AB_2X_4 , in which A and B are cations, and X represents the anions Se, S, Te, and O.¹³ The cubic closed-packed arrangements of anions generate the octahedral and tetrahedral sites, which are filled by the cations.¹⁴ In the crystal structure of spinels, the A^{II} resides in 1/8th of the tetrahedral void, and the B^{III} resides in 1/2nd of the octahedral voids.¹⁵ To check whether the spinel structure is normal or inverse, we follow the specific rule that cations are transitional or non-transitional metals.¹⁶ Spinel chalcogenides have exceptional magnetic characteristics, including high magnetoresistance, which changes the electrical resistance in response to applied magnetic fields, making them suitable for magnetic sensing, data storage, and magnetic field modulation applications. In addition, the attractive thermoelectric (TE) properties enhance their utility for energy conversion and processing.² Spinels have high thermal and chemical stability.¹⁷ In light of existing literature, it has been observed that no research has been done on spinel composition $SrCe_2Z_4$, which has a wide spectrum of tunable properties, making it promising for advanced applications.¹⁸

The previous studies reveal that spinels with rare earth metals are considered emerging breakthroughs for spintronics devices.¹⁹ Researchers are particularly interested in spinels having rare earth metals because of their intense spin polarization, which leads to higher magnetoresistance.²⁰ High magnetoresistance is primarily used in spintronic devices like spin valves, biosensors, magnetic field sensors, and other electronic devices. Hassan *et al.* (2024) reported on the presence of half-metallic ferromagnetism (HMF) with complete spin polarization in Heusler alloys, before moving on to other materials like chalcogenides and spinels.²¹ Similarly, Alburaih *et al.* (2024) found that RE-based $MgSm_2Y_4$ (Y = S, Se) spinels exhibited HM ferromagnetism, high SP, and promising TE characteristics, with $MgSm_2S_4$ showing the highest value of ZT .²² Manjunatha *et al.* (2020) investigated the magnetic and electronic characteristics of $Co_{1-x}Sc_xCr_2O_4$ ($x = 0.0$ and 0.05) nanoparticles by DFT and experimental methods. To better understand the magnetic behavior, field-dependent magnetization and temperature-dependent susceptibility were measured in two magnetic transitions, paramagnetic, collinear ferrimagnetic, and non-collinear spiral states.²³ Maqsood *et al.* (2024) investigated Cd-based spinels $CdSm_2(S/Se)_4$ chalcogenide, and found them suitable for spintronic applications due to their promising magnetic and electrical properties. The total magnetic moment was $10.0 \mu_B$ for both compositions.²⁴ Noor *et al.* (2024) carried out DFT-based research to inspect the mechanical, electronic, and magnetic properties of $HgSm_2S_4$

and $HgSm_2Se_4$ chalcogenides for spintronic applications. Both compounds exhibited a total magnetic moment of $10.0 \mu_B$.²⁵ Kattan *et al.* (2024) investigated the HMF and transport properties of $MgCo_2(S/Se)_4$ chalcogenides for energy harvesting and spintronic implementations. Their study confirmed the half-metallic nature and robust ferromagnetic behavior of these materials, highlighting their potential for high-performance thermoelectric and spintronic devices.²⁶ In another study, Albalawi *et al.* (2023) inspected $MgEr_2(S/Se)_4$ spinels, revealing stable ferromagnetism, full SP, and showing potential in TE characteristics for energy harvesting.²⁷ The $SrCe_2Z_4$ spinels, especially $SrCe_2Te_4$, show exceptional thermoelectric efficiency and magnetic nature, positioning them as superior candidates for future thermoelectric and spintronic devices. Khushi *et al.* (2023) performed first-principles simulations on $CdHo_2Y_4$ (Y = S, Se) spinels, demonstrating their ferromagnetic behavior and suitability for energy storage.²⁸

Ramzan *et al.* (2022) confirmed HMF and favorable transport characteristics in MgV_2S/Se_4 chalcogenides, indicating their promise in thermoelectric and spintronic applications.²⁹ Bilal *et al.* (2022) explored the half-metallic ferromagnetism of spinel $MgFe_2Z_4$ (Z = S, Se) chalcogenides for spintronic implementations. Their results verified these material's half-metallic behavior and robust ferromagnetic ordering, highlighting their suitability for advanced spintronic device applications.³⁰ Alburaih (2021) examined the RE-doped spinels $CdEr_2X_4$ (X = S, Se), reporting strong ferromagnetism and efficient electronic transport for spintronic and energy harvesting applications. The study found that both materials exhibit a total magnetic moment of $5.0 \mu_B$.³¹ Based on the available data, no theoretical analysis has been carried out on the transport and ferromagnetism features of $SrCe_2Z_4$ (Z = Se, S, and Te) spinels. Thus, we theoretically investigated the electrical, magnetic, and transport properties of $SrCe_2Z_4$, where Z corresponds to Se, S, and Te, to realize their suitability for spintronic and energy harvesting device applications.

2. Computational study

The computations on $SrCe_2Z_4$ (Z = S, Se, Te) were performed utilizing the DFT-based FP-LAPW method within WIEN2k,³² which is highly recommended for computing the structural, electronic, and magnetic characteristics. The structural characteristics were calculated using the PBE-GGA approximation.³³ This approximation calculates the structural findings exactly, but underestimates the electronic band gaps and electronic state calculations on which magnetic and thermoelectric characteristics depend. Therefore, the TB-mBJ potential³⁴ was used to compute these compositions' band structure and density of states. This versatile and accurate potential consumes less computational cost and is easier to handle than the hybrid functionals HSE06 and GGA + U potentials. The basis set comprises non-overlapping atomic spheres with muffin tin radii R_{MT} and an interstitial region having a plane wave expansion with wave vector k . The R_{MT} and K_{max} products are set to be 8. The plane wave cutoff value related to the Gaussian factor (G_{max}) was set to 16 during initialization. For the



expansion of the wave function, the maximum value of the angular momentum L_{\max} was set as 10, as it is a dimensionless quantity. For a non-shifted $14 \times 14 \times 14$ grid, a denser k-mesh is utilized for all physical properties. The default energy convergence criteria were set at 10^{-5} Ry. The BoltzTrap code³⁵ was used to compute the transport parameters of the studied compounds. The calculation of the electrical conductivity $\sigma_{\alpha\beta}(T)$ and Seebeck coefficient $S_{\alpha\beta}(T)$ as a function of temperature was performed using the following equations:

$$\sigma_{\alpha\beta}(T) = \frac{1}{Q} \int \sigma_{\alpha\beta}(\varepsilon) \left[\frac{\partial f(T)}{\partial \varepsilon} \right] d\varepsilon \quad (1)$$

$$S_{\alpha\beta}(T) = \left(\frac{1}{eTQ\sigma_{\alpha\beta}(T)} \right) \int \sigma_{\alpha\beta}(\varepsilon)(\varepsilon - \mu) \left[\frac{\partial f(T)}{\partial \varepsilon} \right] d\varepsilon \quad (2)$$

where Q is the unit cell volume, $f(T)$ is the Fermi-Dirac distribution, e is the charge of the electron, and $\sigma_{\alpha\beta}(\varepsilon)$ is the transport distribution function as a function of energy, given by:

$$\sigma_{\alpha\beta}(\varepsilon) = e^2 \sum_{i,k} \tau_{ik} v_{\alpha}(i, k) v_{\beta}(i, k) \delta(\varepsilon - \varepsilon_{i,k}) \quad (3)$$

3. Results and discussions

3.1. Structural properties

For spinel SrCe_2Z_4 (where Z is equal to S, Se, or Te), the face-centered cubic unit cell, having 8 formula units per unit cell, is depicted by a ball-stick model in Fig. 1(a). Sr, Ce, and Z have been represented with blue, brown, and yellow balls in this model, respectively. Sr is divalent (Sr^{2+}) and Ce is trivalent (Ce^{3+}), making them both non-transition cations, thereby classifying the structure as a normal spinel. The configurations have a space group of $Fd\bar{3}m$ (#227). In this unit cell, the atoms Sr, Ce, and Z have coordinates (0.125, 0.125, 0.125), (0.5, 0.5, 0.5), and (0.25, 0.25, 0.25), respectively. Each individual atom, Sr, Ce, and Z, has unique Wyckoff positions, such as 8a, 16d,

and 32e,³⁶ respectively. Fig. 2(b) represents the polyhedral structure, where the anions form an FCC lattice. It can also be observed that the Sr atom occupies the tetrahedral void in SrZ_4 , whereas Ce occupies the octahedral void in CeZ_6 in the FCC lattice.^{37,38} So, from the above information, the coordination numbers of Sr, Ce, and Z in SrCe_2Z_4 are 4, 6, and 4, correspondingly.

The ground state energy (Ryd) and the volume (a.u.³) in AFM and FM states were calculated and plotted using the Murnaghan equation of state.³⁹ Fig. 2 shows the two parabolic curves, with the red one representing the AFM state and the black curve representing the FM state. Fig. 2(a-c) demonstrates the volume optimization graphs of SrCe_2S_4 , SrCe_2Se_4 , and SrCe_2Te_4 . In the AFM state, all compositions release less energy than in the FM state. Therefore, the FM state is energetically more favorable for all compositions. Among all these compositions, SrCe_2Te_4 has the highest lattice parameters and lowest ground state energy. Therefore, it is the most stable.⁴⁰

The lattice constant a_0 (Å) can be calculated from Fig. 2. SrCe_2Te_4 has a higher lattice constant value (13.42 Å) [Table 1] because of the larger ionic radii of Te. The lattice constants for SrCe_2S_4 and SrCe_2Se_4 were 12.01 and 12.52 Å, respectively. As the bulk modulus B_0 (GPa) of the material is inversely proportional to the lattice constant, the bulk moduli decrease with the rise of the lattice constant. The value of B_0 was reported as 53.42 GPa for SrCe_2S_4 , which declined to 42.76 and 33.42 GPa for SrCe_2Se_4 and SrCe_2Te_4 , respectively.⁴¹ The B_0 quantifies the hardness of a material by evaluating its resistance to uniform volumetric compression under applied pressure.⁴² The FM states have higher thermodynamic stability due to their higher enthalpy (H_f) of formation, as the material releases more energy in this state.⁴³ From Table 1, the H_f value of SrCe_2S_4 is -2.20 eV, indicating its higher thermodynamic stability. The values of H_f for the Se and Te-based compositions are noted as -2.05 and -1.94 eV, respectively. The Curie temperatures of all

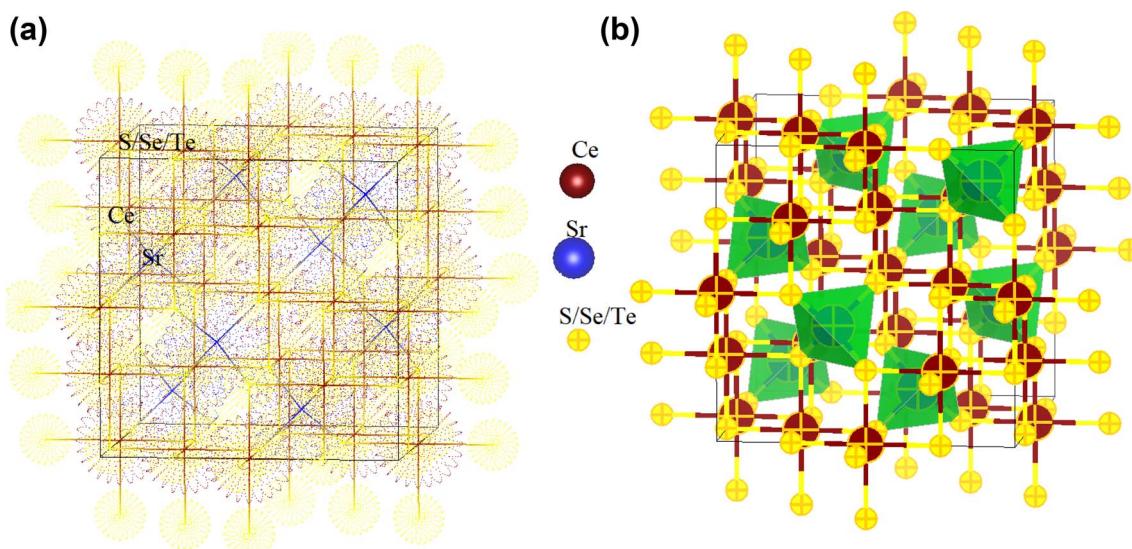


Fig. 1 (a) Illustration of the ball-stick model of the SrCe_2Z_4 crystal structure (with $\text{Z} = \text{S}$, Se, and Te), while (b) depicts the structure of the polyhedron.



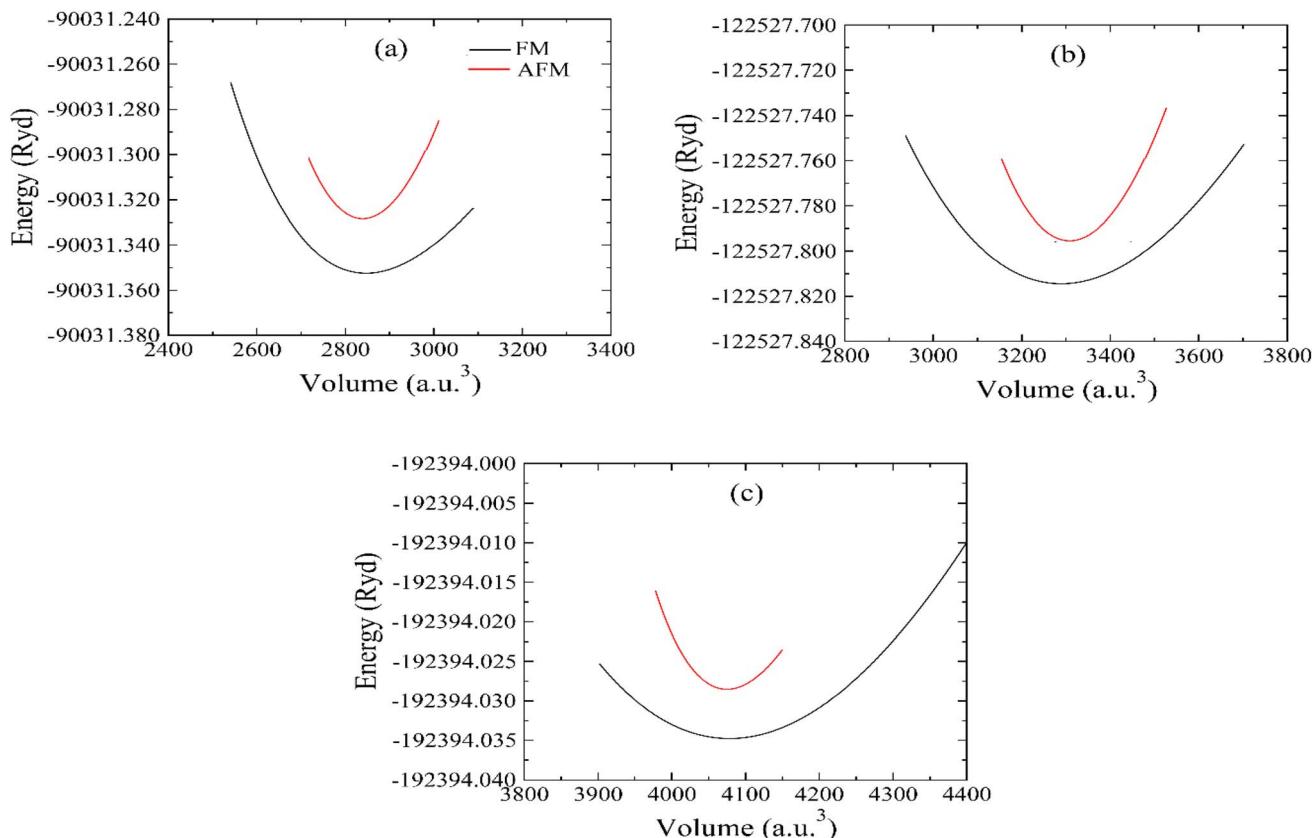


Fig. 2 Energy optimization trends for (a) SrCe_2S_4 , (b) SrCe_2Se_4 , and (c) SrCe_2Te_4 .

Table 1 The computed structural parameters for SrCe_2Z_4 ($\text{Z} = \text{S}, \text{Se}, \text{Te}$)

Parameters	a_0 (Å)	B_0 (GPa)	H_f (eV)	T_c (K)	E_g (eV)	Ref.
SrCe_2S_4	12.01	53.42	-2.2	295	2.20	This work
HgY_2S_4	11.12	76.19	-8.64	—	1.20	44
MgLu_2S_4	10.82	78.03	—	—	2.60	45
MgY_2S_4	11.06	64.88	—	—	1.62	46
LiCr_2S_4	9.73	97.41	-1.18	—	1.40	47
ZnMn_2S_4	9.98	—	-2.86	—	1.55	48
SrCe_2Se_4	12.52	42.76	-2.05	302	1.71	This work
HgY_2Se_4	11.62	63.65	-6.88	—	0.60	44
MgLu_2Se_4	11.32	65.14	—	—	2.00	45
MgY_2Se_4	11.54	53.88	—	—	1.09	46
LiCr_2Se_4	10.24	78.86	—	—	1.10	47
ZnMn_2Se_4	10.57	—	-2.98	—	0.85	48
SrCe_2Te_4	13.42	33.42	-1.94	310	1.30	This work
ZnMn_2Te_4	11.34	—	-3.01	—	0.24	48

compositions are above room temperature, but SrCe_2Te_4 has a higher Curie temperature (310 K). The Curie temperature being near room temperature positions these materials as promising aspirants for energy-efficient data erasing and writing under manageable thermal conditions.³⁶

3.2. Electronics properties

The electrical properties, such as the density of states (DOS) and the band structure (BS), are critical computations to evaluate

the composite's potential for optical applications. Sr-based spinels exhibit exciting electronic properties that verify their FM nature. The TB-mBJ potential is used as the theoretical approach to achieve an accurate bandgap value because of its ability to accurately predict BS, as investigated in previous studies.⁴⁹ The BS properties of three compositions, SrCe_2S_4 , SrCe_2Se_4 , and SrCe_2Te_4 , are demonstrated in Fig. 3(a–c). The dashed line separating the conduction (CB) and the valence bands (VB) represents the Fermi energy (E_f). In all compositions, the VB maxima and CB minima lie on the same symmetry point, showing the direct bandgap nature of these materials.⁵⁰ In Fig. 3(a) and (c), in the $S\uparrow$ orientation, the energy states are close to the E_f , indicating semiconducting behavior. In contrast, the $S\downarrow$ channel shows the insulating behavior due to a large bandgap separating the states of the VB and CBs. This suggests their FM nature with complete spin polarization. Overall, the BS of SrCe_2S_4 and SrCe_2Te_4 indicates that the material behaves as an FM semiconductor.⁵¹ The spin-polarized behavior of both examined compositions is calculated by utilizing this formula:

$$P = \frac{\text{Do}^\uparrow(E_f) - \text{Do}^\downarrow(E_f)}{\text{Do}^\uparrow(E_f) + \text{Do}^\downarrow(E_f)} \times 100 \quad (4)$$

where $\text{Do}^\uparrow(E_f)$ and $\text{Do}^\downarrow(E_f)$ signify the DOS at the E_f for the $S\uparrow$ and $S\downarrow$ channels, correspondingly.⁵² Due to the energy states being slightly above the E_f , the SrCe_2Se_4 in the $S\uparrow$ channel exhibits a metallic nature, as illustrated in Fig. 3(b). The $S\downarrow$



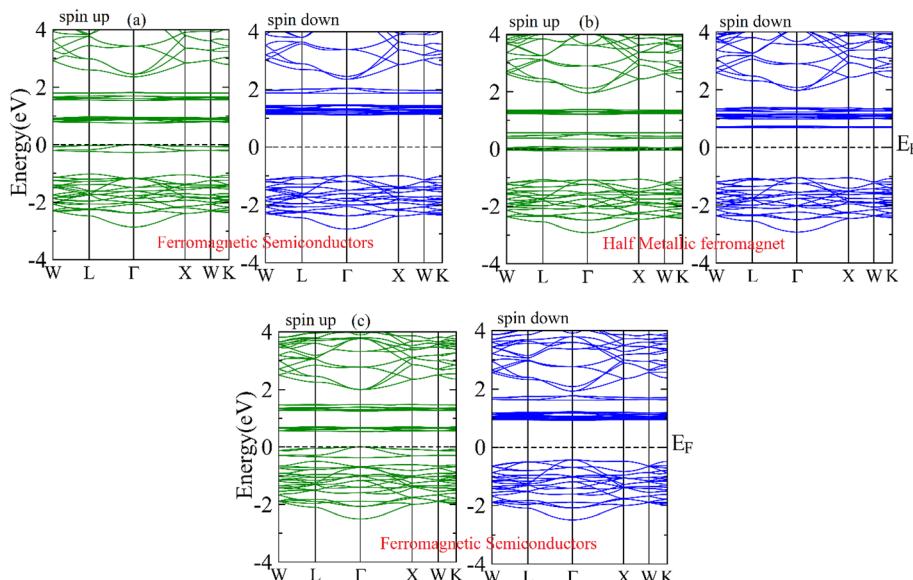


Fig. 3 The band structures in both the spin-up and spin-down channels: (a) SrCe_2S_4 , (b) SrCe_2Se_4 , and (c) SrCe_2Te_4 .

channel shows insulating behavior because the Fermi level lies within these bands.⁵³ So, the overall nature of SrCe_2Se_4 is half-metallic. In Fig. 3(c), the energy difference between the VB and CB indicates that the E_g of SrCe_2Te_4 is minimal. Due to the half-metallic nature, the E_g of SrCe_2Se_4 is not considered.

The total DOS and the partial DOS for each atom are calculated to provide a detailed explanation of the mechanism of ferromagnetism.⁵⁴ Fig. 4 illustrates the TDOS and PDOS of the SrCe_2S_4 composition. The TDOS reflects the electronic BS, and the energy states are shown as peaks. In Fig. 4, the TDOS reflects the combined contributions of all atoms and their corresponding valence orbitals, with VB on the left side and CB on

the other side of the Fermi level. According to the PDOS plot, the VB edge at the Fermi energy is composed of 4f—Ce states and 3p—S states together, while 5s—Sr and 3p—S states firmly hybridize in the VB in the energy range from -2.8 eV to -1 eV. In the CB, near the E_F , 4f—Ce has a significant contribution, ranging from 0.5 to 1.95 eV. So, Ce's overall PDOS has made a substantial contribution to TDOS.

In contrast to earlier compositions, SrCe_2Se_4 demonstrates a half-metallic ferromagnetic nature, as demonstrated by its band structure and DOS analysis. The TDOS and PDOS plots for this composition are highlighted in Fig. 5, which indicates that the 4f—Ce states play a significant role close to the Fermi level,

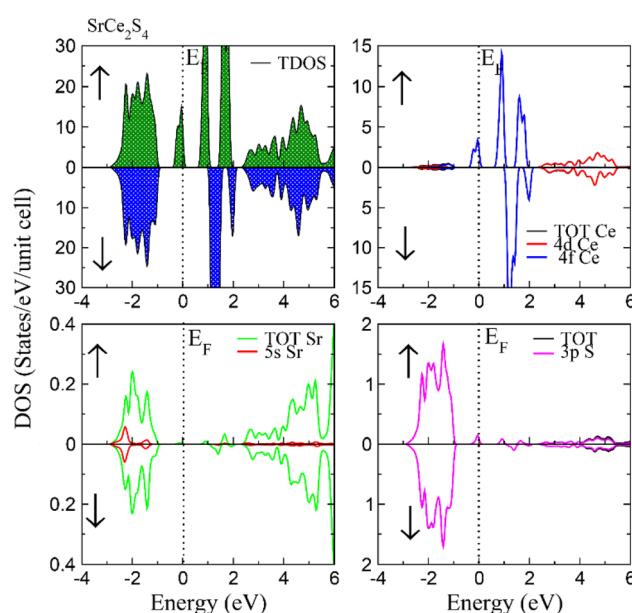


Fig. 4 The TDOS and PDOS of SrCe_2S_4 in the spin-up and spin-down channels.

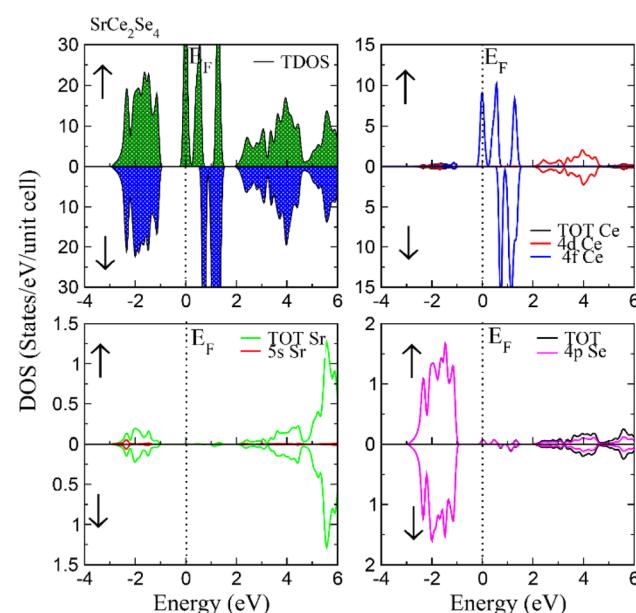


Fig. 5 The TDOS and PDOS of SrCe_2Se_4 in the spin up and spin down channels.



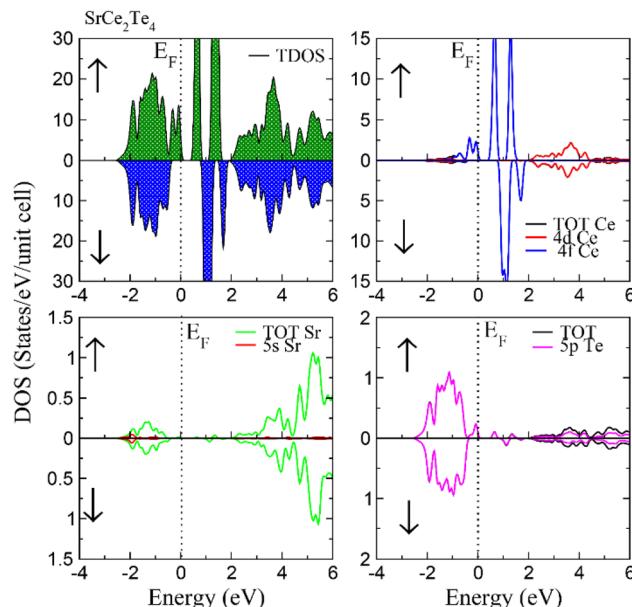


Fig. 6 The TDOS and PDOS of SrCe_2Te_4 in the spin up and spin down channels.

crossing the E_F between -0.2 eV and 0.2 eV and causing the metallic behavior in the spin-up channel. On the other hand, the $4p$ —Se states exhibit insulating properties and contribute little at E_F , but are essential in the valence band (VB) between -2.9 eV and -1 eV. Furthermore, these states lie in the range of 2 – 6 eV in the conduction band. The unique half-metallic behavior is reinforced by the fact that Ce makes the most significant overall contribution to the TDOS. The interaction of energy states is responsible for this behavior, which aligns with observations in similar materials and highlights the importance of composition in controlling electronic properties.⁵⁵

Fig. 6 illustrates the TDOS and PDOS for SrCe_2Te_4 . Like the other two compositions, the Ce element has the maximum involvement in the development of the TDOS. In this case, the energy states near the E_F , extending from -1 eV to the Fermi level, show that a greater number of peaks are present compared to the other two compositions, and there is a slight variance between the highest value of the VB and the minimum value of the CB, indicating the lowest E_g of SrCe_2Te_4 .

3.3. Magnetic properties

The magnetic properties reflect how the material responds to an external magnetic force field. The magnetic nature of the substance can be conceptualized in terms of direct $\Delta_x(f)$ and indirect $\Delta_x(pf)$ exchange energies, crystal field stabilization energy Δ_{CF} , and exchange constants $N_o\alpha$ and $N_o\beta$.⁵⁶ The

geometry of f-orbitals is more complex than that of d orbitals, so the crystal field stabilization energy, Δ_{CF} , cannot be calculated for compositions containing f-block metal cations. For a material to exhibit an FM nature, the value of the direct exchange energy $\Delta_x(f)$ must be higher than the stabilization energy.⁵⁷ The $\Delta_x(f)$ exhibits negative values of -0.32 , -1.047 , and -0.36 eV for SrCe_2Z_4 ($Z = \text{S, Se, Te}$), where SrCe_2S_4 and SrCe_2Te_4 show ferromagnetic semiconducting behavior and SrCe_2Se_4 exhibits a half-metallic nature. The negative sign usually indicates the material's ferromagnetic ordering, confirming its ferromagnetic nature.⁵⁸ This unexpected ferromagnetism is due to the dominance of indirect exchange interaction, such as double exchange or the super exchange mechanism.⁵⁹ The formula can calculate the value of $\Delta_x(f)$ as $\Delta_x(f) = \Delta(f)^\downarrow - \Delta(f)^\uparrow$.⁶⁰ The indirect exchange of energy $\Delta_x(pf)$ is produced by the hybridization between p-block chalcogens (S, Se, Te) and f-block Ce. We can calculate the $\Delta_x(pf)$ from only the VB maximum S and the S channel's maximum peaks. The value of the indirect exchange is negative, indicating the FM behavior in the $S\downarrow$ channel for SrCe_2S_4 , SrCe_2Se_4 , and SrCe_2Te_4 , showing their intense spin polarization.⁶¹ All the calculated values are presented in Table 3.

The interaction in which electrons from CBs exchange with the localized MM is referred to as the exchange constant $N_o\alpha$. The exchange interaction involving holes from the VB and the localized MM is categorized by the exchange constant $N_o\beta$. The following formula can be used to calculate the $N_o\alpha$ and $N_o\beta$:

$$N_o\alpha = \frac{\Delta E_c}{\langle xS \rangle} \quad (5)$$

$$N_o\beta = \frac{\Delta E_v}{\langle xS \rangle} \quad (6)$$

From Table 2, we can observe the value of $N_o\alpha$ and $N_o\beta$. Here, $\Delta E_c = E_c^\downarrow - E_c^\uparrow$ indicates the splitting at the CB edge, and $\Delta E_v = E_v^\downarrow - E_v^\uparrow$ represents the splitting at the VB edge.⁵⁷ Table 2 shows that the obtained results of $N_o\alpha$ and $N_o\beta$ for SrCe_2Z_4 ($Z = \text{S, Se, Te}$) are negative and induce intense spin polarization, leading to the FM order of SrCe_2S_4 and SrCe_2Te_4 . With the influence of the spin-exchange interactions and electronic structure, SrCe_2Se_4 shows half-metallic ferromagnetism.⁶² From the exchange constant equations, the splitting of the CB edge depends on s-f hybridization among the s-Sr and f-Ce orbitals. In contrast, VB maxima splitting relies on the p-f coupling between p-Z ($Z = \text{S, Se, Te}$) and f-Ce orbitals.⁵⁹ The total amount of MM can be determined based on the number of unpaired electrons in the f-orbitals.⁵⁵ From Table 2, the value of total MM for all three compositions is $4 \mu_B$, which indicates that all magnetic spins are equally aligned and have significant

Table 2 List of the computed aspects ($\Delta_x(pf)$, $\Delta_x(f)$, $N_o\beta$, $N_o\alpha$, Sr, Ce, X, Int, and the total magnetic moments) for SrCe_2Z_4 ($Z = \text{S, Se, Te}$)

Compositions	$\Delta_x(f)$ (eV)	$\Delta_x(pf)$ (eV)	$N_o\alpha$	$N_o\beta$	Total (μ_B)	Int (μ_B)	Sr (μ_B)	X (μ_B)	Ce (μ_B)
SrCe_2S_4	-0.32	-0.945	-1.89	-0.732	4	0.151	0.007	0.005	0.952
SrCe_2Se_4	-1.047	-0.75	-1.056	-0.959	4	0.148	0.01	0.012	0.983
SrCe_2Te_4	-0.36	-0.45	-1.463	-0.403	4	0.154	0.008	0.04	0.97



magnetic order, leading to intense spin polarization. The small value of Sr and the considerable value of Ce indicate that Ce makes a greater contribution to the overall composition SrCe_2Z_4 . The value of interstitial MM suggests that the regions between the atomic gaps also contribute to the overall magnetic response of these materials.

3.4. Transport properties

Thermoelectric materials can facilitate heat transformation into electrical power, and their efficiency is measured in the context of the power factor (PF) or Figure of Merit (ZT). These performance-determining parameters are calculated in terms of the thermal conductivity (κ), electrical conductivity (σ), Seebeck coefficient (S), power factor ($S^2\sigma$), and the ZT .^{61,62} The numerical values of these parameters are critical in deciding the applications of materials. Fig. 7 shows how different thermoelectric parameters change with T for SrCe_2S_4 , SrCe_2Se_4 , and SrCe_2Te_4 . Fig. 7(a) demonstrates the graph between σ and T , indicating that σ rises with temperature, attributed to the increase in the thermally generated charge carrier concentration and their mobility.⁶³ Among the compositions studied, SrCe_2Te_4 showed the highest σ values because of its smaller E_g , leading to higher carrier concentration and mobility.

Thermal conductivity (κ) measures how much heat can be transferred through a material. There are two parts of κ ; electronic (κ_e) and lattice thermal conductivity (κ_L).⁶² Here, we can report the κ_e because the lattice part is beyond the computational capabilities of the BoltzTraP function. The variation of κ_e with T has been presented in Fig. 7(b), indicating that κ_e increases with T because more electrons can be thermally excited from the VB to the CB at the elevated temperature.⁴³ This leads to higher carrier concentration and higher mobility, which increases the κ_e .⁶³

Fig. 7(c) shows how the Seebeck coefficient changes with T . The Seebeck coefficient measures how much voltage is produced due to a 1 K temperature change in any material.⁶²

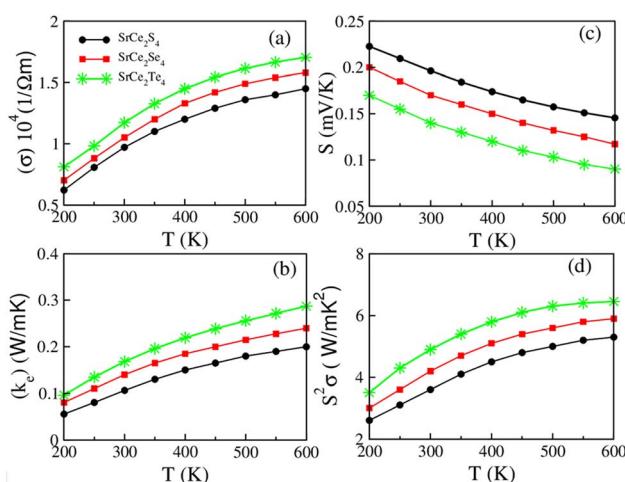


Fig. 7 Temperature-dependent variation of (a) σ , (b) κ_e , (c) S , and (d) $S^2\sigma$ for SrCe_2Z_4 .

$$S = \frac{\Delta V}{\Delta T} \quad (7)$$

At lower temperatures, carrier concentrations are lower, leading to a higher S . So, as the T increases, the S decreases because of an increase in the carrier concentration and higher mobility. Higher mobility causes a reduction in voltage production, leading to a lower S at higher T .⁵⁶ The S value of SrCe_2S_4 is larger than that of other compositions because of its lower carrier concentration, leading to a higher S .⁶³ Fig. 7(b) shows the temperature-dependent electronic part of the thermal conductivity for SrCe_2Z_4 . It is clear that SrCe_2Te_4 showed a higher value of thermal conductivity, which is attributed to a higher carrier concentration, higher mobility, and less phonon scattering as compared to other compositions. ZT and PF are key parameters that are employed to govern the thermoelectric efficiency of any material. The value of PF depends upon the value of σ and the S , and can be expressed as:⁶⁰

$$\text{PF} = \frac{S^2\sigma}{\tau} \quad (8)$$

From Fig. 7(d), we can observe that the reported results of PF confirm the slight upsurges with the elevation of T . The value of PF will be higher when the product of σ and S square is the maximum value in semiconductors.⁶⁰ In Fig. 8(a), it has been observed that there is minimal phonon scattering at lower T , resulting in the usual scattering where the momentum and energy are conserved.⁶⁴ This leads to the elastic scattering of phonons, and there is thus a greater κ_L at the start. However, as T continues to rise, the scattering becomes more pronounced,

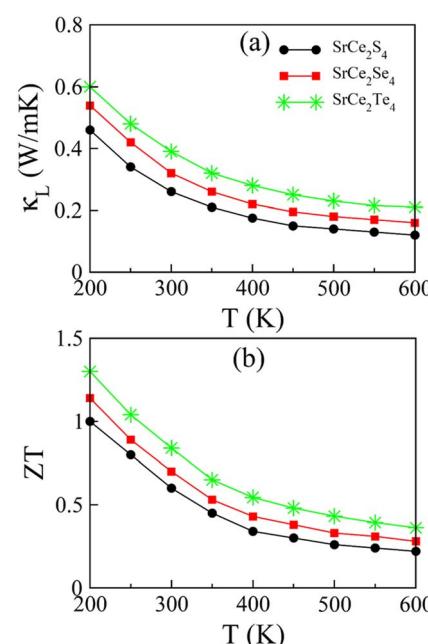


Fig. 8 Temperature-dependent variation of (a) κ_L and (b) ZT for SrCe_2Z_4 .



Table 3 Thermoelectric parameters of SrCe_2Z_4 (where $\text{Z} = \text{S, Se, Te}$) at room temperature

Compositions	σ/τ ($1/\Omega\text{m} \times 10^4$)	κ_e/τ (W mK^{-1})	S (mV K^{-1})	PF (W mK^{-2})	ZT	Ref.
SrCe_2S_4	0.97	0.106	0.14	3.6	0.60	This work
HgY_2S_4	24.1	0.49	223.36	1.20	0.72	44
MgLu_2S_4	1.91	0.46	245.6	1.15	0.74	45
MgY_2S_4	1.381	0.334	242.567	—	0.731	46
LiCr_2S_4	0.88	0.90	-94.43	0.79×10^{-3}	—	47
ZnMn_2S_4	9.48	6.61	7.46	0.05×10^{-3}	—	48
SrCe_2Se_4	1.05	0.14	0.17	4.20	0.70	This work
HgY_2Se_4	17.6	0.40	239.48	1.01	0.75	44
MgLu_2Se_4	1.82	0.42	239.1	1.04	0.75	45
MgY_2Se_4	1.150	0.248	230.585	—	0.739	46
LiCr_2Se_4	1.58	1.67	-64.20	0.66	—	47
ZnMn_2Se_4	11.58	8.11	6.60	0.05×10^{-3}	—	48
SrCe_2Te_4	1.17	0.168	0.196	4.9	0.94	This work
ZnMn_2Te_4	12.10	8.65	10.07	0.12×10^{-3}	—	48

due to which the energy and momentum are no longer conserved, causing a reduction in κ_L .⁵⁴ From Table 3, the value of PF for SrCe_2Te_4 is observed to be 4.90 W mK^{-2} at RT. The value of ZT may be determined based on κ , S , and σ , employing the expression below.⁶⁰

$$ZT = \frac{\sigma S^2 T}{\kappa} \quad (9)$$

From Fig. 8(b), we can observe that with an increase in T , the value of ZT decreases due to the combined effect of κ and S .^{57,60} At low T , the ZT value is higher due to the larger value of S and σ . So, when the T rises, the value of ZT decreases because of the increase of κ .^{64,65} At higher T , the S and σ also decrease, resulting in a lower value of ZT . The calculated values of all thermoelectric parameters for SrCe_2S_4 , SrCe_2Se_4 , and SrCe_2Te_4 at room temperature are listed in Table 3. These values provide a quick reference for the thermoelectric performance of the studied material at room temperature.⁶⁶ The large ZT at room temperature ensures their applications for thermoelectric generators, effectively transforming heat into electrical power.⁶⁷

4. Conclusion

In summary, the structural, electrical, magnetic, and thermoelectric aspects of SrCe_2Z_4 ($\text{Z} = \text{S, Se, Te}$) have been systematically explored to validate their applicability for energy harvesting and spintronic implementations. In optimization, the released energy upon transition to the FM state and negative formation energy collectively ensured their structural and thermodynamic stability in FM states. The analysis of the spin-polarized band structure demonstrated the half-metallic ferromagnetic behavior of SrCe_2Se_4 and the ferromagnetic semiconducting nature of SrCe_2S_4 and SrCe_2Te_4 . The Heisenberg model analysis showed that the Curie temperature ranged from 295–310 K, which is above room temperature, indicating ferromagnetism in these spinels. The DOS confirmed that the strong coupling of p-orbitals of chalcogens and the 4f-states of Ce governed the exchange mechanism of electrons, resulting in

ferromagnetism. The investigation of direct and indirect exchange energy, along with exchange constants, ascertained the dropping of energy of the FM state and stabilized ferromagnetism. Moreover, Ce's magnetic moment distribution to the Sr and S/Se/Te sites was attributed to the electron exchange interactions, rather than the formation of a magnetic cluster of Ce ions. Finally, the bigger electrical and ultra-low thermal conductivity improved the power factor and figure of merit performances. The ZT value of 0.90 at room temperature for SrCe_2Te_4 showcased its potential for thermoelectric devices.

Conflicts of interest

There is no conflict to declare.

Data availability

All data included in this study may be obtained from the corresponding author on reasonable request.

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