



Thermoelectric Performance of CrSSe and CrSeTe Janus Monolayers

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Abstract

In this work, density functional theory-based simulation is used for investigating the structural and electronic properties of Janus monolayers CrSSe and CrSeTe. Electronic bandgap values of 0.85 eV and 0.62 eV are obtained for CrSSe and CrSeTe, respectively. Further, the semiclassical Boltzmann theory is used for assessing the thermoelectric parameters including the Seebeck coefficient, electrical and thermal conductivity, and thermoelectric performance (ZT) of the monolayers. The values of Seebeck coefficient and lattice thermal conductivity for (*n*-type) *p*-type Janus monolayers CrSSe and CrSeTe are (1340) 1390 $\mu\text{V K}^{-1}$, (971) 1010 $\mu\text{V K}^{-1}$, and (11.01) 0.25 W/K, respectively. The ZT values for (*n*-type) *p*-type Janus monolayers CrSSe and CrSeTe are (0.92) 0.93 and (0.95) 0.96, respectively, at room temperature. The thermoelectric performance of these monolayers is higher than for the homogeneous CrSe₂ monolayer due to their unique structural and compositional characteristics. These results contribute valuable insights for the design and optimization of Janus monolayers for advanced thermoelectric applications, and pave the way for promising advancements in sustainable energy harvesting.

Keywords Density functional theory · Boltzmann transport equation · ZT · thermoelectric properties

Introduction

In order to meet the growing need for clean energy and achieve cost-effective sustainable energy, sources of clean energy may help to meet environmental standards. In view of this, researchers are devoting attention as never before to energy conversion materials for both cooling and power generation.^{1,2} Thus, the pressing requirement for improved conversion performance via the Seebeck effect is the direct or reversible conversion of thermal energy into electrical energy, while the Peltier effect determines the amount of cooling.³ Commercially available thermoelectric devices such as thermoelectric coolers are used in computer chips, satellites, sensors, and power generation. These devices have low efficiency which restricts their wider applicability.

Thus, improving these parameters is our main concern in this study. Theoretical predictions of materials that accelerate research towards experiments can yield extremely

efficient TE materials. The ideal path to obtaining the optimal thermoelectric material for commercialization and marketability can be predicted with the use of theoretically predictive modelling.⁴ The thermoelectric efficiency of thermoelectric material can be assessed by a dimensionless quantity, the figure of merit (ZT), which is associated with the contribution of thermopower (*S*), electrical conductivity (σ), and thermal conductivity (κ) that is dependent on both the electron and lattice movement. The figure of merit (ZT) of a thermoelectric material is a key parameter that quantifies its efficiency in converting heat into electricity. This energy conversion parameter which provides the superior performance of materials is formulated as

$$ZT = \frac{S^2 \sigma T}{\kappa_e + \kappa_l} \quad (1)$$

where all the parameters used in this formula are transport parameters.⁵ Due to the rigid intercoupling between these factors, it is extremely difficult to increase the efficiency of thermoelectric material by altering just one of the values in Eq. (1).⁶ However, controlling the Seebeck effect and electrical conductivity at the same time is a significant issue, and band structure tuning is a novel way to increase the ZT. Hence, the band structure can be altered by reducing

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the dimensions to form the nanostructures for variation in thermoelectric performance.⁷

Recent studies have explored the two-dimensional transition metal dichalcogenides (2D TMDCs), which have more exciting physical and chemical properties than their bulk counterparts, and show great prospects as materials for energy harvesting applications.^{8–10}

Since TMDCs have layered structures, a two-dimensional material has been created by considering a specific layer that is also made up of three layers, with a transition metal layer positioned between the two chalcogen atom levels. The weak van der Waals forces that hold these layers together and connect them create a large gap that can accommodate a foreign atom or molecule to produce an intercalated structure. This intercalation plays an efficient and effective role in the manipulation of the electronic band structure. The band-structure valley can be altered through doping,¹¹ alloying,¹² dimension engineering,^{13–15} strain engineering,^{16,17} application of external stress, formation of a Janus monolayer,¹⁸ stacking effects,¹⁵ or the formation of a heterostructure.¹⁹

The Janus monolayers PtSSe, PtSTe, PtSeTe, PdSSe, PdSTe, and PdSeTe were studied sequentially.^{20,21} It was found that PdSeTe and PtSeTe monolayers have a high $ZT \sim 1$ at 300 K. A significant increase in ZT is observed due to a modest increase in S and drastic decrease in lattice thermal conductivity in the PtSSe Janus monolayer as compared with its parent structures, i.e., PtS₂ and PtSe₂. Das et al.²² observed that the enhancement in power factor is mainly due to an increase in the Seebeck coefficient. The obtained values of ZT for the n -type and p -type ZrSSe monolayer are 0.76 and 0.69, whereas the newly investigated Janus monolayers ZrOS and ZrOSe showed maximum ZT values of 0.82 and 0.72, respectively, at 900°C.

In light of the aforementioned research, the current study focusses on the formation of Janus monolayers from Cr-based materials, which exhibit promising features in comparison with CrSe₂ material. Janus monolayers such as CrSSe and CrSeTe have several potential advantages over CrSe₂ monolayers. As Janus monolayers have asymmetry in their atomic structure, which allows the tuning of electronic, optical, and magnetic properties, this can lead to enhanced functionalities tailored for specific applications.²³ When compared with homogeneous monolayers such as CrSe₂, the asymmetric nature of Janus monolayers may help to improve stability. This stability is crucial for practical applications of these monolayers in electronic and optoelectronic devices.²⁴

Janus monolayers often exhibit novel physical phenomena that are not observed in homogeneous monolayers. For example, they can have unique electronic band structures or optical properties that make them attractive for fundamental research and technological innovation.^{25,26} Due to their dual composition, Janus monolayers may exhibit multifunctionality, combining different properties such as

optical and semiconducting behaviour in a single material. This versatility is advantageous for developing multifunctional devices.^{27,28} Overall, Janus monolayers like CrSSe and CrSeTe offer a wider range of tuneable properties and potential applications, making them promising candidates for future research and technological development.²⁹

Computational Details

The framework of first-principles calculations was studied in Quantum Espresso (QE) software³⁰ to determine the structural and electronic properties of Cr-based Janus monolayers using density functional theory (DFT). The Kohn-Sham equation, which is solved iteratively, forms the foundation of this software. The generalized gradient approximation (GGA) in its Perdew-Burke-Ernzerhof (PBE) form was used to incorporate exchange-correlation functionals of electrons.³¹

The norm-conserving pseudopotentials were used for Cr, S, Se, and Te, in which the d -orbital of transition metals and the p -orbital chalcogen atoms play a vital role. To prevent the spurious interactions of neighbouring layers, an optimized value of vacuum = 20 Å was considered along the z -direction. Throughout the calculations, the optimized value of energy cutoff for electronic wavefunction and electron charge density were set with values of 85 Ry and 340 Ry for CrSSe and 90 Ry and 360 Ry for CrSeTe, respectively. Using these values, the optimized geometry of Monkhorst–Pack for k -points was used as $13 \times 13 \times 1$ and $14 \times 14 \times 1$ for CrSSe and CrSeTe, respectively, for sampling the Brillouin zone. To determine the accurate transport parameters, which are based on the density of states, a dense k -point mesh of $50 \times 50 \times 1$ was selected. The semiclassical Boltzmann transport theory-based BoltzTraP code³² interfaces with these highly dense densities of states. Its foundation is the constant scattering time approximation (CSTA), which has a minor dependence on group velocity and energy but a strong dependence on the density of states contribution. However, this assumption does not hold true for all materials, and hence the deformation potential theory which was briefly discussed in earlier work³³ is used to calculate the value of relaxation time (τ).

The electronic band structure and density of states obtained from DFT calculations provided the critical information about carrier effective masses, mobility, type and concentration of charge carriers. This information was further employed for studying the electronic transport properties, Seebeck coefficient, electrical conductivity, and electronic thermal conductivity using the BoltzTrap code.

This code computed the electronic transport properties, σ , S , and κ_e , which can be expressed by a tensor integral (κ_n) given as

$$\kappa_n = \frac{2}{(2\pi)^3} \sum_i \int d^3k \tau_i(k) v_i(k) \otimes v_i(k) [\epsilon_i(k) - \mu]^n \frac{\partial f(\mu, T, \epsilon_i)}{\partial \epsilon_i}, \quad (2)$$

where $v_i(k)$, ϵ_i , μ , and $\tau_i(k)$ represent the electron group velocity, electronic energy eigenvalue, chemical potential, and electronic relaxation time with wave vector k and band index i . Other parameters including σ , S , and κ_e can be expressed in terms of tensor κ_n as

$$\sigma = e^2 \kappa_0, \quad (3)$$

$$S = \frac{1}{eT} \kappa_1 \kappa_0^{-1}, \quad (4)$$

$$\kappa_e = \frac{e^2}{\pi}. \quad (5)$$

Phonopy code was used to create a phonon dispersion curve to assess the thermodynamic stability of these selected Janus monolayers.³⁴ Using the Phonopy code³⁵ interfaced with QE, a $3 \times 3 \times 1$ supercell sampled using a $6 \times 6 \times 1$ k-point mesh was used to extract the second- and third-order force constants. This was used to calculate lattice thermal conductivity while considering a $25 \times 25 \times 1$ q-mesh. The transport parameters for energy conversion applications were computed using all parameters.

Structural and Electronic Properties

CrSeTe and CrSSe are both members of the transition metal dichalcogenide (TMD) family, and exhibit distinctive structural and electronic properties owing to their asymmetric atomic composition. Cr-based TMDCs have a 2H-MoS₂ type structure, with hexagonal unit cells of space group number 187 with space group P-6m2.

These materials exhibit interesting structural and electronic properties due to their layered crystal structure and the presence of transition metal atoms combined with chalcogen atoms (S, Se, Te). The layers are held together by weak van der Waals forces, making them prone to cleavage and exfoliation into thin layers, as shown in Fig. 1a and b. The obtained optimized lattice parameters for the CrSSe and CrSeTe Janus monolayers are $a = b = 3.13$ Å and $a = b = 3.35$ Å, respectively. The relaxed lattice parameter of the CrSe₂ monolayer is 3.22 Å, as studied in previous work,¹³ which lies in between the two Janus monolayers, and results show good agreement with the literature for W-based Janus monolayers.³⁶ To prevent interaction between the layers, a vacuum of 20 Å was considered along the z-direction. All the optimized parameters are presented in Table I.

CrSeTe and CrSSe monolayers typically exhibit a direct bandgap at the k-points of the Brillouin zone. In CrSSe, chromium atoms are bonded to sulphur on one side and selenium on the other, whereas CrSeTe features chromium atoms bonded to selenium and tellurium atoms on opposite sides, introducing further asymmetry and modifying the bandgap relative to CrSe₂.

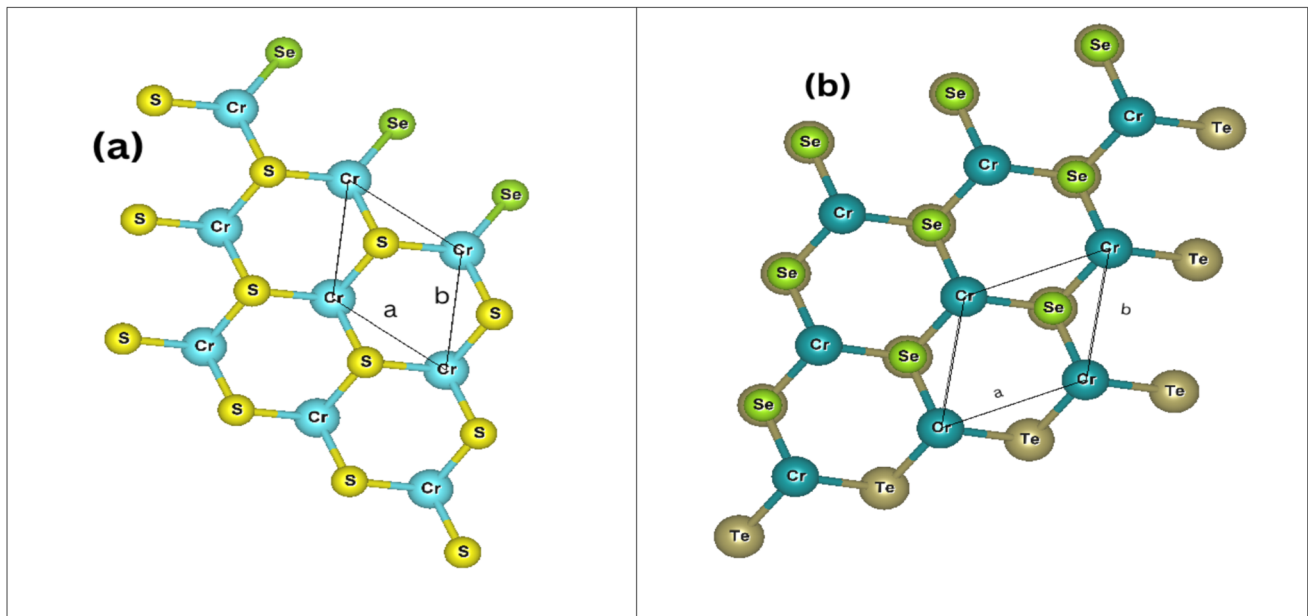


Fig. 1 Optimized structure of Janus monolayers (a) CrSSe and (b) CrSeTe.

Table 1 Optimized lattice parameters height (h), d_{MSe} (band length between M and Se), d_{MX} (band length between M and X), θ_1 and θ_2 (angle between Se-Cr-Se and X-Cr-X) of Janus monolayer CrSSe and CrSeTe, and their energy bandgap (E_g)

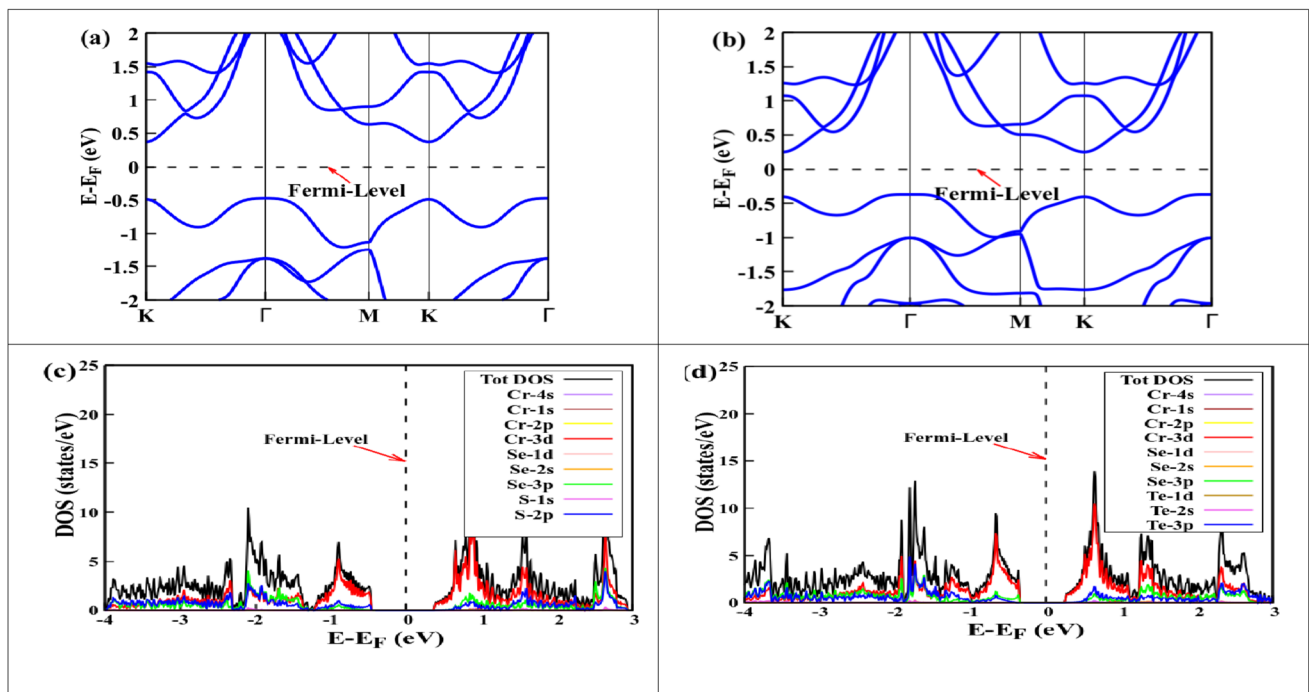
Janus monolayer	$a=b$ (Å)	h (Å)	d_{MSe} (Å)	d_{MX} (Å)	θ_1 (°) (Se-Cr-Se)	θ_1 (°) (X-Cr-X)	E_g (eV)
CrSSe (MXSe)	3.13	3.0437	2.4220	2.3016	80.376	85.540	0.84
CrSeTe (MSeX)	3.35	3.2824	2.4521	2.6286	86.289	79.274	0.62

These structural configurations lead to unique electronic characteristics, influencing the material's suitability for various applications, including optoelectronics and thermoelectrics. The bandgap can vary depending on the specific composition of CrSSe or CrSeTe, with values of 0.84 eV or 0.62 eV, respectively, as shown in Fig. 2a and b, whereas the bandgap of the CrSe₂ monolayer is 0.75 eV.^{13,37} Due to their layered nature, these materials often show anisotropic electronic properties. As seen in Fig. 2c and d, the electronic states in the density of states (DOS) plot close to the Fermi level are affected by both the chalcogen p-orbitals and the transition metal d-orbitals. In general, the bandgap shrinks when tellurium (Te) is used in place of sulphur (S). Adding other chalcogens can also cause changes in charge carrier mobility and electrical conductivity.

Thermodynamic Stability

The thermodynamic stability of materials is crucial for their applicability in various technological advancements, including nanoelectronics and optoelectronics. Janus monolayers such as CrSSe and CrSeTe exhibit unique properties due to their asymmetrical atomic arrangement, which can influence their structural integrity and vibrational characteristics. The thermodynamic stability of these materials is investigated using Phonopy code.

The thermodynamic stability of CrSSe and CrSeTe Janus monolayers was evaluated by analysing the phonon dispersion curves. A material is considered dynamically stable if all phonon frequencies are real and positive throughout the Brillouin zone. Imaginary frequencies indicate unstable modes, suggesting potential structural distortions or phase transitions. For both CrSSe and CrSeTe Janus monolayers, the phonon dispersion curves were carefully examined, as

**Fig. 2** Variation of electronic band structure by replacing the chalcogen atom for (a) CrSSe and (b) CrSeTe, and the corresponding density of states (DOS) for (c) CrSSe and (d) CrSeTe.

shown in Fig. 3a and b. The absence of imaginary frequencies across the entire Brillouin zone indicates that both materials are dynamically stable under ambient conditions. The reliability of the calculations can also be verified by calculating the cohesive energy which can be formulated⁵ as

$$\Delta E_c = [E(\text{Monolayer})^{2D} - nE(\text{M})^{\text{atom}} - mE(\text{X})^{\text{atom}}]/(n + m), \quad (6)$$

where $E(\text{Monolayer})^{2D}$, $E(\text{Cr})^{\text{atom}}$, and $E(\text{X})^{\text{atom}}$ denote the energy of the Janus monolayer two-dimensional unit cell, isolated Cr atom, and isolated chalcogen atom, and n , m denotes the number of atoms of transition metal and chalcogenide, respectively. Using the above relation, we obtained values of -6.250 eV/atom and -5.597 eV/atom for the cohesive energy of the CrSSe and CrSeTe Janus monolayers, which indicates that the chosen material is stable.

The electronic band structure and density of states provide critical information about carrier effective mass, mobility, type, and concentration of charge carriers, which play an important role for calculating the Seebeck coefficient, electrical conductivity, and electronic thermal conductivity.

Phonon dispersion relations and phonon density of states obtained from DFT-based phonon calculations enable the estimation of lattice thermal conductivity by capturing phonon group velocities and stability of the Janus monolayers. Furthermore, these calculations are helpful for calculating the thermoelectric figure of merit (ZT).

Lattice Thermal Conductivity

The lattice thermal conductivity of Janus monolayers such as CrSSe and CrSeTe exhibits intriguing variations compared to the well-studied CrSe_2 .¹³ Janus monolayers, which possess asymmetric layers due to the different elements on either side of the crystal, generally exhibit reduced lattice thermal conductivity compared to their counterparts like CrSe_2 , as shown in Fig. 4. This reduction is attributed to enhanced phonon scattering mechanisms induced by the asymmetry and the presence of different types of atoms, which disrupt the phonon transport pathways.

For instance, the incorporation of sulphur and tellurium in CrSSe and CrSeTe, respectively, introduces additional mass and bonding variations that increase phonon-phonon

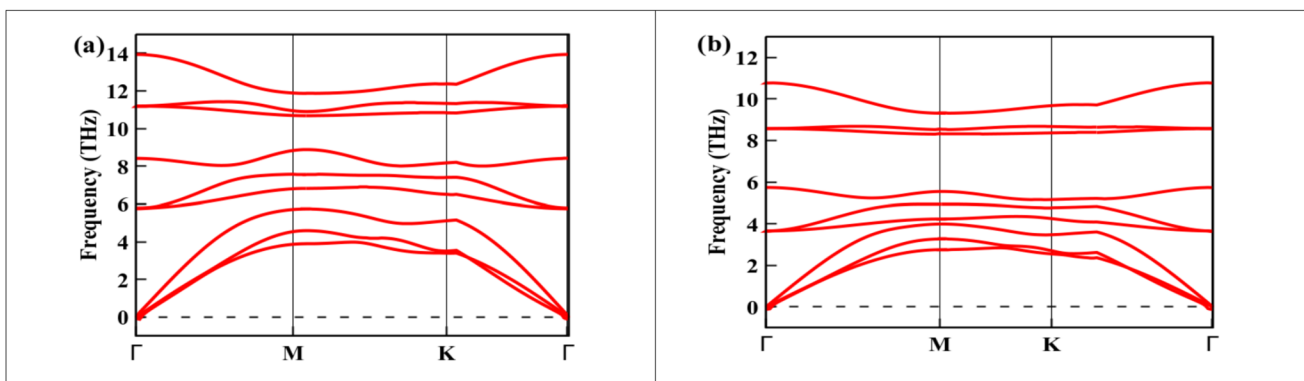


Fig. 3 Variation in behaviour of phonon dispersion curve of (a) CrSSe and (b) CrSeTe Janus monolayers.

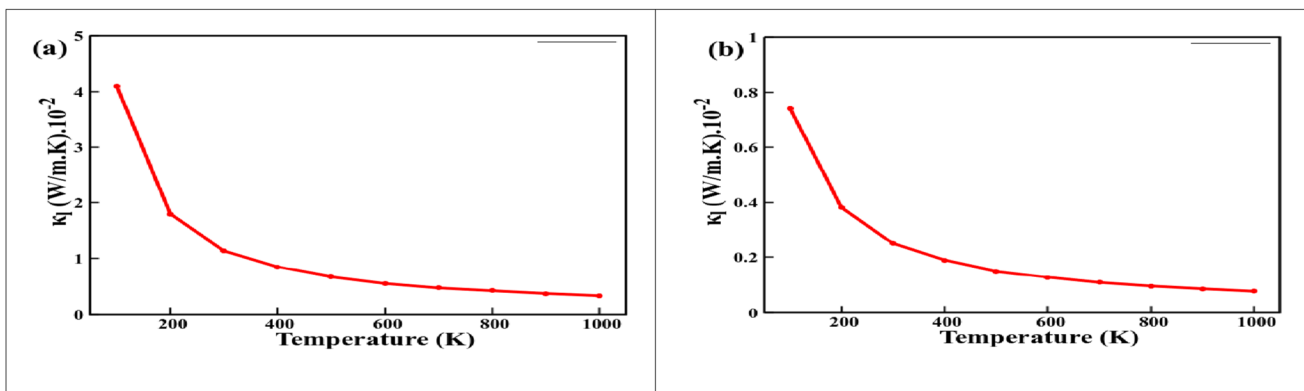


Fig. 4 Decreasing variation of lattice thermal conductivity with respect to temperature for (a) CrSSe and (b) CrSeTe Janus monolayers.

scattering and impede efficient thermal transport. As shown in Fig. 3, the curvature of optical phonon curve is nearly linear, which confirms that the contribution of optical phonon scattering is negligible, whereas acoustic phonon curves are not linear. Therefore, the main role is of acoustic phonon scattering up to moderate temperatures. If there is a further increase in temperature, then lattice thermal conductivity decreases as shown in Fig. 4 due to increased phonon scattering. The main idea of the present study is to investigate the thermoelectric behaviour of Janus monolayers at room temperature.

The obtained values of lattice thermal conductivity are 11.01 W/K, 6.7 W/K, and 4.2 W/K for CrSSe and 0.25 W/K, 0.15 W/K, and 0.10 W/K for CrSeTe, at 300 K, 500 K, and 800 K, respectively. Consequently, while CrSe₂ maintains a relatively higher lattice thermal conductivity due to its more symmetric structure and uniform atomic interactions, Janus monolayers such as CrSSe and CrSeTe typically demonstrate lower thermal conductivity, highlighting their potential for applications where low thermal energy is required.

Effective Mass and Relaxation Time Using Deformation Potential Theory

Understanding the effective mass of charge carriers in 2D materials like Janus monolayers (CrSSe and CrSeTe) is crucial for predicting their electronic transport properties. Firstly, the electronic band structures of CrSSe and CrSeTe Janus monolayers were computed, which involved optimizing the crystal structure and calculating the electronic band structure to determine the energy dispersion of electrons and holes, as shown in Fig. 2a and b. The effective masses of electrons and holes were calculated using the relevant band curvature data near the band extrema (valence band maximum and conduction band minimum). Analysing the effective masses provides insights into the charge carrier mobility and conductivity of CrSSe and CrSeTe Janus monolayers. Lower effective masses indicate higher carrier mobility and better electronic transport properties, desirable for applications such as high-speed electronics or efficient photovoltaics. The average effective masses of electrons and holes in CrSSe and CrSeTe Janus monolayers were determined as given in Table II. These values provide critical information

on the material's electronic transport capabilities, guiding future research and development efforts.

Relaxation time is a crucial parameter in determining the transport properties of charge carriers in semiconductors and 2D materials. In this study, the deformation potential theory is applied to analyse the relaxation time of charge carriers in Janus monolayers (CrSSe and CrSeTe).

This theory sheds light on how lattice vibrations impact the overall conductivity and scattering mechanisms of these materials. According to this theory, the interaction with lattice vibrations (phonons), which are defined by deformation potential constants, is related to the scattering rate of carriers. A previous work³³ provides a brief explanation of how to compute the relaxation period of electrons and holes using the deformation potential constants and elastic constants listed in Table II. Table II shows the computed relaxation time values for the CrSSe and CrSeTe Janus monolayers at various temperatures.

Thermoelectric Properties of Janus CrSSe and CrSeTe Monolayers

The bandgap of the material affects both the electrical conductivity and Seebeck coefficient. Janus monolayers may have different band structures compared to CrSe₂ due to their asymmetric composition, potentially altering the bandgap and electronic properties crucial for thermoelectric performance. Differences in the band structure can influence the effective mass of charge carriers and carrier concentration, affecting electrical conductivity and thermoelectric power factor ($S^2\sigma$).

When considering the formation of Janus monolayers like CrSSe and CrSeTe from CrSe₂, several factors can affect the Seebeck coefficient. Tellurium has different electronegativity and atomic size compared to sulphur. This substitution alters the electronic band structure of the Janus monolayers CrSSe and CrSeTe. Specifically, the position and width of the valence and conduction bands may change, affecting the density of states near the Fermi level. The DOS near the Fermi level can be asymmetrically distributed due to the different atomic species in Janus monolayers. This asymmetry affects the distribution of charge carriers and their effective mass influences the Seebeck coefficient. Substituting Te for S can influence the carrier concentration and

Table II Calculated deformation potential constant (E_β), elastic constant (C_{11}), average effective mass (m_d), and relaxation time (τ) at different temperatures for the two Janus monolayers

Janus monolayer	Carriers	E_β (eV)	C_{11} (J/m ²)	m_d (m_e)	τ (10 ⁻¹⁴ s)		
					300 K	500 K	800 K
CrSSe	h	-4.46	122.97	0.97	7.73	4.64	2.90
	e	-9.97	122.97	0.52	2.88	1.73	1.08
CrSeTe	h	-4.64	95.68	1.04	5.17	3.10	1.93
	e	-9.64	95.68	0.61	2.04	1.23	0.76

mobility within the material. Replacing sulphur (S) with tellurium (Te) in the CrSSe Janus monolayer (forming CrSeTe) alters its electronic band structure and carrier properties, and consequently, the Seebeck coefficient decreases to $1010 \mu\text{V/m}$ ($971 \mu\text{V/m}$) from $1390 \mu\text{V/m}$ ($1340 \mu\text{V/m}$), for p -type (n -type) carriers at room temperature, as shown in Fig. 5a and b. The dependence of S on carrier concentration (n) shows that S is almost constant with carrier concentration (n), i.e., for both n -type and p -type, and expressed as $S \propto (1/n)^{2/3}$.³⁸ These changes are pivotal for optimizing the thermoelectric performance of the material and exploring its potential in energy harvesting applications.

The introduction of different elements (S, Se, Te) in Janus monolayers alters the bandgap and the distribution of

electronic states. This modification can influence the carrier concentration and mobility, impacting electrical conductivity as shown in Fig. 5c and d.

Janus monolayers, like other TMDs, possess multiple valleys in their electronic band structure near the Fermi level. Charge carrier transport is affected by the scattering between these valleys, i.e., due to inter-valley scattering. The inter-valley scattering in the present Janus monolayers is negligible, because the inter-valley scattering requires large momentum transfer. In acoustic phonon scattering, the wavelength is longer, which is not sufficient for inter-valley scattering. Therefore, in the case of Janus monolayers, the band valley has low depth as compared to the CrSe₂ monolayer,

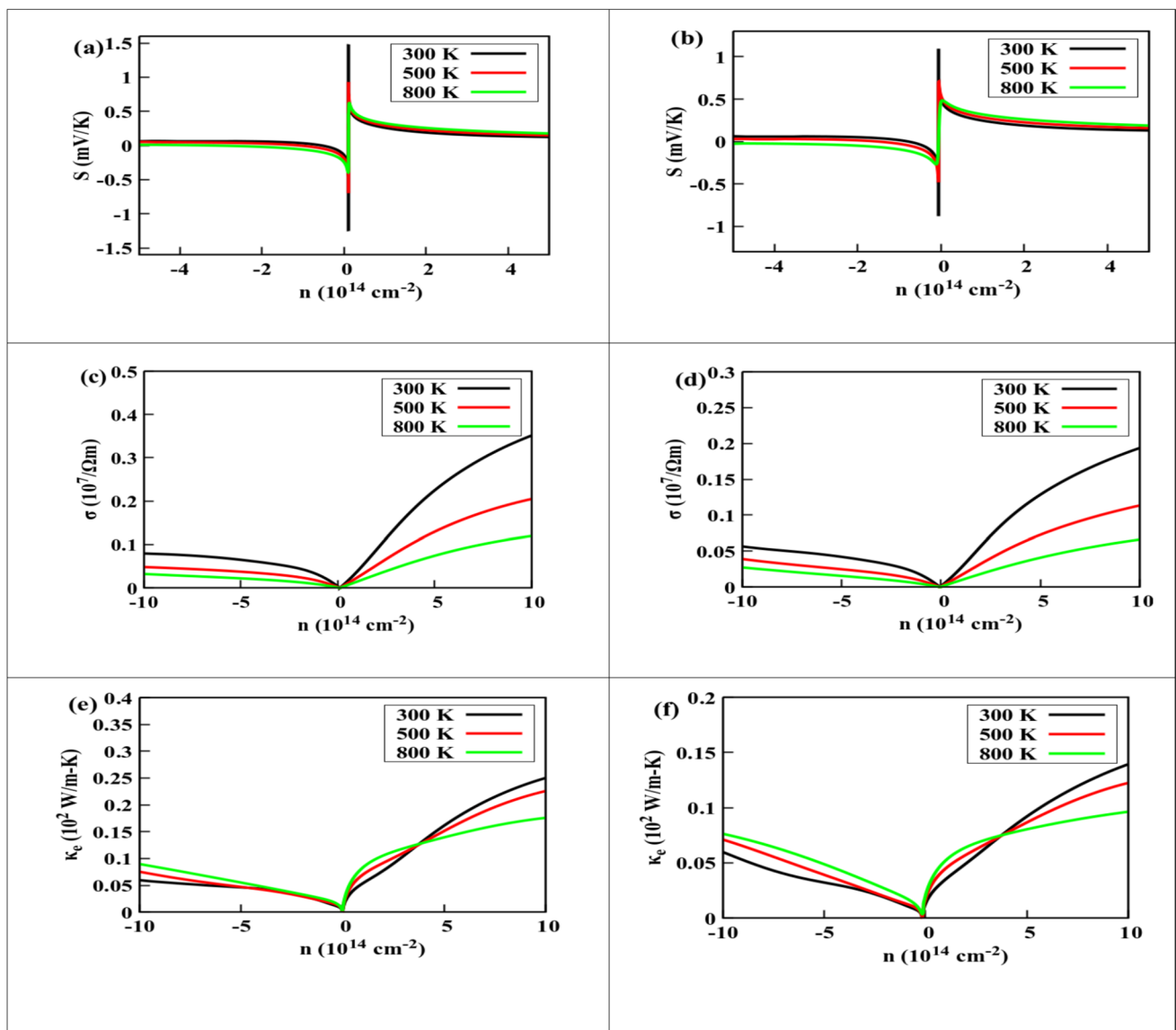


Fig. 5 Seebeck coefficient for (a) CrSSe and (b) CrSeTe Janus monolayers, electrical conductivity for (c) CrSSe and (d) CrSeTe, and electronic lattice thermal conductivity for (e) CrSSe and (f) CrSeTe.

which results in negligible inter-valley scattering, resulting in higher electrical conductivity.^{5,39}

Thus, interfaces between different atomic species in Janus monolayers can introduce additional scattering mechanisms and the electrical conductivity of Janus monolayers like CrSSe and CrSeTe differs from CrSe₂ due to their unique structural and compositional characteristics. These differences impact carrier mobility, carrier concentration, and the overall electronic properties of the material, thereby influencing its electrical conductivity.

The variation of electronic thermal conductivity in Janus monolayers such as CrSSe and CrSeTe is intricately linked to their electrical conductivity due to the fundamental relationship outlined by the Wiedemann-Franz law,⁴⁰ which is expressed as $\kappa_e = L\sigma T$. This law states that the electronic thermal conductivity (κ_e) is proportional to the electrical conductivity (σ) and temperature (T), with the proportionality constant being the Lorenz number (L), whose value is $1.5 \times 10^{-8} \text{ W}\cdot\Omega \text{ K}^{-2}$ for non-degenerate semiconductors.⁴¹ Consequently, materials with higher electrical conductivity tend to exhibit higher electronic thermal conductivity, as shown in Fig. 5e and f.

The power factor (PF) is a crucial parameter in assessing the thermoelectric performance of a material, when

considering the formation of Janus monolayers like CrSSe and CrSeTe from the CrSe₂ monolayer. The variation in the power factor of Janus monolayers is shown in the Fig. 6a and b. The power factor temperature dependence is closely related to S and σ . Changes in the electronic properties and band structure of Janus monolayers can affect how these parameters vary with temperature, thereby influencing the overall thermoelectric performance.

The figure of merit (ZT) of Janus monolayers like CrSSe and CrSeTe compared to CrSe₂ is influenced by their altered electronic band structure, changes in carrier transport properties, and variations in thermal conductivity. These factors collectively determine the material thermoelectric efficiency and its potential for practical applications in energy conversion technologies. Fig. 6c and d shows that, the figure of merit i.e. ZT is higher for CrSeTe Janus monolayer as compared to CrSSe, because of low lattice thermal conductivity of CrSeTe as compared to CrSSe. Highest value of ZT has been attained for CrSSe and CrSeTe with value 0.93 and 0.96 for p-type carriers, respectively, at room temperature, as listed in Table III.

To emphasize the significance of studying Janus monolayers CrSSe and CrSeTe, it is essential to compare their thermoelectric performance with other transition metal

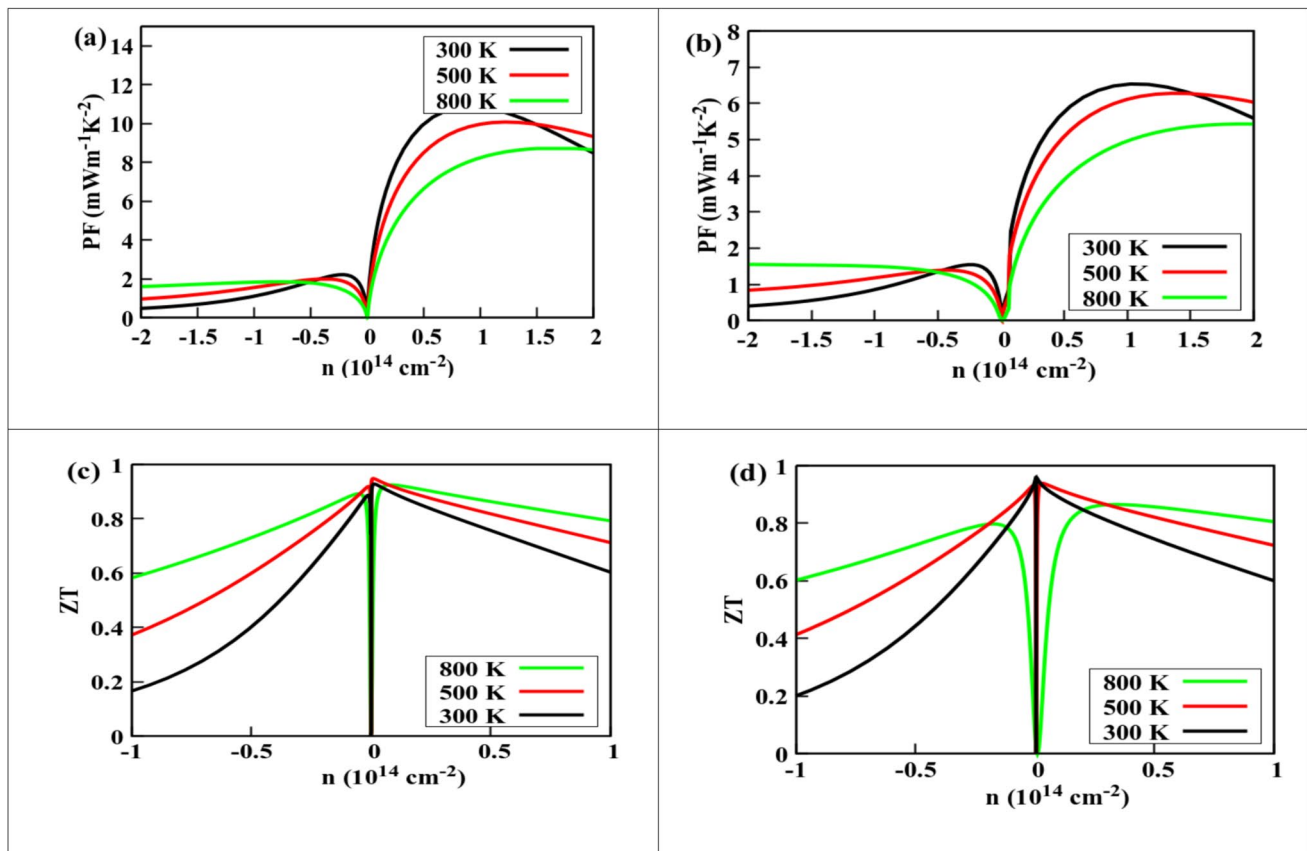


Fig. 6 Variation of power factor for (a) CrSSe and (b) CrSeTe, and figure of merit (ZT) for (c) CrSSe and (d) CrSeTe at different temperatures.

Table III Variation of S and ZT for *p*-type and *n*-type carriers at 300 K, 500 K, and 800 K

Janus monolayer	Carriers	S ($\mu\text{V K}^{-1}$)			ZT		
Temp (K)		300 K	500 K	800 K	300 K	500 K	800 K
CrSSe	p	1390	840	531	0.93	0.93	0.92
	n	1340	787	481	0.92	0.92	0.90
CrSeTe	p	1010	615	394	0.96	0.94	0.86
	n	971	570	358	0.95	0.93	0.80

dichalcogenide (TMD)-based Janus structures, particularly those based on Zr, Mo, and W. The Janus CrSSe and CrSeTe monolayers exhibit moderate Seebeck coefficients and ultralow lattice thermal conductivity. The Mo- and W-based Janus monolayers, such as WSSe and particularly WSTe, achieve substantially higher ZT values up to ~ 2.56 at 1200 K owing to ultralow lattice thermal conductivity and high Seebeck coefficients ($\sim 322 \mu\text{V/K}$ at 300 K).³⁶ Meanwhile, Zr- and Hf-based Janus TMDs (e.g., ZrSeTe, HfSeTe) have also been predicted to deliver outstanding thermoelectric performance: bandgaps ~ 0.56 – 0.90 eV, thermal conductivities around 3 – $5 \text{ W/m}\cdot\text{K}$ at 300 K, and ZT up to ~ 0.94 at 300 K rising to ~ 3.6 at 900 K for ZrSeTe under optimal *n*-type doping.⁴²

However, Cr-based Janus monolayers hold potential advantages in terms of stability and simplicity of composition, which can lead to more accessible material engineering and tuning strategies. Also, the low thermal conductivity of CrSSe and CrSeTe Janus monolayers indicates that these materials are promising candidates for future low-temperature or flexible thermoelectric devices.

Conclusions

The structural and electronic properties of Janus monolayers CrSSe and CrSeTe were studied by employing density functional theory. Electronic bandgap values of 0.85 eV and 0.62 eV were obtained for CrSSe and CrSeTe, respectively. The values of Seebeck coefficient and lattice thermal conductivity for (*n*-type) *p*-type CrSSe and CrSeTe are (1340) $1390 \mu\text{V K}^{-1}$, (971) $1010 \mu\text{V K}^{-1}$, and (11.01) 0.25 W/K , respectively. These parameters were investigated using the semiclassical Boltzmann transport theory. The value of ZT for (*n*-type) *p*-type Janus monolayers CrSSe and CrSeTe are (0.92) 0.93 and (0.95) 0.96 , respectively, at room temperature. The thermoelectric performance of these monolayers was also studied at high temperature, which revealed that the performance of these monolayers is higher than that of the homogeneous CrSe₂ monolayer. The bandgaps and thermoelectric properties of the studied Janus monolayers make them suitable for use in nanoelectronic devices such as photovoltaics, light-emitting diodes (LEDs), and sensors.

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Conflict of interest All the authors declare that they do not have any conflict of interest.

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