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THE STRUCTURAL AND THERMOELECTRIC PROPERTIES OF MAGNESIUM SULPHIDE (MGS_2) CHALCOGENIDE

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Abstract: The pursuit of efficient and sustainable energy conversion technologies has led to a growing interest in the exploration of novel materials with enhanced thermoelectric properties. In this study, we employ first-principles calculations to investigate the structural and thermoelectric characteristics of Magnesium Sulfide (MgS2) Perovskites Chalcogenide, a promising candidate for thermoelectric applications. Our investigation begins with a comprehensive examination of the structural properties of MgS2, delving into the crystal structure, lattice parameters, and bond lengths. Utilizing density functional theory (DFT) and ab initio simulations, we elucidate the electronic structure of MgS2, uncovering crucial insights into its band structure, density of states, and band gap. The electronic properties are explored to understand the nature of charge carriers and their mobility within the material. Furthermore, the thermoelectric properties of MgS2 are thoroughly analyzed, including the Seebeck coefficient, electrical conductivity, and thermal conductivity. Through the calculation of the figure of merit (ZT), we assess the thermoelectric efficiency of MgS2 under varying conditions, such as temperature and doping levels. Our study aims to identify optimal parameters for enhancing the thermoelectric performance of MgS2, which is crucial for applications in waste heat recovery and power generation. The investigation extends to the impact of different crystal structures, chemical compositions, and external factors on the thermoelectric behavior of MgS2, providing a comprehensive understanding of its potential in diverse thermoelectric applications. Insights gained from this study contribute to the ongoing effort to develop efficient and sustainable materials for thermoelectric devices, thereby facilitating advancements in energy harvesting and utilization. In conclusion, our first-principles study of MgS2 Perovskites Chalcogenide sheds light on its structural and thermoelectric properties, offering valuable guidance for the design and optimization of materials in the quest for improved thermoelectric performance.
Keywords: Thermoelectric properties; Chalcogenide; DFT calculations; BoltzTrap

1 INTRODUCTION

Thermoelectric materials have gained considerable attention in recent years for their potential applications in converting waste heat into electricity and solid-state cooling devices. -based materials are particularly promising due to their tunable properties. In this study, we focus on the Magnesium sulfide [MgS2] as a candidate for thermoelectric applications. Using a first principles approach based on density functional theory (DFT), we investigate its structural stability, electronic band structure, and thermoelectric transport properties. Thermoelectric materials are crucial for converting waste heat into usable electrical energy and for solid-state cooling applications. -based compounds have garnered interest due to their tunable electronic and thermal properties. In this study, we focus on the Magnesium Sulfide chalcogenide [MgS2] as a potential thermoelectric material. The first principles approach using density functional theory (DFT) is employed to explore its structural stability, electronic band structure, and thermoelectric transport properties. The pursuit of efficient thermoelectric materials has been fueled by the growing need for sustainable energy solutions. Thermoelectric materials can directly convert heat into electricity, making them vital for waste heat recovery and solid-state cooling applications. -based materials have gained considerable attention due to their tunable properties, offering a promising avenue for enhancing thermoelectric performance. In this project, we delve into the exploration of the Magnesium Sulfide [MgS2] as a potential candidate for thermoelectric applications.
The importance of thermoelectric materials lies in their ability to address critical energy challenges, such as waste heat recovery from industrial processes and vehicle exhausts. These materials can also be used in compact solid-state cooling devices, reducing the reliance on energy-intensive and environmentally harmful refrigeration technologies. Thus, there is a pressing need to identify novel thermoelectric materials with enhanced performance and stability [1] . compare interhemispheric exchange periods with sulfur hexafluoride (SF_6) age to assess interhemispheric transport simulations. The researchers examine how well the dynamics of air exchange between the Northern and Southern Hemispheres are captured by the models that are currently in use. Their results point to differences between simulation projections, indicating that greater modeling is required to comprehend atmospheric transport processes. The bandgap, an essential parameter for thermoelectric materials, was found to be within the desirable range for efficient energy conversion, as reported by[2]. Several studies have investigated the thermoelectric transport properties of [MgS2][3]. reported a

significant positive Seebeck coefficient, suggesting the material can convert temperature gradients into electrical voltage efficiently.

Additionally, they highlighted the inherently low thermal conductivity of [MgS2], a crucial factor for thermoelectric materials, which further enhances its thermoelectric performance. On the other hand [4], explored the electrical conductivity and carrier mobility of [MgS2], providing insights into its charge transport capabilities. Efforts to enhance the thermoelectric performance of [MgS2] have been explored by several researchers. [5] investigated the potential benefits of alloying and doping in [MgS2], demonstrating improved thermoelectric properties through suitable chemical modifications. This suggests that optimization strategies could further elevate the material's performance. As the push for sustainable energy technologies grows, evaluating the environmental impact of materials like [MgS2] becomes essential. [6] conducted a life cycle assessment (LCA) to analyze the environmental sustainability of [MgS2]-based thermoelectric devices. Their study emphasized the need to consider not only the material's thermoelectric properties but also its ecological implications in the context of green energy technologies. First-principles techniques and the Boltzmann transport equation are used by [6] to determine the thermoelectric coefficients of n-doped silicon. A thorough grasp of the electrical characteristics influencing thermoelectric performance is provided by their research, which also offers suggestions for improving silicon-based thermoelectric materials. Recent developments in thermoelectric materials that improve waste heat recovery and renewable energy generating efficiency are reviewed by [7] , which Their results demonstrate how these materials have a great deal of promise to support environmental preservation and energy sustainability. An alternative green solution for turning waste thermal energy into electrical power is thermoelectric power generation, as discussed by [8] . Reviewing current patents and the fundamentals of thermoelectric production, their research emphasizes the benefits of increasing energy conversion efficiency without taking into account the cost of thermal energy intake. The ability of thermoelectric generators to transform waste heat into useful electricity is highlighted in [9] investigation of their potential as renewable energy sources. The study emphasizes how thermoelectric technology is effective in promoting sustainable energy solutions and how it improves the environment. The potential of thermoelectric materials to improve energy sustainability through waste heat recovery systems is covered by [10]. While conventional energy conversion techniques frequently result in substantial heat waste, the chapter emphasizes that thermoelectric generators (TEGs) can effectively capture this lost energy in a variety of applications, such as residential buildings and industrial processes. The goal of continuous research and development in thermoelectric materials is to enhance their performance and scalability for broad applications, notwithstanding obstacles such as high costs and low efficiency. [11] gives a summary of solar energy as a vital renewable resource, outlining its uses, methods, and possibilities in relation to the world's energy requirements. In addition to highlighting continuous developments in solar technology to improve efficiency and accessibility, the chapter emphasizes the significance of solar energy in lowering reliance on fossil fuels. The characteristics and uses of thermoelectric materials, which make it easier to convert heat into electricity and vice versa, are examined by [12]. The basic ideas underlying thermoelectric performance are covered in the article, along with developments in material design that attempt to increase efficiency for energy harvesting and cooling applications. The ecological and socioeconomic effects of oil spills are reviewed by [13], who highlight the long-term effects on ecosystems and communities. The authors offer a framework to direct preparation and response activities with the goal of improving readiness and lessening the negative social and environmental impacts of future spills. According to [14] , solar thermal energy has a lot of promise for effective energy production and heating applications but is sometimes disregarded in talks of renewable energy. In comparison to photovoltaic technology, solar thermal systems are more cost-effective and efficient. The study emphasizes these benefits and urges greater investment in this often-overlooked energy source. When [15] examine the electrical characteristics and stability of octagon-nitrogen (ON), a novel two-dimensional material, they discover that it is a dynamically stable semiconductor with an indirect band gap of 4.7 eV. The work shows that methods including stacking, biaxial tensile strain, and applying an external electric field can be used to efficiently design the band gap, indicating possible uses in electronics and optoelectronics. The structural, electrical, and thermodynamic characteristics of magnesium chalcogenide ternary alloys are examined by [16] . Their findings show that the composition of these materials significantly affects their band gaps and thermal stability. Since these alloys' characteristics may be adjusted, the work sheds light on their possible uses in optoelectronic devices. Using density functional theory, [17]calculate the electronic structures of the magnesium chalcogenides MgS and MgSe in order to examine their band structures and electronic characteristics. Regarding their applicability in semiconductor applications, the study concludes that both materials display unique electronic properties. The structural, magnetic, optical, electronic, and thermoelectric characteristics of Gd_2MgS_4 and Tm_2MgS_4 spinel sulfides are investigated by [18] using first-principles calculations. The study highlights the tunable capabilities of these materials based on compositional alterations, revealing interesting traits for possible use in thermoelectric devices. Using density functional theory, [19] do a first-principles investigation of the structural, electrical, elastic, and optical characteristics of the magnesium chalcogenides MgS, MgSe, and MgTe. The results reveal unique optical properties and electrical structures for every material, indicating their possible use in a range of fields, such as optoelectronics and catalysis.

The primary goal of this work was to examine the thermoelectric and structural characteristics of magnesium sulfide (MgS2) chalcogenide. In order to evaluate whether MgS2 chalcogenide is a good thermoelectric material appropriate for use in high-voltage or low-voltage devices, the study attempts to identify other aspects that may affect or influence its structural and thermoelectric capabilities. Whether magnesium sulfide (MgS2) has sufficient structural and thermoelectric qualities to be appropriate for electrical applications is the main research question. The central research

question is whether magnesium sulphide (MgS2) possesses adequate structural and thermoelectric properties to be suitable for electrical applications.

2 METHOD

This investigation thoroughly analyzed the Magnesium Sulphide (MgS2) compound, concentrating on its structural characteristics through Quantum Espresso in Density Functional Theory (DFT) simulations utilizing the PBE pseudopotential. The electronic structures underwent optimization to determine the ground state properties, with a cut-off energy of 80 Ry and a K-mesh order of 4x4x4 for optimal convergence. Following this, an examination of thermoelectric properties was carried out using the Boltzmann conductivity equation. All thermoelectric properties presented in this study were computed using the BoltzTraP code, covering transport properties such as the Seebeck coefficient, electrical conductivity, Power Factor, and thermal conductivity, as outlined in the work by [20].

2.1 Structural Properties

The below figure 1 depicts the crystallographic structure of Magnesium Sulphide in an orthorhombic form.

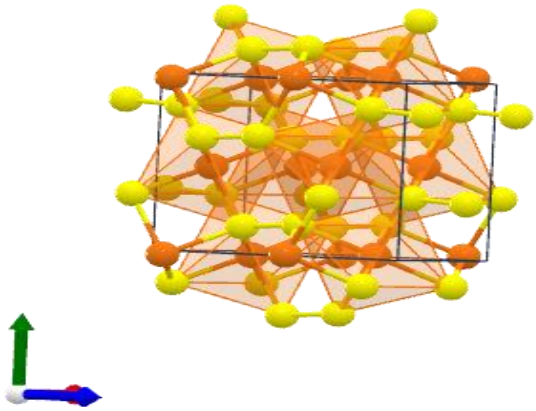

Figure 1 The Crystallographic Structure of MgS2

The crystal structure of MgS2, adopting the orthorhombic Pnma space group, is illustrated below. All essential attributes of chalcogenides are presented. The visualization of the three-dimensional structure is utilized [21] . recommended software, X-Window Crystalline Structure and Densities (XcrySDen). Specifically, the program XcrySDEN, designed for displaying crystalline and molecular structures, was employed to represent iso-surfaces and outlines of the molecules, as depicted in Fig. 1. Graphs were generated using the XMGRACE plotting program. The obtained results closely align with the theoretical and experimental values of lattice parameters observed in related chalcogenides.The stability of the compounds was assessed using the Goldschmidt tolerance factor, calculated as

$$T = \frac{(r_A + r_B)}{\sqrt{2}(r_B + r_X),} \quad (1)$$

where rA, rB, and rX represent the ionic radii of the elements A, B, and X in the structure, respectively. The values are crucial for assessing the stability and distortion of crystal structures. The obtained results affirm the stability of the material, confirming its stable orthorhombic crystal structure.

2.2 Thermoelectric Properties

Boltzmann's transport theory offers a method for estimating thermoelectric transport coefficients with minimal computational efforts. This theory is particularly useful when studying the thermoelectric voltage generated by a temperature difference between two distinct materials. The phenomenon resulting from this temperature gradient, known as the Seebeck effect, gives rise to a voltage of several microvolts per Kelvin [9]. In the case of the MgS2 compound, both charge and thermal transport properties were analyzed using the generalized BoltzTraP program. This program relies on the electronic band structure to derive various transport coefficients, including the Seebeck coefficient denoted as S (measured in V K^{-1}). The Seebeck coefficient represents the ratio of the induced voltage to the temperature gradient and plays a crucial role in understanding a material's thermoelectric properties. The generalized BoltzTraP program facilitates the estimation of the Seebeck coefficient as a function of temperature (T). By examining the Seebeck coefficient's variation with absolute temperature and chemical potential (μ), the program provides valuable insights into the material's thermoelectric behavior. The integration of the transport equation is a key step in these calculations, enabling a comprehensive understanding of how the Seebeck coefficient evolves under different temperature and chemical potential conditions.

This approach allows researchers to explore and characterize the thermoelectric performance of MgS2 efficiently, shedding light on its suitability for applications involving thermoelectric energy conversion. The Seebeck coefficient, as

determined through Boltzmann transport theory, serves as a fundamental metric for evaluating the thermoelectric efficiency and potential applications of materials in the realm of energy harvesting and conversion. The integration of the transport equation enables the calculation of the Seebeck coefficient as a function of both absolute temperature (T) and chemical potential (μ). This process provides a comprehensive understanding of how the Seebeck coefficient varies under different temperature and chemical potential conditions, offering valuable insights into the material's thermoelectric behavior[6]. The Seebeck coefficient as functions of absolute temperature T and chemical potential μ can be calculated by integrating the transport equation.

$$\boldsymbol{S_{\alpha\beta}(\mathrm{T},\mu)} = \frac{1}{eT\,\Omega\sigma_{\alpha\beta}\,(\mathrm{T},\mu)} \int \boldsymbol{\sigma_{\alpha\beta}(\mathcal{E})(\mathcal{E}-\mu)}[\frac{\delta f_{\mu}(T,\mathcal{E})}{\delta\mathcal{E}}]\boldsymbol{d\mathcal{E}} \quad (2)$$

Where the energy projected conductivity tensor, denoted as $\sigma_{\alpha\beta}(\mathcal{E})$, encapsulates system-specific information and is expressed in terms of various parameters. Here, Ω represents the volume of the unit cell, *f* is the Fermi–Dirac distribution function, and *e* denotes the elementary charge. This tensor provides insights into the electrical conductivity of the system as a function of energy $(\mathcal{E})$, offering a means to characterize the material's electronic transport properties. The energy projected conductivity tensor, $\sigma_{\alpha\beta}$ (ε), which contains the system-dependent information, can be expressed as:

$$\boldsymbol{\sigma_{\alpha\beta}(\mathcal{E})} = \frac{e^2}{N}\sum_{i,\,k} \boldsymbol{\tau_{i,k} v_{i,k}(i,k) v_{\beta}(i,k)} \frac{\delta(\varepsilon - \varepsilon i,k)}{\delta\varepsilon} \quad (3)$$

In the given expression, where *N* is the number of k-points, *i* is the band index, *k* represents the wave vector, is the relaxation time dependent on the wave vector, and v_{α} *(i,k)* denotes the group velocity. The group velocity, an essential parameter, can be derived from the calculation of the band structure, providing valuable information about the material's electronic transport behavior.

$$\boldsymbol{v_{\alpha}(i,\,k)} = \frac{1}{\hbar}\frac{\delta\mathcal{E}_{i,k}}{\delta k_{\alpha}} \quad (4)$$

where $\hbar$ is the Planck's constant.

3 RESULTS AND DISCUSSION

As shown in Table 1-5, the calculated thermoelectric figure of merit in this study surpasses the experimental values, and one plausible explanation for this disparity lies in the fact that only electronic thermal conductivity was considered in the calculations. In practice, the total thermal conductivity, encompassing both electronic and phonon contributions, would likely lead to a lower experimentally measured figure of merit. It is worth noting that, in semiconductors, the dominance of electronic thermal conductivity at high temperatures is expected to be a contributing factor to the observed trends.

Table 1 MgS2 Structure Details

Energy Above Hull	0.005 eV/atom
Space Group	$Cmc2_1$
Band Gap	1.01 eV
Predicted Formation Energy	-1.149 eV/atom
Magnetic Ordering	Non-magnetic
Total Magnetization	0.00 μB/f.u.
Experimentally Observed	No

Table 2 Lattice (Conventional)

a	3.94 Å
b	6.82 Å
c	9.15 Å
α	90.00 °
β	90.00 °
ɣ	90.00 °

Volume	245.93 Å³

Table 3 Atomic Positions

Wyckoff	Element	x	y	z
4a	Mg	1/2	0.013605	0.722525
4a	S	1/2	0.344614	0.858485
4a	S	1/2	0.677021	0.585733

Table 4 Symmetry

Crystal System	Orthorhombic
Lattice System	Orthorhombic
Hall Number	C 2c -2
International Number	36
Symbol	$Cmc2_1$
Point Group	mm2
Number of Atoms	12
Density	2.39 g·cm^{-3}
Dimensionality	3D
Possible Oxidation States	Mg^{2+}, S^{-}

Table 5 Chemical Environment

Wyckoff	Species	Environment	IUPAC	CSM
2a	Mg^{2+}	Octahedron	OC-6	1.291

The results obtained from the computational properties, structural properties, and thermoelectric properties are explained in this section. In Figure 2 below, shown that the convergence point for the lattice is taken as 5 at a cell volume of about -328Å³, the space group is P1, the system being triclinic we have a = 3.9412 Å, b = 6.8214 Å, c = 9.1478 Å, 6 sites were used for the asymmetric unit, and it has a crystal structure type. In this section, we delve into the investigation of several thermoelectric properties specifically, electrical conductivity, thermal conductivity, Seebeck coefficient, power factor, and the thermoelectric figure of merit *(ZT)* as depicted in Figure 6. These properties are derived from the energy band gap and the electronic band structure, as thoroughly analyzed in the preceding sections. The material under scrutiny exhibits an indirect band gap that undergoes modification with temperature due to the thermal excitation of electrons and holes. From the analyzed electronic structure, including the band structure and energy density of states, we can readily derive the electrical conductivity spectrum σ_{ave} as a function of temperature, assuming a constant relaxation time.

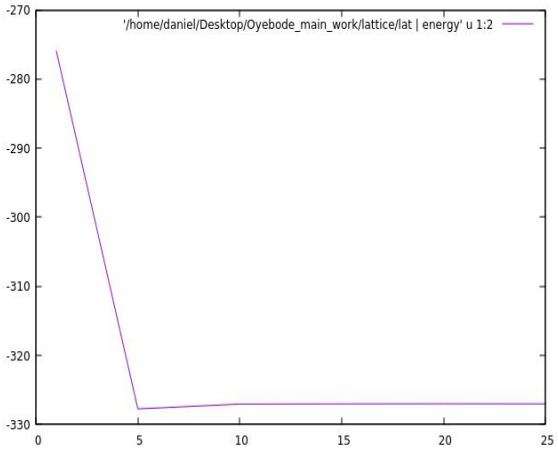

Figure 2 Lattice constant curve of MgS2

For the following figures 3 below, kindly note that μ - $\mathcal{E}_f$ [Ha] is the temperature (T)

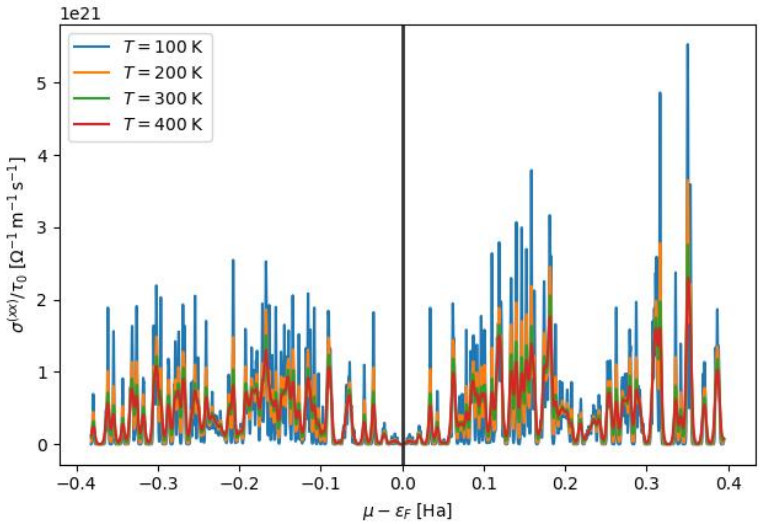

Figure 3 Electrical Conductivity(σ) against Temperature(T)

In Figure 4 below, the temperature range of 300 to 800 K illustrates the variation in the Seebeck coefficient (S) . The (S) values exhibit sensitivity to both carrier concentration and temperature. Figure 4 strongly supports the characterization of MgS2 as a p-type semiconductor, a conclusion drawn from the position of the Fermi level concerning the top of the valence band or the bottom of the conduction band. The (S) spectrum demonstrates a notable decrease in magnitude with the temperature increasing from 100 to 400 K, reflecting the concurrent rise in carrier concentration. At 100 K, the Seebeck coefficient stands at 1.5 × 10−3 V K^{-1}, while at 400 K, the (S) value reduces to 5.00 × 10−4 V K^{-1}. Furthermore, observations from Figure 4 underscore the (S) spectrum's high sensitivity to temperature and carrier concentration variations. The reasonably dispersive nature of the energy bands around the Fermi level contributes to small effective mass values for electrons and holes. This characteristic leads to a diminished Seebeck coefficient, explaining the observed variation in its magnitude with temperature.

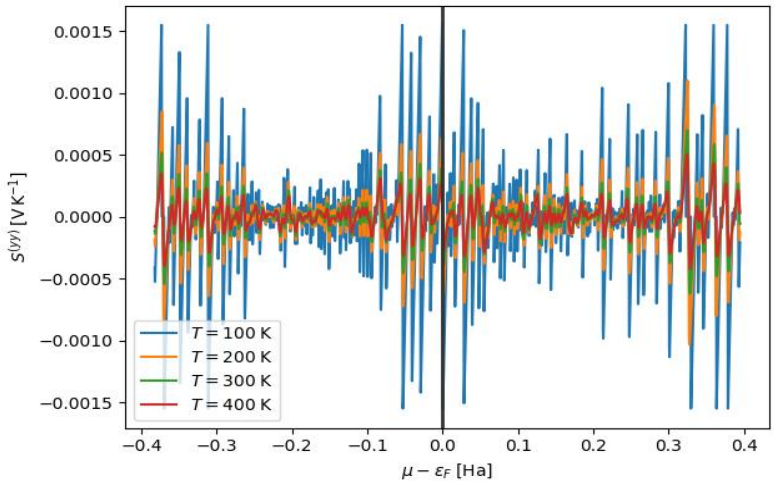

Figure 4 Seebeck(S) against Temperature(T)

The total thermal conductivity is the sum of contributions from both lattice and electronic components, and these components exhibit distinct temperature dependencies. In our investigation, we specifically focused on the electronic component of thermal conductivity (*K*). Essentially, (*K*) is directly proportional to the carrier concentration, electrical conductivity, and mobility of charge carriers, expressed by the equation ($K = \sigma\mu_n$). For the MgS2 compound in this study, the (*K*) component is determined to be 5.0×10^{15} W m^{-1} K^{-1} s^{-1} at 100K and 1.5×10^{16} W m^{-1} K^{-1} s^{-1} at 400K. The temperature-dependent electronic thermal conductivity, as illustrated in Figure 5, exhibits a linear increase in magnitude within the temperature range of 100 K to 400 K. This observed behavior reflects the direct influence of temperature on carrier concentration, electrical conductivity, and charge carrier mobility, collectively contributing to the enhancement of (*K*) as the temperature rises.

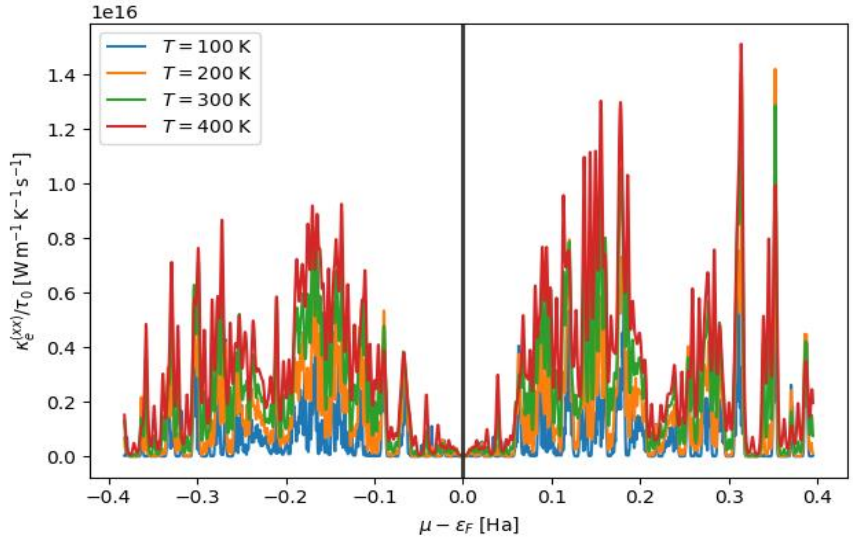

Figure 5 Thermal Conductivity (K) against Temperature(T)

The σ_{ave} spectrum, illustrated in Figure 6 below, reveals a linear increase in magnitude with temperature ranging from 100 to 400 K. This observed behavior in the σ_{ave} spectrum at its maximum can be attributed to the excitation of carriers from the occupied valence band to the unoccupied conduction band at the highest temperature considered in this study (400 K). This excitation process leads to an augmented number of carrier concentrations available for electrical conduction, thereby influencing the observed increase in the electrical conductivity magnitude. Differences in volume observed in comparison to other theoretical findings could be attributed to the choice of pseudopotential[22]. The utilization of PBEsol is noteworthy as it enhances the structural characteristics of compounds in contrast to alternative pseudopotentials. This underscores the efficacy of the generalized gradient approximation (GGA) over the local density approximation (LDA), as demonstrated by [23] . After these calculations, the derived results were employed in determining the various physical properties of the investigated compounds. The power factor ($S^2\sigma$), depicted in Figure 6, is computed from the product of the Seebeck coefficient and electrical conductivity. As the temperature ascends from 100 K to 400 K, there is an increase in ($S^2\sigma$). Specifically, at low temperatures (100 K), the ($S^2\sigma$) value is 5.8×10^{13} W m^{-1} K^{-2} s^{-1}, while at high temperatures (400 K), it reaches approximately 2.5×10^{13} W m^{-1} K^{-2} s^{-1}. This decrease in ($S^2\sigma$) is primarily attributed to the thermally induced elevation in carrier concentration, leading to an enhancement in

electrical conductivity in semiconductors. The substantial magnitude of the ($S^2\sigma$) parameter for the MgS2 compound suggests that it may not be an ideal candidate for applications in thermoelectric devices. The observed characteristics indicate limitations in its thermoelectric potential. The thermoelectric figure of merit ($ZT = \frac{S^2\sigma T}{K}$) illustrated in Figure 7, exhibits interesting and distinctive characteristics. As the temperature undergoes an increment from 100 K to 400 K, the spectrum initially displays a linear increase, reaching its maximum value before subsequently decreasing. This trend observed consistently at each temperature within the 100 K to 400 K range, suggests a complex interplay between temperature and doping concentration. However, with further temperature increase, the magnitude of *ZT* begins a gradual descent, ultimately reaching values close to zero.

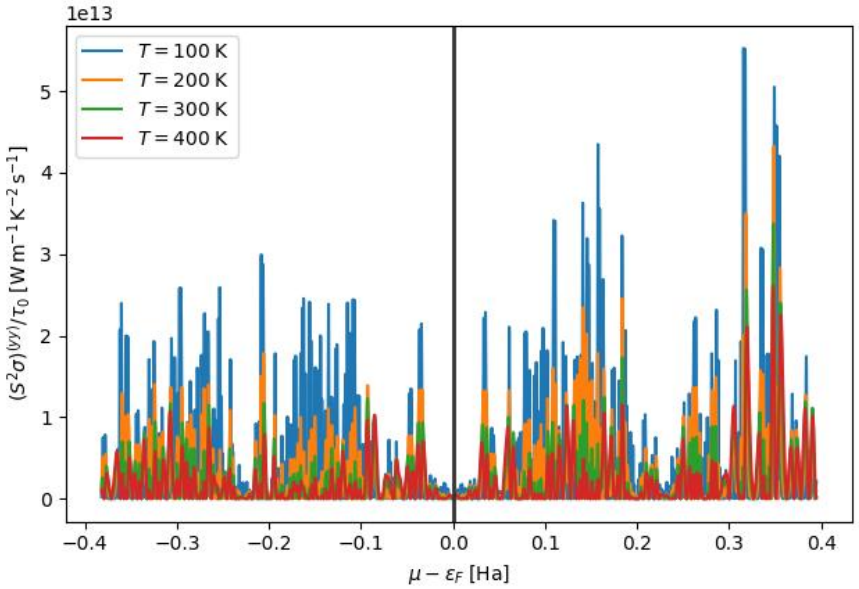

Figure 6 Power Factor (PF) against Temperature(T)

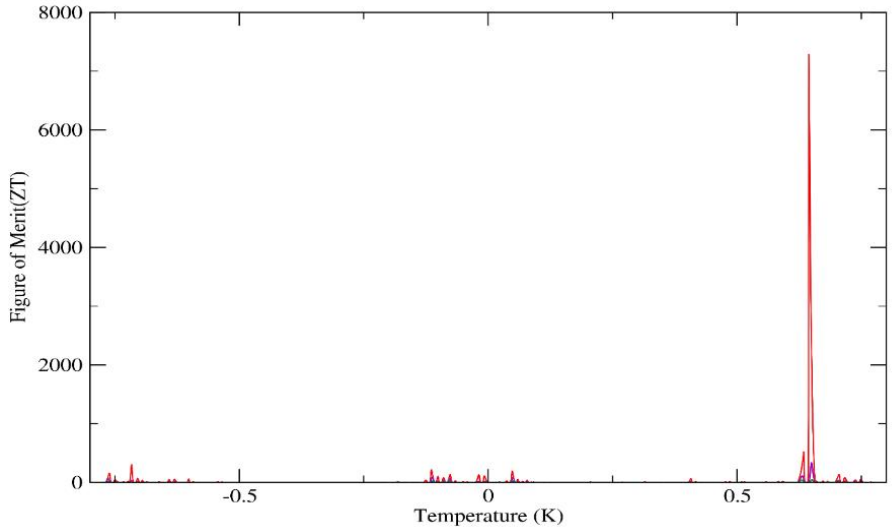

Figure 7 Figure of Merit(ZT) against Temperature(T)

Figure 7 underscores that the *ZT* spectrum is influenced by both temperature and doping concentration. A higher *ZT* value is predominantly derived from a combination of elevated electrical conductivity and reduced thermal conductivity. The interplay between these factors contributes to the nuanced behavior observed in the *ZT* spectrum across varying temperature ranges. The findings suggest that the studied compound holds promise for applications in both cooling devices and other relevant thermoelectric applications. The significant dependence of the ($S^2\sigma$) spectrum on temperature is particularly noteworthy, representing a valuable thermoelectric property. It is important to note that the thermoelectric figure of merit presented in this study focuses solely on electronic thermal conductivity.In insulating systems, where heat is primarily conducted by phonons, the electronic contribution becomes more pronounced with increasing temperature, as demonstrated in Figure 5. In contrast, the contribution from lattice vibrations is expected to sharply decrease at higher temperatures. It should be acknowledged that the presented thermoelectric figure of merit might be somewhat overestimated, as it only considers the electronic thermal conductivity. In reality, the total thermal

conductivity encompasses both electronic and phonon thermal conductivities. This could lead to a reduction in the experimentally measured figure of merit. Notably, in semiconductors, the electronic thermal conductivity tends to increase with temperature, while the phonon thermal conductivity substantially decreases at sufficiently high temperatures (beyond the Debye temperature). Consequently, at elevated temperatures, the thermoelectric figure of merit is anticipated to be predominantly influenced by electronic thermal conductivity. The calculated thermoelectric figure of merit in this study surpasses the experimental values, and one plausible explanation for this disparity lies in the fact that only electronic thermal conductivity was considered in the calculations. In practice, the total thermal conductivity, encompassing both electronic and phonon contributions, would likely lead to a lower experimentally measured figure of merit. It is worth noting that, in semiconductors, the dominance of electronic thermal conductivity at high temperatures is expected to be a contributing factor to the observed trends.

4 CONCLUSION

The investigation of MgS_2's electronic structure and thermoelectric properties through Density Functional Theory (DFT) calculations has provided significant insights. The compound exhibits an indirect band gap that changes with temperature, influencing its thermal conductivity, which is primarily determined by the electronic component. Notably, MgS_2 shows promising thermoelectric properties, highlighted by a substantial figure of merit (ZT) at elevated temperatures and a temperature-dependent power factor ($S^2\sigma$) that indicates its potential as a p-type semiconductor. While the calculated ZT values are higher than experimental results due to an overestimation that considers only electronic thermal conductivity, this underscores the need to account for all thermal conductivity components. Overall, MgS_2 is a promising candidate for thermoelectric applications, and further experimental studies could enhance its practical use in sustainable technologies.

5 RECOMMENDATIONS

The suggestions for improving our knowledge and use of MgS_2 in thermoelectric technology include a number of important steps. First, theoretical predictions regarding the thermoelectric characteristics of MgS_2 under carefully monitored laboratory settings must be verified by a thorough experimental validation procedure. Secondly, to offer a more precise estimate of the thermoelectric figure of merit (ZT), a comprehensive examination of both electronic and phonon thermal conductivities should be carried out. The properties of the material can also be optimized for particular applications by in-depth research on temperature-dependent behavior and the impacts of doping and alloying... Lastly, an environmental effect assessment and an evaluation of MgS_2's practical uses in thermoelectric devices will assist guarantee its viability and sustainability in practical settings.

COMPETING INTERESTS

The authors have no relevant financial or non-financial interests to disclose.

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