FIRST-PRINCIPLES STUDY OF THE THERMOELECTRIC PROPERTIES OF TWO-DIMENSIONAL MATERIALS SiS_X (X = 1, 2)

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ABSTRACT

In this study, density functional theory, combined with the Quantum ESPRESSO simulation package, was employed to investigate the thermoelectric properties of two-dimensional materials SiS and SiS_2. The results show that the Seebeck coefficient of SiS reaches its optimal value at T = 400 K, while that of SiS_2 is maximized at T = 300 K. This indicates that both materials exhibit great potential for converting thermal energy into electrical energy. Specifically, the Seebeck coefficient of SiS is 2.53 mV/K, which is higher than that of SiS_2 at 2.22 mV/K. The electronic thermal conductivity of SiS is 8.39×10^{14} W/mK, significantly higher than that of SiS_2, which is 1.42×10^{14} W/mK. In addition, other characteristic parameters such as electrical conductivity and power factor were also analyzed to provide a more comprehensive evaluation of the thermoelectric performance of SiS and SiS_2. These findings not only shed light on the thermoelectric characteristics of two-dimensional SiS and SiS_2 but also suggest promising applications of these materials in advanced energy technologies.

NGHIÊN CỨU TỪ NGUYÊN LÝ ĐẦU VỀ TÍNH CHẤT NHIỆT ĐIỆN CỦA VẬT LIỆU HAI CHIỀU SiS_X (X = 1, 2)

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TỪ KHÓA

Tính chất nhiệt điện
Lý thuyết phiếm hàm mật độ
Hệ số Seebeck
Vật liệu 2D
Vật liệu nhiệt điện

TÓM TẮT

Trong nghiên cứu này, lý thuyết phiếm hàm mật độ, kết hợp với gói mô phỏng Quantum ESPRESSO, đã được sử dụng để khảo sát các tính chất nhiệt điện của vật liệu hai chiều SiS và SiS_2. Kết quả cho thấy hệ số Seebeck của SiS đạt giá trị tối ưu tại T = 400 K, trong khi đó của SiS_2 đạt cực đại tại T = 300 K. Điều này cho thấy cả hai vật liệu đều thể hiện tiềm năng lớn trong việc chuyển đổi năng lượng nhiệt thành năng lượng điện. Cụ thể, hệ số Seebeck của SiS là 2,53 mV/K, cao hơn so với SiS_2 ở mức 2,22 mV/K. Độ dẫn nhiệt điện tử của SiS là $8,39\times10^{14}$ W/mK, cao hơn đáng kể so với SiS_2 ở mức $1,42\times10^{14}$ W/mK. Ngoài ra, các đại lượng đặc trưng khác như độ dẫn điện và hệ số công suất cũng được phân tích nhằm đánh giá toàn diện hơn hiệu suất nhiệt điện của SiS và SiS_2. Những phát hiện này không chỉ làm sáng tỏ các đặc tính nhiệt điện của SiS và SiS_2 hai chiều mà còn gợi mở những ứng dụng triển vọng của các vật liệu này trong các công nghệ năng lượng tiên tiến.

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1. Introduction

Two-dimensional (2D) materials with efficient thermoelectric energy conversion capabilities play a crucial role in optimizing energy use and minimizing environmental impact. Due to their unique electronic-and thermal properties, numerous 2D materials, such as graphene and phosphorene, have demonstrated potential to enhance thermoelectric performance through optimization of microstructure and electronic characteristics [1]. Notably, metal chalcogenide compounds like MoS_2 and WS_2 stand out for their exceptional electrical conductivity, unlocking possibilities for applications in optoelectronics and transistors [2]. Additionally, hexagonal boron nitride (*h*-BN), with its excellent insulating properties and high thermal stability, contributes to improving the performance of semiconductor devices [3]. Beyond thermoelectrics, 2D materials are also utilized in diverse fields such as biosensors, drug delivery systems, and renewable energy solutions, including photovoltaic panels and long-lasting batteries [4], [5]. Thanks to their structural and property diversity, these materials are paving the way for new technological breakthroughs, revolutionizing energy management approaches and driving sustainable solutions [6].

Among 2D materials, monolayer SiS has garnered significant attention due to its outstanding properties, including a lattice constant of 3.29 Å and an energy bandgap of 2.18 eV [7]. Another study indicates that SiS exhibits higher electron mobility than hole mobility, making it suitable for applications in electron or hole separation [8]. Furthermore, research by Y. Guan and colleagues reveals that the energy bandgap of SiS_2 is 1.39 eV, with the maximum valence band (VBM) and minimum conduction band (CBM) located at high-symmetry points [9].

In this study, the density functional theory (DFT) method is employed to analyze the thermoelectric properties of the 2D materials SiS and SiS_2, revealing their significant potential in modern devices. The findings not only confirm their ability to convert energy and improve device performance but also open new savenues for the development of sensors, energy-absorbing materials, and advanced applications in electronics and clean energy technologies.

2. Calculation method

The theoretical calculations in this study were performed using the Quantum ESPRESSO software [10], employing the density functional theory (DFT) with norm-conserving pseudopotentials for Si and S elements. The structures of the 2D SiS and SiS_2 materials were optimized with an energy cutoff of 60 Ry and a charge density cutoff of 600 Ry [11]. The *k*-point grid was selected as 12×12×1 for both SiS and SiS_2 using the Monkhorst-Pack method [12], with a vacuum region along the z-direction set to a thickness of 20 Å [13]. The PBE (Perdew-Burke-Ernzerhof) exchange-correlation functional was used within the GGA approximation. Calculations were performed to investigate the electronic and thermal properties of the materials at various temperatures. The structural optimization process was carried out at 0 K, with forces on each atom limited to less than 5×10^{-3} Ry/a.u. and stress not exceeding 5×10^{-2} GPa [14], ensuring accurate equilibrium states of the monolayer SiS and SiS_2 structures, providing a foundation for the thermoelectric property analysis.

3. Results and discussion

To fully evaluate the thermoelectric properties of the 2D materials SiS and SiS_2, computational studies were conducted on key parameters such as the Seebeck coefficient (*S*), electrical conductivity (σ), electronic thermal conductivity (*K*e), and power factor (*PF*). These parameters were calculated using the following formulas [15]:

$$S = \frac{\Delta V}{\Delta T} \quad (1) \qquad \sigma = \frac{1}{\rho} \quad (2) \qquad \kappa_e = L.\sigma.T \quad (3) \qquad PF = S^2.\sigma \quad (4)$$

where ΔV is the voltage difference across the material (V), ΔT is the temperature difference across the material (K), ρ is the resistivity (Ω·m), L is the Lorenz constant ($L \approx 2.45\times10^{-8}$ WΩK^{-2}) and T is the absolute temperature (K).

3.1. Seebeck coefficient

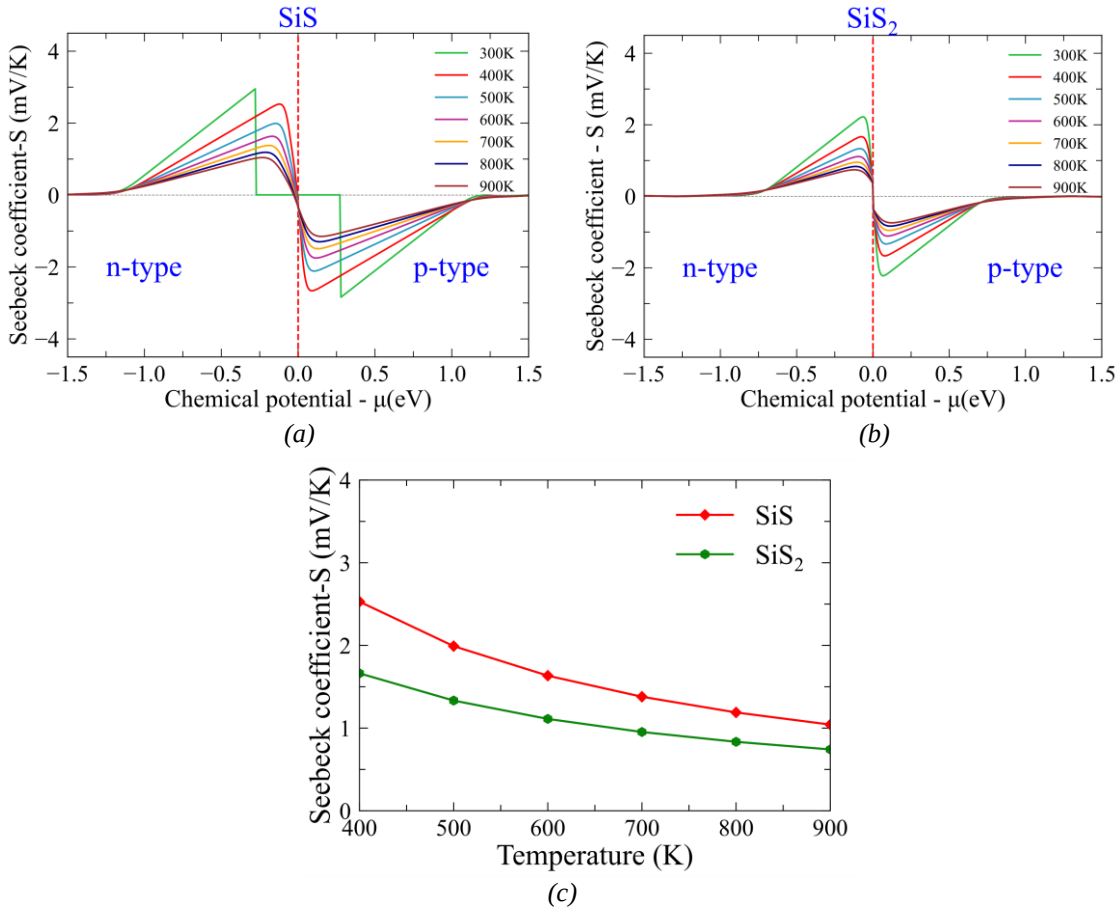

Figure 1. *Seebeck coefficient of 2D materials: (a) SiS; (b) 2D SiS_2; (c) Relationship between temperature and Seebeck coefficient of 2D materials SiS and SiS_2*

Figure 1 illustrates the dependence of the Seebeck coefficient (S) on temperature (T) for two 2D materials, SiS and SiS_2. Specifically, at room temperature (300 K), the 2D SiS material does not generate a voltage difference ($S = 0$), indicating no ability to convert thermal energy into electrical energy. As the temperature rises to 400 K, a voltage difference ($S \neq 0$) begins to appear, indicating thermoelectric conversion capability, as shown in Figure 1a. In contrast, SiS_2 generates a voltage difference ($S \neq 0$) even at room temperature, demonstrating better thermoelectric conversion performance than SiS under normal conditions, as shown in Figure 1b. This indicates that SiS_2 performs more efficiently at room temperature, while SiS requires higher temperatures to achieve optimal performance. Specifically, the Seebeck coefficient of SiS reaches a maximum of 2.53 mV/K at 400 K, which is higher than that of SiS_2 at 2.22 mV/K at 300 K. This suggests that while SiS requires higher temperatures to exhibit thermoelectric conversion and it has a higher Seebeck coefficient than SiS_2 when ideal conditions are reached. Both materials show a decrease in S as temperature increases, reflecting an inverse relationship between S and T, which reduces energy conversion efficiency at higher temperatures (Figure 1c).

The analysis results show that both SiS and SiS_2 exhibit symmetrical *n*-type and *p*-type characteristics, meaning the positive and negative values of *S* are equal in magnitude, reflecting electrical balance between free electrons and holes. At room temperature, SiS_2 converts thermal energy into electrical energy more efficiently, making it suitable for thermoelectric sensors in standard environments. Meanwhile, SiS achieves its highest efficiency at 400 K, making it suitable for thermoelectric applications in high-temperature environments, such as waste heat recovery or high-power electronic devices.

3.2. Electrical conductivity

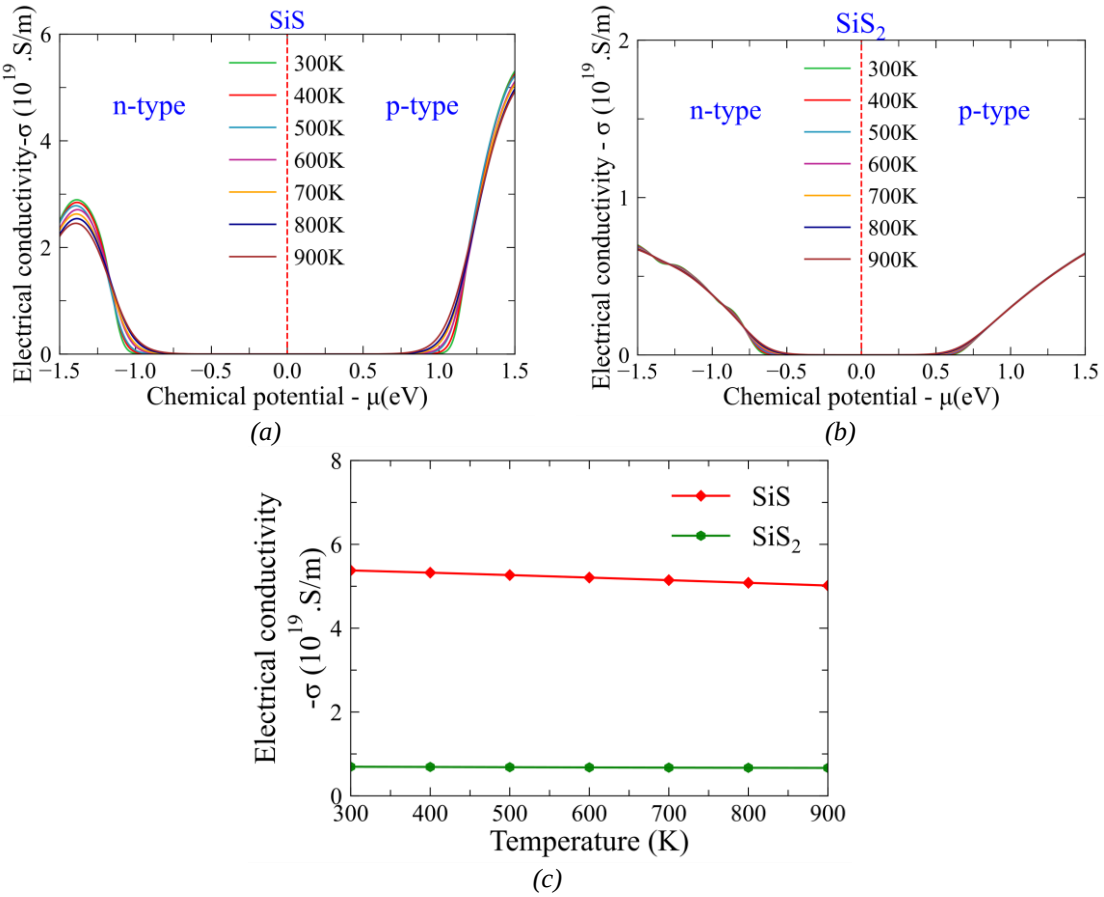

Figure 2. *Electrical conductivity of 2D materials: (a) SiS; (b) SiS_2; (c) Electrical conductivity values as a function of temperature for 2D SiS and SiS_2*

The research results on the conductivity (σ) of 2D materials SiS and SiS_2 as a function of temperature are presented in Figure 2. For SiS, σ begins to appear and increases when the chemical potential exceeds ± 0.7 eV. Additionally, σ in the *p*-type region is greater than in the *n*-type region, indicating that holes play a dominant role in conduction. Temperature has a stronger effect on σ in the *p*-type region, as shown in Figure 2a. Meanwhile, the 2D material SiS_2 exhibits conductivity when the chemical potential is at ± 0.5 eV and tends to increase, particularly in the *n*-type region, suggesting that free electrons are the main contributors to conduction. This reflects SiS_2's more rapid and stable electrical conductivity in high-temperature environments, as shown in Figure 2b.

Moreover, the maximum conductivity of SiS reaches 5.38×10^{19} S/m at T = 300 K, significantly higher than that of SiS_2 at 0.7×10^{19} S/m. Notably, the conductivity (σ) of both

materials is nearly temperature-independent, ensuring stability across over a wide temperature range, as seen in Figure 2c.

Thus, it can be observed that the 2D material SiS has superior conductivity (σ), making it suitable for devices that require strong and stable conduction. Conversely, SiS_2, with its ability to conduct at room temperature, is ideal for low-temperature sensor applications or devices operating under standard environmental conditions. The choice of material will depend on the specific requirements regarding operating temperature and electrical conductivity for each application.

3.3. Electronic thermal conductivity

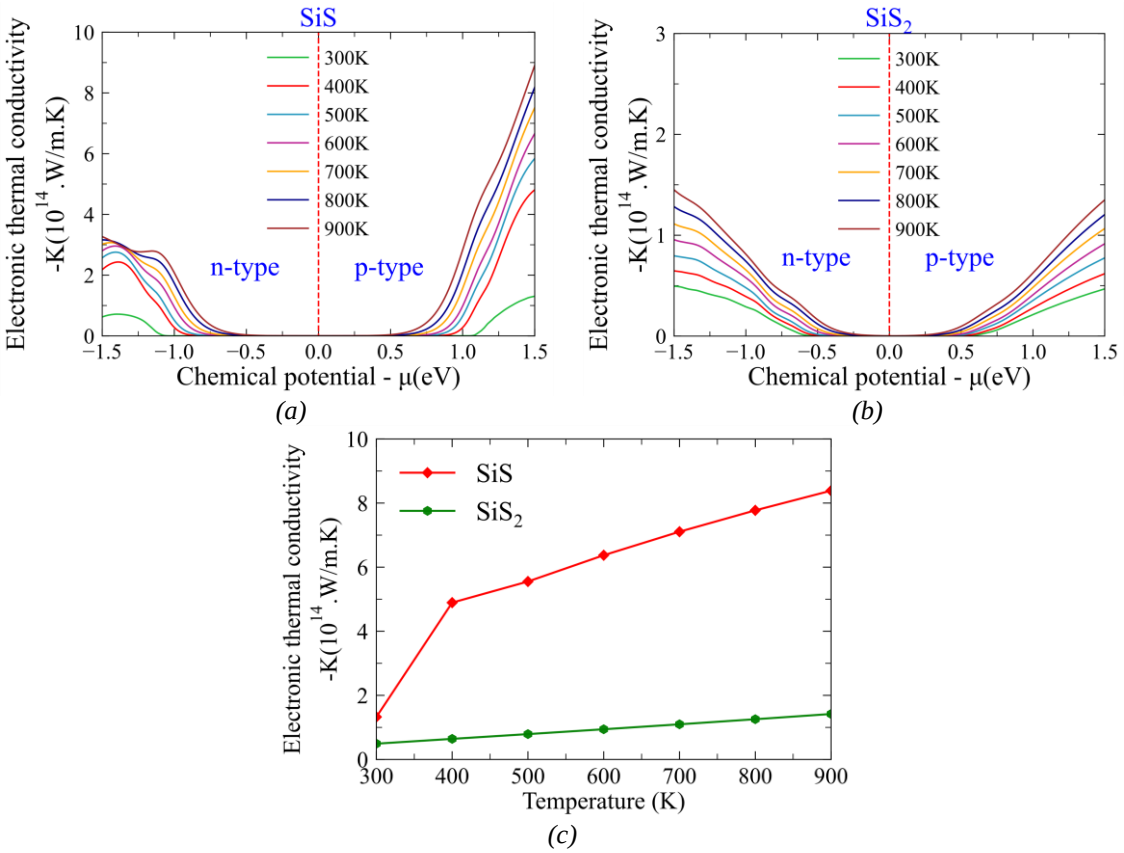

Figure 3. *Electronic thermal conductivity of 2D materials: (a) SiS; (b) SiS_2; (c) Electronic thermal conductivity values as a function of temperature for 2D SiS and SiS_2*

The research results show that, within the temperature range from 300 K to 900 K, the 2D material SiS does not have the ability to conduct heat when the chemical potential is in the range of ± 0.0 ÷ ± 0.6 eV, acting as an electronic insulator. When the chemical potential exceeds ± 0.6 eV, SiS begins to conduct heat, with the *p*-type region having higher thermal conductivity than that in the *n*-type region, as holes play a dominant role. Temperature has a more pronounced effect in the *p*-type region, as shown in Figure 3a. For the 2D material SiS_2, the thermally insulating region is within ± 0.0 ÷ ± 0.3 eV. When the chemical potential exceeds ± 0.3 eV, the ability to conduct heat appears, mainly due to free electrons in the *n*-type region, which can move faster due to their low effective mass, as shown in Figure 3b. The results also show that the electronic thermal conductivity of SiS reaches a maximum of 8.39×10^{14} W/mK at 900 K, significantly higher than that of SiS_2 (1.42×10^{14} W/mK at 900 K). Both materials exhibit an increase in electronic thermal conductivity with rising temperature, indicating a direct relationship, as shown in Figure 3c.

In general, SiS has higher electronic thermal conductivity, making it suitable for applications that require thermal insulation. However, since high electronic thermal conductivity can reduce thermoelectric efficiency, SiS_2, with its lower electronic thermal conductivity, would be more suitable for thermoelectric devices that require efficient thermal management.

3.4. Power factor

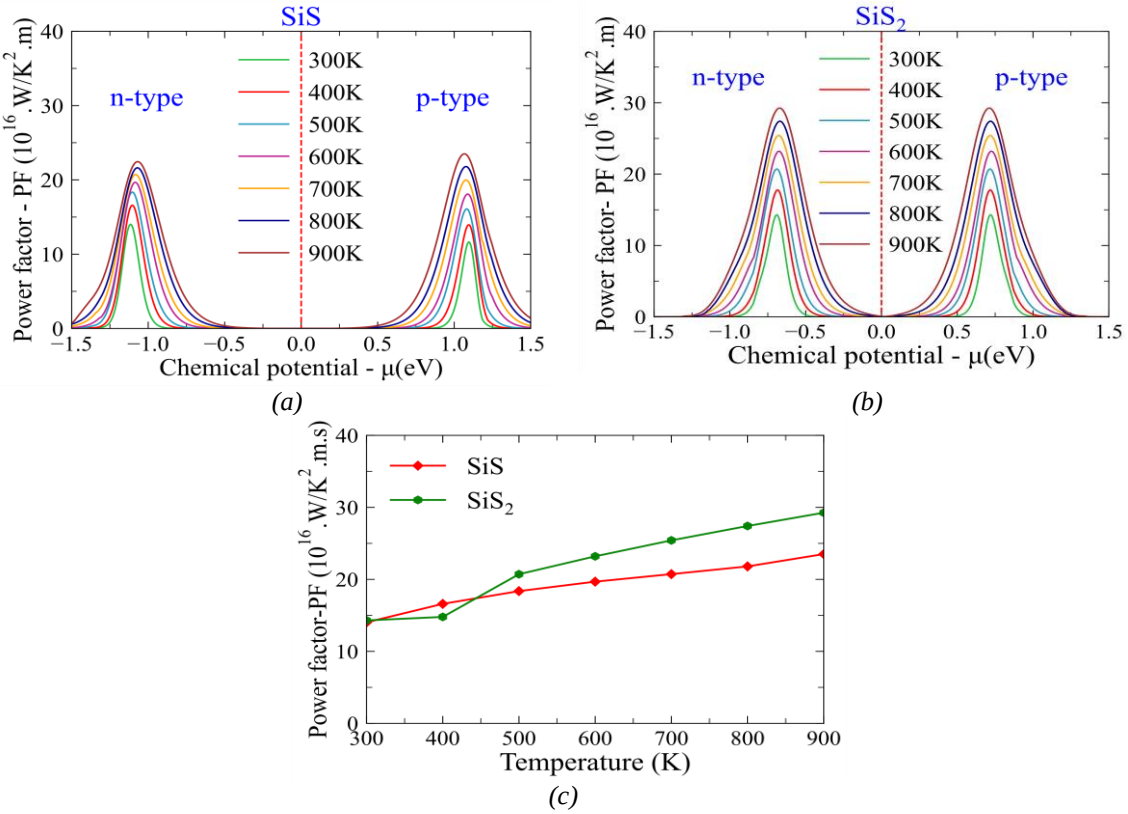

Figure 4. *Power factor of 2D materials: (a) SiS; (b) SiS_2; (c) Power factor values as a function of temperature for 2D SiS and SiS_2*

The research results show that the power factor (PF) of 2D materials SiS and SiS_2 increases with temperature and exhibits symmetry between the *n*-type and *p*-type regions, as illustrated in Figure 4. For SiS, *PF* starts to appear and increases sharply within the chemical potential range of ± 0.5 to ± 1.15 eV, then gradually decreases, as shown in Figure 4a. For SiS_2, *PF* increases within the range of ± 0.1 to ± 0.65 eV and then decreases, as shown in Figure 4b. This indicates that at higher temperatures, the power factor increases at lower chemical potential in both regions, reflecting the temperature dependence of the thermoelectric conversion process.

The maximum power factor for SiS is 23.51×10^{16} W/K²m at T = 900 K, while SiS_2 achieves a maximum value of 29.26×10^{16} W/K²m also at *T* = 900 K, as shown in Figure 4c. Thus, the *PF* of SiS_2 is significantly higher than that of SiS, indicating that SiS_2 has greater thermoelectric conversion potential. Notably, both materials exhibit equivalent power factors in the *n*-type and *p*-type regions, demonstrating symmetry in their thermoelectric properties, which enhances stability and flexibility in applications. The *PF* of both materials increases directly with temperature, enabling devices to achieve higher performance at elevated temperatures. SiS_2 has a broader optimal chemical potential range than SiS, making it more suitable for thermoelectric devices at a range of temperatures, while SiS achieves optimal performance at 400 K for its Seebeck coefficient, and SiS_2 performs optimally at 900 K for its power factor.

4. Conclusion

This study provides a comprehensive theoretical assessment of the thermoelectric behavior of two-dimensional SiS and SiS_2 using first-principles calculations. It highlights the distinct emperature-dependent behavior of each material to, particularly in terms of charge transport and heat conduction. While SiS demonstrates superior performance in properties such as electrical and electronic thermal conductivity, SiS_2 exhibits a more favorable power factor at elevated temperatures. These contrasting yet complementary properties underscore the tunability and functional potential of both materials in thermoelectric applications. Importantly, their temperature-dependent behavior and responsiveness to chemical potential variations suggest their suitability for devices operating across a broad temperature range. Overall, the insights gained from this work pave the way for future experimental validation and integration of 2D SiS and SiS_2 into next-generation energy conversion systems, contributing to the advancement of sustainable and efficient technologies.

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