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The Effect of Biaxial Strain on The Thermoelectric Properties of 2D SiBi

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Abstract

By employing Density Functional Theory (DFT) calculations, the electronic and thermoelectric properties of 2D silicon bismuth (SiBi) materials were analyzed. The 2D SiBi structure was identified as a semiconductor with a bandgap of approximately 0.67 eV. Using Boltzmann transport equations for thermoelectric characterization, we determined that 2D SiBi exhibited significant Seebeck coefficients, reaching values of 1243.79 and 1217.23 μV/K for p-type and n-type doping, respectively. Notably, subjecting the material to a biaxial compressive strain of -1% under ambient conditions results in a considerable enhancement in the Seebeck coefficients, reaching 1361.75 and 1371.85 μV/K for p-type and n-type doping, respectively. These observations indicate that the strategic application of mechanical strain provides a practical pathway for improving the thermoelectric efficiency of 2D SiBi, thereby demonstrating its potential for integration into advanced thermoelectric devices.

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Abstrak

Telah dilakukan analisis sifat elektronik dan termoelektrik material silikon bismut (SiBi) dua dimensi (2D) dengan menggunakan metode perhitungan Density Functional Theory (DFT). Struktur SiBi 2D merupakan semikonduktor dengan celah pita sekitar 0,67 eV. Dengan menggunakan persamaan transport Boltzmann untuk sifat termoelektrik, ditemukan bahwa SiBi 2D menunjukkan koefisien Seebeck yang tinggi, mencapai 1243,79 dan 1217,23 μV/K berturut-turut untuk doping tipe-p dan tipe-n. Menariknya, penerapan regangan tekan dua arah sebesar -1% pada suhu ruang menghasilkan peningkatan yang cukup besar pada koefisien Seebeck, mencapai 1361,75 dan 1371,85 μV/K berturut-turut untuk doping tipe-p dan tipe-n. Temuan ini menunjukkan bahwa penerapan regangan mekanis merupakan salah satu cara efektif untuk meningkatkan efisiensi termoelektrik material SiBi 2D, sehingga menunjukkan potensinya untuk diintegrasikan ke dalam perangkat termoelektrik canggih.

1. Introduction

Since graphene was first isolated in 2004, scientific interest in two-dimensional (2D) materials has been growing owing to their unique structural, mechanical, optical, electrical, and thermal properties [Novoselov et al., 2004]. For instance, graphene and transition-metal dichalcogenides have shown potential applications in areas related to optoelectronics, spintronics, and thermoelectric (TE) devices [Affandi et al., 2018; Affandi & Absor, 2022; Hanna et al., 2020]. Due to the increasing need to enhance the energy efficiency of electronic devices, TE devices have gained prominence.

TE devices facilitate the direct transformation of thermal energy into electrical energy and vice versa, offering potential applications in diverse areas, such as cooling systems, power generation, and refrigeration [Goldsmid, 2016]. Optimal TE materials require a specific set of features such as high electrical conductivity, a substantial Seebeck coefficient, and low thermal conductivity [Wang et al., 2022]. Achieving this delicate tradeoff is a major

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challenge for researchers. The effectiveness of thermoelectric materials is generally assessed by their unitless figure-of-merit (ZT) [Yang et al., 2016], which can be represented as:

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

where S, σ, T, and κ denote the Seebeck coefficient, electrical conductivity, absolute temperature, and thermal conductivity, respectively. High ZT values are ideally achieved through a large power factor ($S^2\sigma$) and a reduced thermal conductivity (κ).

Numerous investigations have concentrated on exploring the thermoelectric characteristics of two-dimensional (2D) materials, including those composed of group IV–V elements such as XBi (X = Si, Ge, Sn) [Wang et al., 2019]. These materials exhibit a hexagonal structure with an A_2B_2 chemical arrangement and are known to possess narrow bandgaps, thereby promising elevated thermoelectric coefficients at higher temperatures [Slack & Tsoukala, 1994; Singh & Pickett, 1994; Sales et al., 1996; Tritt, 2001]. Strategies for further enhancing these properties include modulation of the electronic band structure through, for instance, pressure tuning [Pei et al., 2012; Bartkowiak & Mahan, 1999; Jones et al., 1998; Itskevich et al., 1997; Sologub et al., 1980].

The silicon bismuthide (SiBi) monolayer is a promising 2D material for thermoelectric applications due to its low thermal conductivity, which is essential for efficient performance. However, its moderate bandgap and low power factor [Bafekry et al., 2020] limit its practical use. While strain engineering has been shown to enhance the thermoelectric properties of other materials—such as a ZT value of 3.25 for HfS_2 monolayers at 6% biaxial strain [Patel et al., 2021] and 4.88 for Janus ZrSSe monolayers under 6% tensile strain [Huang et al., 2023]—the effect of strain on SiBi remains largely unexplored. This leaves a significant gap in understanding how strain can improve SiBi's thermoelectric performance.

This gap is significant because experiments struggle to isolate and measure the effects of strain on the electronic and thermoelectric properties of silicon bismuth (SiBi). This difficulty leads to unclear performance metrics, such as variations in the Seebeck coefficient and bandgap tuning. Our research addresses these challenges by utilizing density functional theory (DFT) calculations and Boltzmann transport equations. By analyzing the impact of biaxial strain on SiBi's electronic structure and thermoelectric efficiency, we clarify these ambiguities and reveal the mechanisms that drive performance improvements.

Several studies have investigated the effect of strain on the thermoelectric properties of two-dimensional materials, including the SiBi monolayer. The study conducted by [Bafekry et al., 2020] found that the application of uniaxial and biaxial strain on SiBi monolayer can induce a transition from a semiconductor to a metal, demonstrating the potential for controlling electronic properties through strain engineering. However, existing research on SiBi monolayer under strain is still limited and often focuses only on general electronic behavior without a comprehensive analysis of thermoelectric efficiency across a broad range of strain conditions. Therefore, there remains a clear research gap in systematically understanding how various strain types and magnitudes affect the thermoelectric performance of SiBi monolayers. This study aims to address this gap by providing an in-depth computational investigation of the strain-induced modifications in the thermoelectric properties of SiBi, thereby contributing to the development of more efficient thermoelectric materials.

We found that applying a biaxial compressive strain of -1% significantly enhances the thermoelectric efficiency of SiBi by improving both the Seebeck coefficient and the power factor. These findings position SiBi as a strong candidate for advanced thermoelectric devices, particularly for applications at room temperature. This study not only demonstrates the practical potential of SiBi but also advances our understanding of strain-engineered thermoelectrics, addressing important gaps in both theoretical and experimental knowledge.

2. Research Methods

DFT simulations were conducted in this research using the Quantum ESPRESSO package [Giannozzi et al., 2017] to achieve structural optimization and analyze the electronic properties of the 2D SiBi material. The exchange-correlation functional used in this study was the Perdew-Burke-Ernzerhof (PBE) form of the Generalized Gradient Approximation (GGA) [Perdew et al., 1996], with a kinetic energy cutoff set to 60 Ry. The SiBi monolayer has a hexagonal honeycomb structure consisting of four three-coordinate Si and four-fold coordinate Bi atoms, as shown in **Figure 1**.

In our DFT calculations, we represented the SiBi monolayer as a periodic slab with a substantial 20 Å vacuum layer to prevent interactions between neighboring layers. In this case, we used a 12 × 12 × 1 k-point mesh, and the crystal geometries underwent full relaxation until the force on each atom was less than 1×10^{-5} eV/Å. The optimized structural parameters from these calculations are shown in **Table 1**.

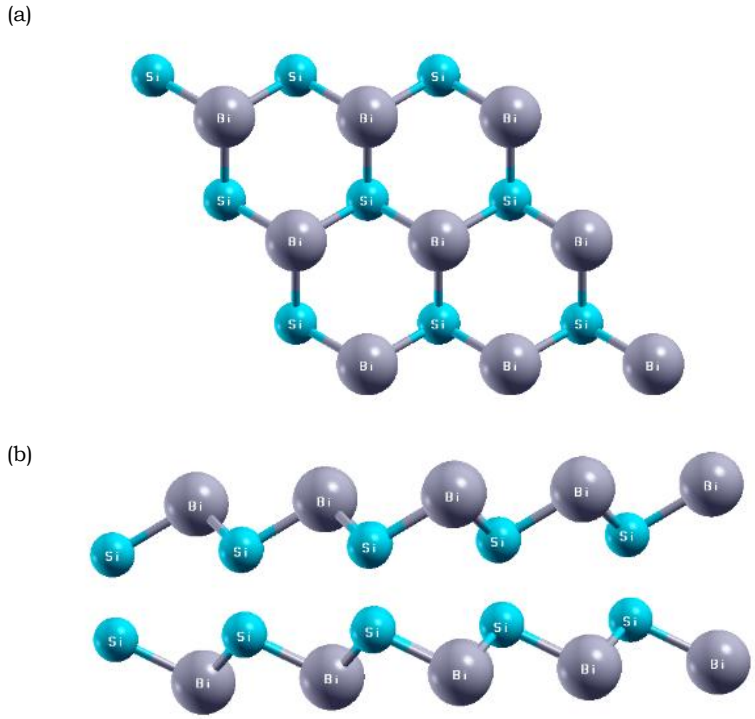


Figure 1. Atomic structure of the SiBi monolayer, visualized using XCrySDen software, shown from (a) a top view and (b) a side view.

Table 1. Structural-related in the SiBi monolayer.

a(Å)	d_{Si-Bi}(Å)	**Ref**
4.122	2.6966	This work
4.160	2.6900	Ref.[Somaiya et al., 2020]
4.090	2.6900	Ref.[Bafekry et al., 2020]

We obtained an optimized lattice constant of 4.122 Å for a SiBi monolayer. The bond length of Si-Bi ($d_{\text{Si-Bi}}$) in the SiBi monolayer was 2.6966 Å. Overall, we observe that these parameters align well with the findings from prior studies [Somaiya et al., 2020; Bafekry et al., 2020].

The thermoelectric properties of this material were determined using the Boltzmann transport equation via the BoltzTrap code [Madsen & Singh, 2006]. According to this equation, the Seebeck coefficient and electrical conductivity can be expressed as follows:

$$S(\mu,T) = \frac{ek_B}{\sigma}\int d\varepsilon\left(-\frac{\partial f_\mu(\varepsilon,T)}{\partial\varepsilon}\right)\Xi(\varepsilon)\frac{\varepsilon-\mu}{k_BT} \tag{2}$$

$$\sigma(\mu,T) = e^2\int d\varepsilon\left(-\frac{\partial f_\mu(\varepsilon,T)}{\partial\varepsilon}\right)\Xi(\varepsilon) \tag{3}$$

where k_B is Boltzmann constant and μ is the chemical potential. The transport distribution function Ξ(ε) and the Fermi Dirac distribution function $f(\varepsilon,T)$ are given as [Kaur et al., 2019]:

$$f(\varepsilon,T) = \frac{1}{(\exp\left(\frac{\varepsilon-\mu}{k_BT}\right)+1)} \tag{4}$$

$$\Xi(\varepsilon) = \sum_k \tau_k\delta(\varepsilon-\varepsilon_k)v_k^\alpha v_k^\beta \tag{5}$$

3. Results and Discussions

The electronic band structures of the SiBi monolayers are shown in **Figure 2**. without considering spin-orbit coupling. Our results show that the SiBi monolayer exhibits the characteristics of a direct-gap semiconductor featuring an energy gap of 0.67 eV. This outcome aligns with the latest findings regarding the electronic structure of the SiBi monolayer with an energy gap of 0.674 eV [Somaiya et al., 2020].

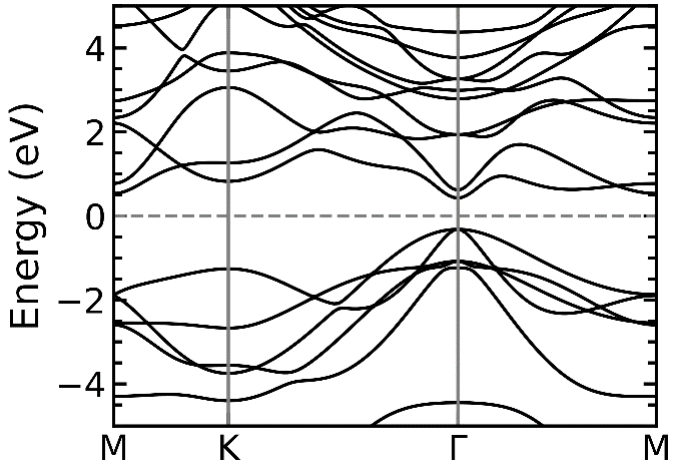


Figure 2. The Electronic Band Structure of SiBi Monolayer

We will now focus on examine the impact of isotropic biaxial strains, which are defined as $\varepsilon = \left(\frac{(a-a_0)}{a_0}\right)$, where a_0 and a represent the lattice constants for the pristine and strained cases. For hexagonal crystal geometries (where $a = b$), we introduce strain by changing the system lattice constant within the range of ±7% at an interval of 1%. **Figure 3** shows the changes in the band structure under different applied biaxial strains.

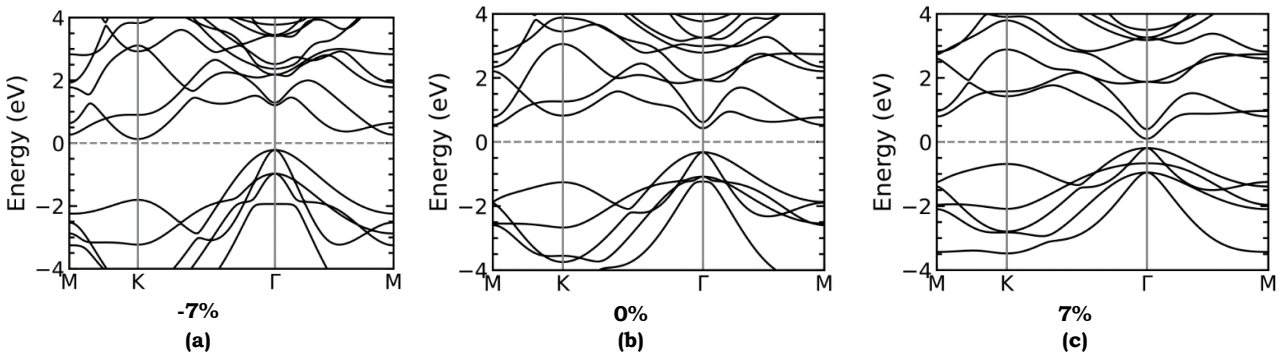


Figure 3. The Electronic Band Structure of SiBi Monolayer under biaxial (a) compressive and (c) tensile strain

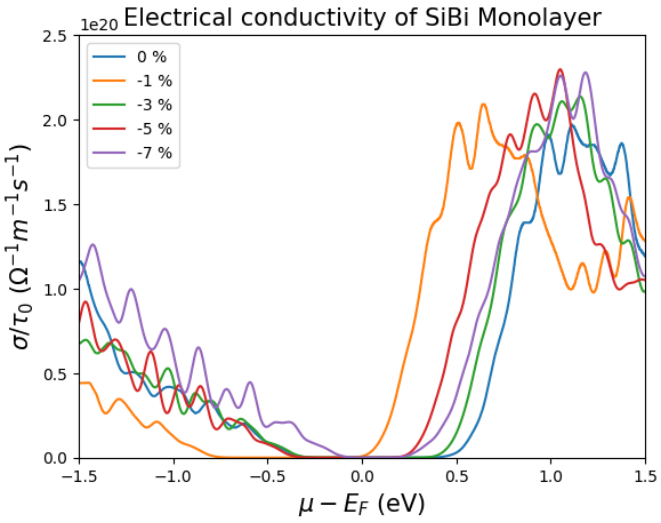
Based on **Figure 3**, it can be observed that applying biaxial compressive strain in the range of 0% to -7% increases the bandgap value, shifting the material towards insulating behavior. Meanwhile, applying biaxial tensile strain in the range of 0% to +7% also increases the bandgap value, resembling conductive properties. However, under both biaxial compressive and tensile strain, the 2D SiBi material retains its direct bandgap characteristics.

Our calculations revealed that applying biaxial compressive or tensile strain can also influence the energy gaps of the SiBi monolayer. **Table 2** lists the energy gaps of the 2D SiBi under biaxial strain. From the table, it is found that the energy gap reaches 0.76 eV by applying biaxial compressive strain (-1%) at room temperature. The decrease in energy gap observed in the SiBi monolayer under compressive strain (-3% to -7%) can be attributed to several key factors related to lattice deformation and electronic structure modifications. Compressive strain reduces the interatomic distance, enhancing orbital hybridization between Si and Bi, which leads to band broadening and a narrower band gap. Additionally, strain-induced lattice symmetry distortion shifts the energy levels of the conduction band (CB) and valence band (VB) closer together, further reducing the gap. Overall, the narrowing of the energy gap in 2D SiBi under compressive strain is primarily driven by enhanced orbital interactions, band structure modifications, and quantum mechanical effects within the crystal lattice.

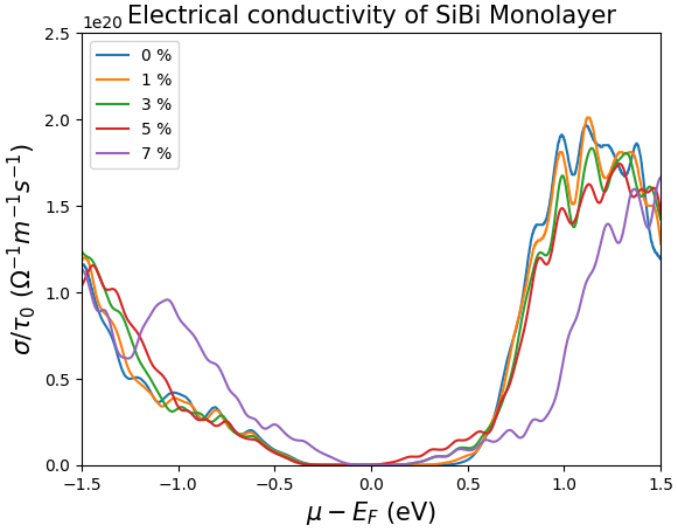
The thermoelectric properties of SiBi monolayers were examined using a constant relaxation time approximation within the semi-classical Boltzmann approach [Goldsmid, 2016]. BoltzTrap [Madsen & Singh, 2006] was used to compute parameters dependent on relaxation time, such as electrical conductivity (σ/τ) and the electronic component of thermal conductivity. Figure 4 shows the electrical conductivity of the SiBi monolayer under biaxial strain.

Table 2. The Energy gap of SiBi Mololayer under biaxial strain

Strain (%)	Energy Gap (eV)
7	0.22
5	0.33
3	0.45
1	0.59
0	0.67
-1	0.76
-3	0.66
-5	0.55
-7	0.28



(a)



(b)

Figure 4. The electrical conductivity of SiBi monolayer under biaxial (a) compressive and (b) tensile strain

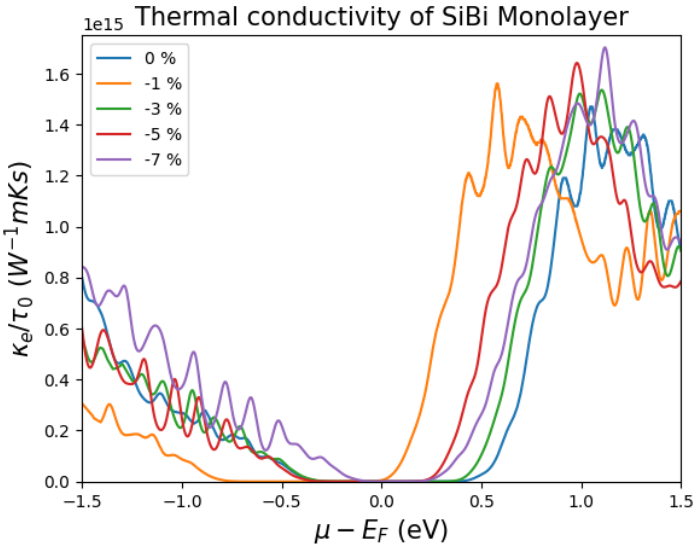
Figure 4 shows that the electrical conductivity of the SiBi monolayer is highest under a biaxial compressive strain of -1% at ambient temperature. This improvement is due to changes in the electronic band structure, such as a narrower bandgap and energy levels shifting closer to the Fermi level, which enhance carrier mobility. Compressive strain reduces carrier scattering and increases the density of states near the Fermi level, resulting in better conductivity. In contrast, tensile strain broadens the bandgap, reducing carrier transport and lowering conductivity.

Figure 5 depicts the thermal conductivity of SiBi under biaxial strain, peaking at -7% compressive strain at room temperature. This can be explained by improved phonon transport properties. Compressive strain reduces

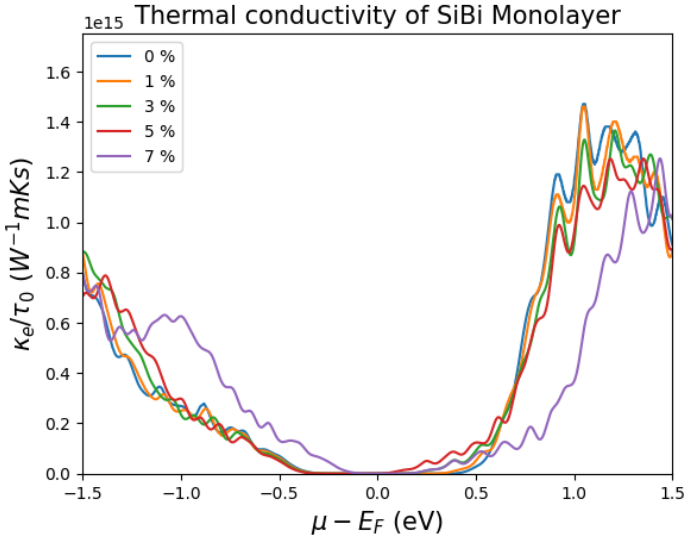
anharmonic phonon scattering, allowing phonons to move more efficiently and increasing thermal conductivity. However, excessive compressive strain can disrupt the atomic arrangement, decreasing lattice integrity and thermal conductivity. On the other hand, tensile strain increases anharmonicity, hindering phonon transport and reducing thermal conductivity.

The changes in electrical and thermal conductivity are closely linked to the material's electronic and vibrational properties when under strain. The relationship between carrier mobility and phonon scattering under various strain conditions demonstrates the tunability of SiBi's thermoelectric properties. Further research utilizing advanced models, such as Boltzmann transport theory that incorporates full phonon and electron interactions, could offer a deeper understanding of the effects of strain on SiBi's behavior.

Additionally, the variation of the Seebeck coefficient (S) with chemical potential (μ) at different temperatures, depicted in **Figure 6**, reflects the sensitivity of thermoelectric properties to carrier concentration and temperature. The Seebeck coefficient increases as the electronic band structure under strain favors asymmetry in carrier distribution, enhancing thermopower. These results highlight the interplay between strain and material properties, suggesting that controlled biaxial strain can be an effective strategy to tune the thermoelectric performance of SiBi monolayers.



(a)



(b)

Figure 5. The thermal conductivity of SiBi monolayer under biaxial (a) compressive and (b) tensile strain

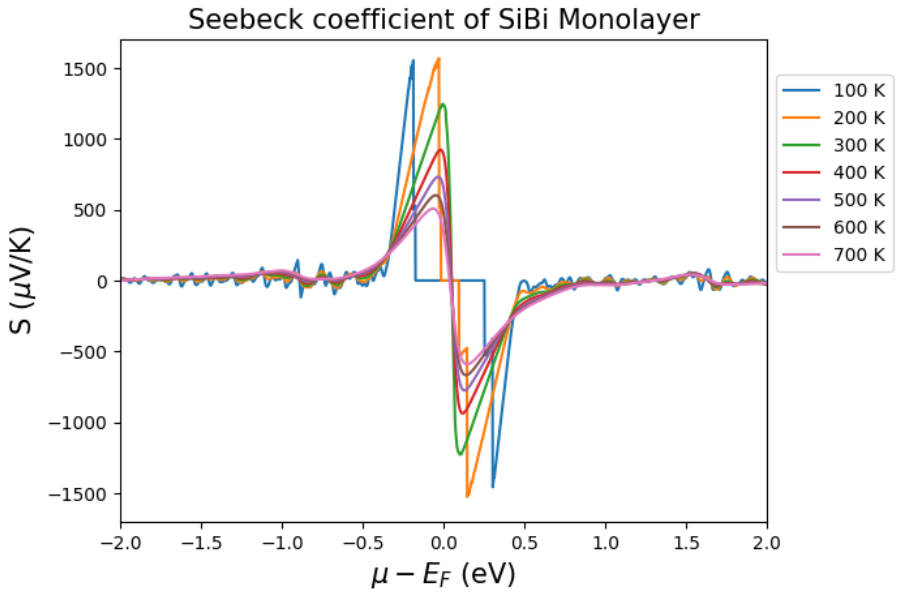


Figure 6. Variation of Seebeck coefficient as chemical potential of SiBi monolayer at different temperature

Figure 6 illustrates two distinct peaks in the Seebeck coefficient (S) near the Fermi level across varying temperatures, indicative of optimized thermoelectric behavior for both p- and n-type doping. At 300 K, the Seebeck coefficient attains its highest values of 1243.79 μV/K for p-type doping and 1217.23 μV/K for n-type doping, attributed to the asymmetry in the electronic density of states around the Fermi level. However, these values decline significantly with increasing temperature, reaching 507.48 μV/K and 589.60 μV/K, respectively, at 700 K. This decrease is likely due to enhanced carrier excitation at higher temperatures, which reduces the thermoelectric voltage per unit temperature gradient.

In **Figure 7**, the application of -1% biaxial compressive strain at room temperature further amplifies the Seebeck coefficient, achieving peaks of 1361.75 μV/K for p-type doping and 1371.85 μV/K for n-type doping. This enhancement can be attributed to strain-induced modifications in the electronic band structure, such as the sharpening of energy bands or an increase in the asymmetry of carrier distribution, which strengthens the thermopower. These findings underscore the critical role of strain engineering in optimizing thermoelectric performance, particularly for achieving high Seebeck coefficients in SiBi monolayers under varying doping conditions.

After determining the values for thermal and electrical conductivity, as well as the Seebeck coefficient, we calculated the power factor (PF) using the equation:

$$PF = S^2\sigma \tag{6}$$

We evaluated the PF based on the chemical potential at various temperatures, as depicted in **Figure 8**. Notably, the PF increases with rising temperature. The peak value of PF was found to be 2.24×10^{11} W/K²ms at T=300 K for n-type doping. At T=700 K, the peak value of PF reached 5.34×10^{11} W/K²ms.

We then plotted the PF as a function of the chemical potential at different biaxial strains at T = 300 K, as shown in **Figure 9**. An interesting finding is that biaxial strain affects PF of the SiBi monolayer. These findings indicate that SiBi monolayers are promising candidates for thermoelectric materials that can be tuned by strain.

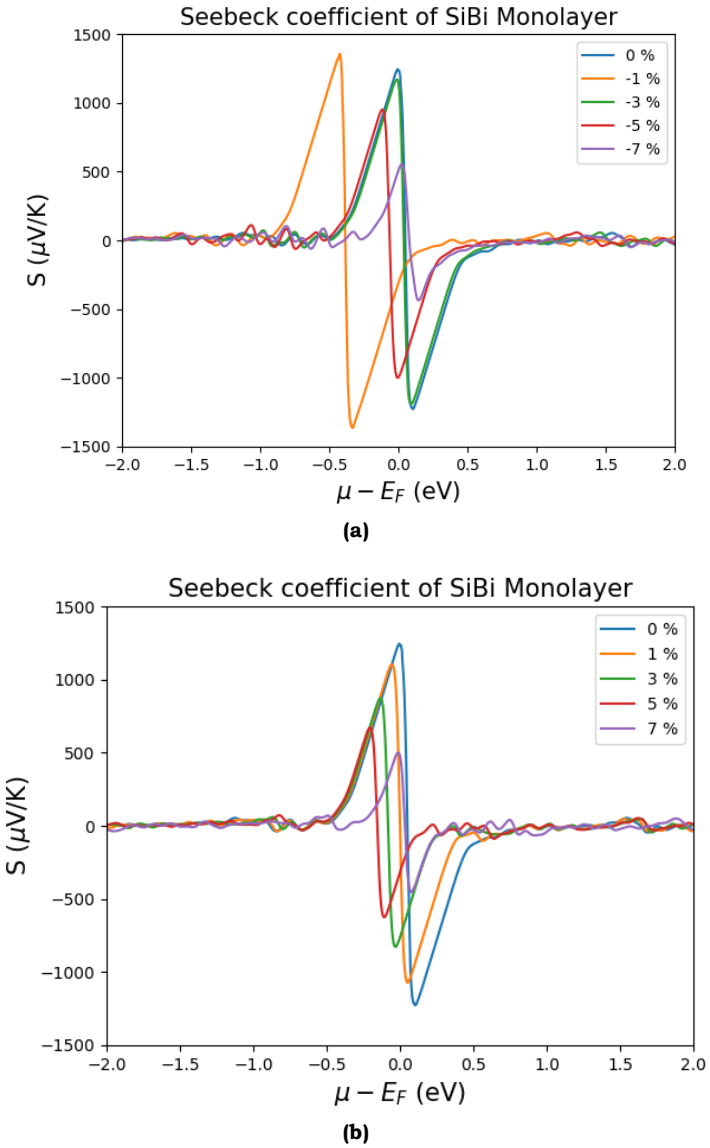


Figure 7. The Seebeck coefficient of SiBi monolayer under biaxial (a) compressive and (b) tensile strain

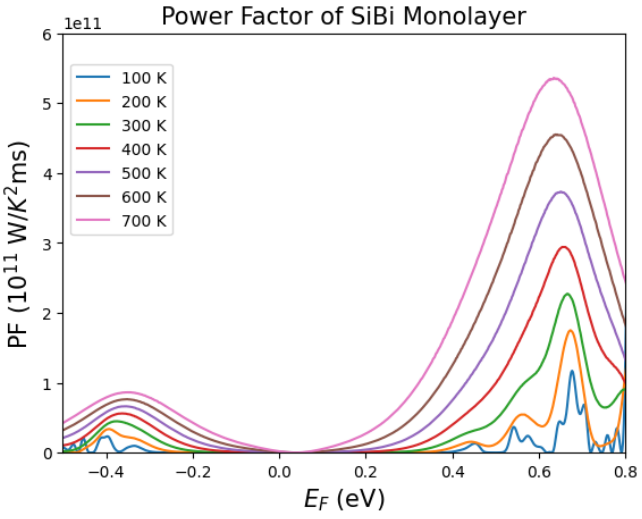


Figure 8. The Power Factor of SiBi monolayer at different temperature

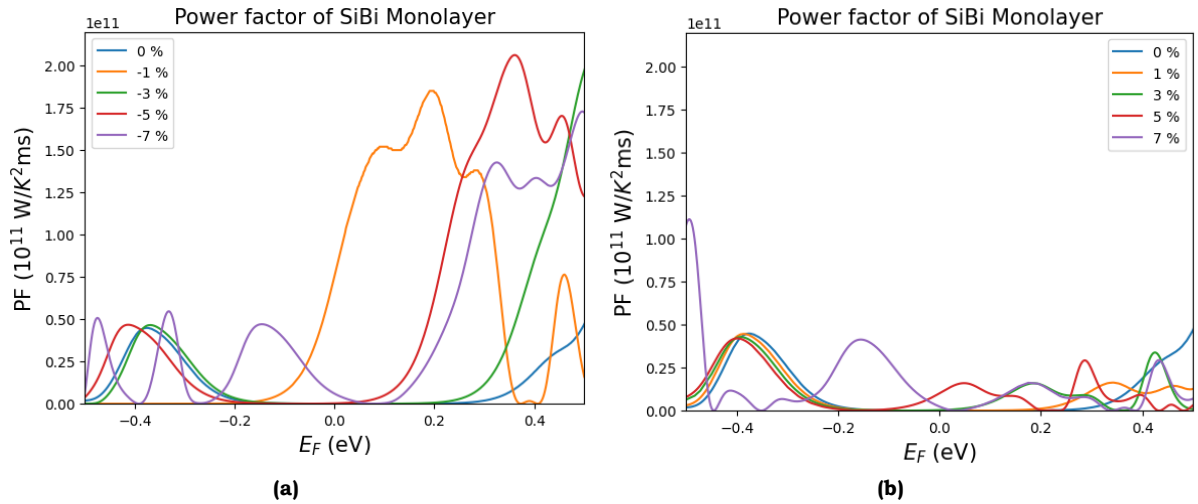


Figure 9. The Power Factor of SiBi monolayer under biaxial (a) compressive and (b) tensile strain

4. Conclusions

Using both DFT calculations and semiclassical Boltzmann transport analysis, we investigated the structural, electronic, and thermoelectric (TE) properties of hexagonal SiBi monolayers. Our findings indicate that SiBi is a direct-gap semiconductor, with an energy gap of 0.67 eV that can be increased to 0.76 eV at room temperature under biaxial compressive strain of -1%. The Seebeck coefficients decreased with increasing temperature, whereas the power factor increased, exhibiting promising prospects for SiBi as a thermoelectric material. Under the same compressive strain, the Seebeck coefficient peaked at 1361.75 μV/K for p-type doping and at 1371.85 μV/K for n-type doping at room temperature. These attributes make SiBi monolayers promising candidates for strain-tuneable thermoelectric applications.

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6. Bibliography

Affandi, Y., Absor, M. A. U., & Abraha, K. (2018). Effect of external electric field on spin-orbit splitting of the two-dimensional tungsten dichalcogenides. *Journal of Physics: Conference Series, 1011*(1), 012070. https://doi.org/10.1088/1742-6596/1011/1/012070

Affandi, Y., & Absor, M. A. U. (2022). Electric field-induced anisotropic Rashba splitting in two-dimensional tungsten dichalcogenides. *Journal of Physics: Condensed Matter, 34*(15), 155502. https://doi.org/10.1088/1361-648X/ac476e

Bafekry, A., Shojaei, F., Obeid, M. M., Ghergherehchi, M., Nguyen, C., & Oskouian, M. (2020). Two-dimensional silicon bismotide (SiBi) monolayer with a honeycomb-like lattice: First-principles study of tuning the electronic properties. *RSC Advances, 10*(53), 31894–31900. https://doi.org/10.1039/D0RA05026A

Bartkowiak, M., & Mahan, G. D. (1999). In *Proceedings of the 18th International Conference on Thermoelectrics* (p. 71). Piscataway, NJ.

Giannozzi, P., et al. (2017). Advanced capabilities for materials modelling with QUANTUM ESPRESSO. *Journal of Physics: Condensed Matter, 29*, 465901.

Goldsmid, H. J. (2016). *Introduction to thermoelectricity* (2nd ed.). Springer. https://doi.org/10.1007/978-3-662-49256-7

Hanna, M. Y., Hasdeo, E. H., Suprayoga, E., & Nugraha, A. R. T. (2020). Thermoelectric properties of two-dimensional hydrogenated borophene: A first-principles study. *AIP Conference Proceedings, 2256*, 5. https://doi.org/10.1063/5.0014610

Huang, S.-Z., Fang, C.-G., Feng, Q.-Y., Wang, B.-Y., Yang, H.-D., Li, B., Xiang, X., Zu, X., & Deng, H.-X. (2023). Strain tunable thermoelectric material: Janus ZrSSe monolayer. *Langmuir, 39*(7), 2719–2728.

Itskevich, E. S., Kashirskaya, L. M., & Kraidenov, V. F. (1997). Anomalies in the low-temperature thermoelectric power of p-Bi_2Te_3 and Te associated with topological electronic transitions under pressure. *Semiconductors, 31*(3), 276–278. https://doi.org/10.1134/1.1187126

Jones, W., Regan, K. A., & DiSalvo, F. J. (1998). Thermoelectric properties of the doped Kondo insulator: NdxCe3−x. *Physical Review B: Condensed Matter, 58*(24), 16057–16063. https://doi.org/10.1103/physrevb.58.16057

Kaur, K., Murali, D., & Nanda, B. R. K. (2019). Stretchable and dynamically stable promising two-dimensional thermoelectric materials: ScP and ScAs. *Journal of Materials Chemistry A, 7*(20), 12604–12615.

Madsen, G. K. H., & Singh, D. J. (2006). BoltzTraP: A code for calculating band-structure dependent quantities. *Computer Physics Communications, 175*(1), 67–71. https://doi.org/10.1016/j.cpc.2006.03.007

Novoselov, K. S., Geim, A. K., Morozov, S. V., Jiang, D., Zhang, Y., Dubonos, S. V., Grigorieva, I. V., & Firsov, A. A. (2004). Electric field effect in atomically thin carbon films. *Science, 306*(5696), 666–669. https://doi.org/10.1126/science.1102896

Patel, A., Singh, D., Sonvane, Y., Thakor, P. B., & Ahuja, R. (2021). Improved thermoelectric performance of monolayer HfS_2 by strain engineering. *ACS Omega, 6*(44), 29820–29829.

Pei, Y., Wang, H., & Snyder, G. J. (2012). Band engineering of thermoelectric materials. *Advanced Materials, 24*(46), 6125–6135. https://doi.org/10.1002/adma.201202919

Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. *Physical Review Letters, 77*(18), 3865–3868. https://doi.org/10.1103/PhysRevLett.77.3865

Sales, B. C., Mandrus, D., & Williams, R. K. (1996). Filled skutterudite antimonides: A new class of thermoelectric materials. *Science, 272*(5266), 1325–1328. https://doi.org/10.1126/science.272.5266.1325

Singh, D. J., & Pickett, W. E. (1994). Skutterudite antimonides: Quasilinear bands and unusual transport. *Physical Review B, 50*(15), 11235–11238. https://doi.org/10.1103/physrevb.50.11235

Slack, G. A., & Tsoukala, V. G. (1994). Some properties of semiconducting compounds with high thermal conductivity. *Journal of Applied Physics, 76*(3), 1665–1671. https://doi.org/10.1063/1.357747

Sologub, V., Shubnikov, M., Itskevich, E., Kashirskaya, L., Parfen'ev, R., & Goletskaya, A. (1980). Change of Bi_2Te_3 band structure under hydrostatic compression. *Soviet Physics JETP, 52*(6), 1203.

Somaiya, R. N., Sonvane, Y., & Gupta, S. K. (2020). Exploration of the strain and thermoelectric properties of hexagonal SiX (X = N, P, As, Sb, and Bi) monolayers. *Physical Chemistry Chemical Physics, 22*, 3990–3998.

Tritt, T. M. (2001). *Recent trends in thermoelectric materials research III.* Academic Press.

Wang, H., Zhang, X., & Zhao, X. (2019). First-principles investigation of electronic, mechanical, and thermoelectric properties of graphene-like XBi (X = Si, Ge, Sn) monolayers. *Physical Chemistry Chemical Physics, 21*(34), 18556–18565. https://doi.org/10.1039/C9CP03432E

Wang, K., Xu, J., Xia, Z., & Jia, Y. (2022). Remarkable thermoelectric performance in BaPdS via pudding-mold band structure, band convergence, and ultralow lattice thermal conductivity. *Journal of Materials Chemistry A, 10*(35), 18693–18702. https://doi.org/10.1039/D2TA04552H

Yang, J., et al. (2016). On the tuning of electrical and thermal transport in thermoelectrics: An integrated theory-experiment perspective. *npj Computational Materials, 2*(October 2015), 15. https://doi.org/10.1038/npjcompumats.2015.15