The Verification of Thermoelectric Performance Obtained by High-Throughput Calculations: The Case of GeS₂ Monolayer From First-Principles Calculations

Xiaolian Wang¹, Wei Feng¹, Chen Shen², Zhehao Sun³, Hangbo Qi², Mao Yang¹, Yonghui Liu¹, Yuchen Wu¹ and Xiaoqiang Wu¹*

¹School of Mechanical Engineering, Chengdu University, Chengdu, China, ²Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany, ³School of Energy and Power Engineering, Dalian University of Technology, Dalian, China

Electronic fitness function (EFF, achieved by the electrical transport properties) as a new quantity to estimate thermoelectric (TE) performance of semiconductor crystals is usually used for screening novel TE materials. In recent years, because of the high EFF values, an increasing number of two-dimensional materials have been predicted to have the potential for TE applications via high-throughput calculations. Among them, the GeS₂ monolayer has many interesting physical properties and is being used for industrial applications. Hence, in this work, we systematically investigated the TE performance, including both electronic and thermal transport properties, of the GeS₂ monolayer with first-principles calculations. The results show that the structure of the GeS₂ monolayer at 700 K is thermally unstable, so we study its TE performance only at 300 and 500 K. As compared with other typical TE monolayers, the GeS₂ monolayer exhibits excellent electronic transport properties but a relatively high lattice thermal conductivity of 5.71 W m⁻¹ K⁻¹ at 500 K, and thus an unsatisfactory ZT value of 0.23. Such a low ZT value indicates that it is necessary to consider not only the electron transport properties but also the thermal transport properties to screen the thermoelectric materials with excellent performance through high-throughput calculations.

Keywords: GeS₂ monolayer, thermoelectric, transport property, high-throughput calculations, first-principles calculations

INTRODUCTION

In the past decades, the development of environment-friendly renewable energy has been the main task since it has alleviated the current global energy crisis and the greenhouse effect to some extent (Biswas et al., 2012; Wang and Wu, 2012; Tan et al., 2016). Thermoelectric (TE) materials, which are capable of converting waste heat into electricity directly and reversibly without air pollution, have attracted intense attention (Bell 2008; Wang et al., 2016; Wang et al., 2017). The conversion efficiency is characterized by a dimensionless figure of merit, \( ZT = S^2 T \sigma / (k_e + k_l) \) (Snyder and Toberer, 2008), where the \( S \), \( T \), \( \sigma \), \( k_e \), and \( k_l \) represent the Seebeck coefficient, absolute temperature, electrical conductivity, and electronic and lattice thermal conductivity, respectively. However, it is extremely difficult to simultaneously increase the power factor \( PF \) (\( S^2 \sigma \)) while reducing the thermal...
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conductivity $\kappa (\kappa_e + \kappa_i)$ due to the conflicting properties of TE materials. Therefore, improving the conversion efficiency of TE materials is a challenging and desirable task. Some semiconductors with great TE performance have been found so far. For example, a high $ZT$ value of 2.6 ± 0.3 at 923 K in a promising thermoelectric material, SnSe single crystals, was reported due to the strong anharmonicity, and thus the exceptionally low lattice thermal conductivity (0.23 W m$^{-1}$ K$^{-1}$) (Zhao et al., 2014). Besides, another promising candidate of TE materials, PbTe, exhibits a high $ZT$ value above 1.5 at 773 K (Heremans et al., 2008). However, it is necessary to further improve their TE performance to achieve industrial applications. Therefore, some methods like doping (Liu et al., 2008), alloying (Row et al., 1981), and nanostructuring (Yuan et al., 2018) were reported to enhance the $ZT$ value. Except for these approaches, screening new TE materials is also an effective strategy to improve the $ZT$ value via experimental research (Nielsen et al., 2013; Tang et al., 2015; Li et al., 2018) and theoretical predictions [such as first-principles calculations (Wang et al., 2017; Ouyang et al., 2018) and high-throughput computations (Chen et al., 2016; Li M. et al., 2019; Li R. et al., 2019; Ortiz et al., 2019)].

High-throughput computations are usually used to screen high-performance functional materials according to their EFF (electronic fitness function) values, which is a new quantity to estimate TE performance of materials, such as SnSe$_2$ (Jia et al., 2020) and SnO (Miller et al., 2017). As a chalcogenide material, GeS$_2$ has interesting physical properties and is being used for industrial applications, such as photodetection (Yang et al., 2019), photoresistor, or antireflection coating (Málek and Sháňelová, 1999). Especially, glassy germanium disulfide has been heavily studied for many years (Lucovsky et al., 1974; Tichý et al., 1982; Weinstein et al., 1982) and was still the subject of recent experimental investigations (Petri and Salmon, 2001). Besides, the 1T-CdI$_2$-type GeS$_2$ monolayer was recently reported to have potential as a promising TE material due to its highest peak EFF value (0.3 × 10$^{-19}$ W$^{−2/3}$ ms$^{1/3}$ K$^{-2}$) for p-type carriers (Sarikurt et al., 2020). However, the high EFF value only reflects its strong electron transport performance, but the thermal transport property of the GeS$_2$ monolayer is not yet clear. Most importantly, there has not been a focus on the TE performance of GeS$_2$ monolayers that integrate electronic transport and thermal transport. Consequently, the further exploration of the electronic and thermal transport properties of the GeS$_2$ monolayer is quite reasonable and desirable.

In this work, the TE properties of two-dimensional (2D) isotropic GeS$_2$ are comprehensively studied based on first-principles calculations combined with the Boltzmann transport theory. The results show that this monolayer exhibits great electronic properties, for example, high PF value (3.4 mW m$^{-1}$ K$^{-2}$) at 300 K, which is consistent with the high EFF values obtained with high-throughput computations. However, due to the unsatisfactory thermal transport properties, the $ZT$ value of 2D GeS$_2$ can only reach 0.23 at 500 K. This study suggests that the GeS$_2$ monolayer has poor TE performance, thus proving that the method of predicting high-efficiency TE materials according to the EFF values obtained via high-throughput computations may be incomplete.

**COMPUTATIONAL DETAILS**

In this study, our first-principles calculations are performed by using density functional theory (DFT), as implemented in the Vienna Ab initio Simulation Package (VASP) (Kresse and Hafner, 1993; Kresse and Furthmüller, 1996a; Kresse and Furthmüller, 1996b). The generalized gradient approximation (GGA) (Perdew et al., 1996; Zhang et al., 2018) with Perdew–Burke–Ernzerhof (PBE) parametrization (Qiao et al., 2018) is applied as the exchange–correlation potential. For obtaining the accurate electronic structure, the Heyd–Scuseria–Ernzerhof hybrid functional (HSE06) (Heyd et al., 2003) is adopted to describe the exchange–correlation energy. The cutoff energy of 550 eV is set for the plane-wave basis, and the Brillouin zones are sampled with $15 \times 15 \times 1$ Monkhorst–Pack special k-point meshes for 2D GeS$_2$. The convergence criteria for energy and force are $1 \times 10^{-3}$ eV and $1 \times 10^{-4}$ eV/Å, respectively, which is accurate enough and used in many studies (Sun et al., 2003). To avoid the effect of layer–layer interactions, a sufficiently large vacuum layer of 20 Å is constructed perpendicular to the layer plane in all the calculated structures.

In order to obtain $\kappa_i$, the second- and third-order interatomic force constants (IFCs) are calculated, first using the Phonopy code and the Thirdorder.py script, respectively (Togo et al., 2008; Li et al., 2014). Then $\kappa_i$ can be derived from the mode-resolved phonon properties based on the obtained harmonic and anharmonic IFCs by solving the Boltzmann transport equation as implemented in the ShengBTE code (Li et al., 2014), which is expressed as follows:

$$\kappa_i = \frac{1}{k_B T^2 \Omega N} \sum_x n_0 (n_0 + 1)(\hbar \omega_x)^2 v_x^\alpha v_x^\beta \tau_x, \quad (1)$$

where $\alpha$ and $\beta$ are the Cartesian components of $x$, $y$, or $z$, and $k_B$, $h$, $\Omega$, $N$, $\lambda$, $n_0$, $\omega_x$, $\tau_x$, and $v_x$ are the Boltzmann constant, Planck constant, volume of the unit cell, number of phonon wave vectors, phonon mode, Bose–Einstein distribution function, phonon frequency, phonon lifetime, and phonon group velocity, respectively. For calculating the accurate $\kappa_i$, the cutoff value and the Q-grid mesh are set to the 14th and $25 \times 25 \times 1$, respectively.

The electronic transport properties are obtained by employing the Boltzmann transport equation combined with the relaxation time approximation (RTA) via the BoltzTraP2 code with a denser $31 \times 31 \times 1$ k-point sampling (Madsen et al., 2018). Although RTA tends to overestimate power factors, because of computational convenience, we still adopt this approximation. It was also used in a study on the electronic transport properties of two-dimensional triphosphides (InP$_3$, GaP$_3$, SbP$_3$, and SnP$_3$) (Sun et al., 2020). The relaxation time $\tau$ is calculated using deformation potential (DP) theory combined with the effective
mass approximation (Bardeen and Shockley, 1950) as shown below:

\[
\tau = \frac{\mu m^*}{e} = \frac{2h^2 C}{3k_B T m^* E_1^2}.
\]

(2)

where \( h, k_B, m^*, C, \) and \( E_1 \) are the Planck constant, Boltzmann constant, effective mass, elastic constant, and DP constant, respectively. For the electronic thermal conductivity \( \kappa_e \), in this study, it is obtained using the Wiedemann–Franz law, that is, \( \kappa_e = L_0 T \) (Jonson and Mahan, 1980) Besides, \( \kappa_e \) can also be obtained directly from the BoltzTraP2 code, that is, \( \kappa_e = \kappa_0 - T\sigma S^2 \) (Madsen et al., 2018) A recent study put forward that the results which were obtained from the output of BoltzTraP and from using the Wiedemann–Franz law agree very well with each other (Li M. et al., 2019).

RESULTS AND DISCUSSION

Geometrical Characteristics and Electronic Structures

The optimized structure of 2D GeS\(_2\) possesses a trigonal structure, with the P\(_3\)m1 space group consisting of 1 Ge and 2 S atoms in the primitive unit cell, as shown in Figures 1A, B. The optimized lattice constants are \( a = b = 3.45 \) Å with the PBE method, which is consistent with the previous first-principles results, which are \( a = b = 3.45 \) Å (Sarikurt et al., 2020). Then based on the optimized structure, the electronic band structure and density of states (DOS) distributions are obtained by using the HSE06 functional near the Fermi level of the Ge\(_2\) monolayer, and then we compare the band structures with the HSE06 and PBE functionals, and the results are given in Figure 1C. The calculated results show that an indirect bandgap of 1.47 eV with HSE06 is twice over that of 0.73 eV with PBE, which is large enough to overcome the bipolar conduction effect and thus avoid the decreasing of the Seebeck coefficient (Shi et al., 2015). As for DOS distribution, it is contributed by both \( s \) orbitals of the Ge atom and \( p \) orbitals of the S atoms near the CBM, and around the VBM, it is only dominated by the \( p \) orbitals of the S atoms.

Stability and Phonon Dispersion

To confirm the thermal stability of monolayer Ge\(_2\), \textit{ab initio} molecular dynamics (AIMD) simulations are performed between 300 and 700 K with a time period up to 4 ps. The results as given in Figure 2 show that the average values of the total energy remain nearly constant after 1 ps at 300 and 500 K. However, the curve at 700 K still declines after 1 ps. Besides, the structures are well maintained and all the atoms in monolayer Ge\(_2\) are vibrating around their equilibrium positions at 300 and 500 K, but the atom distribution is disordered at 700 K, which suggests that the structure is unstable at 700 K. Consequently, we choose 300 and 500 K as the typical temperatures to study the TE properties of the Ge\(_2\) monolayer.

Next, we focus on the thermal properties of the Ge\(_2\) monolayer and figure out the phonon spectrum and phonon DOS as given in Figure 3 to confirm its dynamic stability. There are nine phonon branches found in the phonon dispersion since there are three atoms in the unit cell. Among them, the three
lowest vibration frequency branches are the out-of-plane flexural acoustic branch (ZA), the in-plane linear transverse acoustic branch (TA), and the longitudinal acoustic branch (LA), respectively. From Figure 3, one can see that no imaginary phonon branches are observed in the phonon dispersion, suggesting that the GeS2 monolayer is dynamically stable. It is noted that there is no overlapped part among acoustic and optical branches, which suggests that the coupling effect of acoustic–acoustic modes and acoustic–optical modes is extremely weak. This phenomenon may lead to high lattice thermal conductivity. Also, the phonon DOS distribution shows that the acoustic branches are dominated by the heaviest Ge atoms, and the relatively light S atoms mostly contribute to the optical branches.

**Thermal Transport Properties**

Next, the thermal transport properties of the GeS2 monolayer are obtained based on the second- and third-order IFCs. The lattice thermal conductivities in the temperature range of 200–700 K are shown in Figure 4A. It shows that the calculated intrinsic $\kappa_l$ of the isotropic GeS2 monolayer at 300 K is 9.52 Wm$^{-1}$ K$^{-1}$, which is larger than those of most well-known 2D TE materials like SnSe (2.02 Wm$^{-1}$ K$^{-1}$) (Wang et al., 2015), PbTe (2.01 Wm$^{-1}$ K$^{-1}$) (Zhang et al., 2009), and LaCuOSe (1.73 Wm$^{-1}$ K$^{-1}$) (Wang et al., 2020), suggesting that its thermal transport properties may not be satisfactory for TE application. In addition, the lattice thermal conductivity of monolayer GeS2 decreases as temperature increases, typically following a $1/T$ dependence, which is a common behavior exhibited in the $\kappa_l$ of crystalline materials and mainly attributed to the intrinsic enhancement in phonon–phonon scattering with temperature (Yang et al., 2016).

To further understand the thermal transport behavior of the GeS2 monolayer, $\kappa_l$ is studied using the following formula (Hicks and Dresselhaus, 1993):

$$\kappa_l = \frac{1}{3} C_V V_g l,$$  \(3\)

where $C_V$, $V_g$, and $l$ are the lattice heat capacity, phonon group velocity, and phonon mean free path (MFP), respectively. The phonon lifetime and group velocity with respect to frequency are plotted in Figures 4B, C. It can be seen that the calculated phonon lifetime is about 1–10$^2$ ps at the range of vibration frequency of acoustic phonons (0–3 THz), which is comparable with rhombohedral GeSe (1–10$^2$ ps) (Yuan et al.,...
and SnP$_3$ ($< 10^2$ ps) (Sun et al., 2020) monolayers. Also, Figure 4C shows that the maximum group velocity for the acoustic modes is about 6.2 km/s. Then the cumulative $\kappa_l$ as a function of the MFP for the GeS$_2$ monolayer is plotted in Figure 4D. It is found that the phonon MFP (180 nm) is much larger than those of many materials with high TE performance, such as SnSe (100 nm) (Carrete et al., 2014), SnS (70 nm) (Guo et al., 2015), and PbTe (10 nm) (Tian et al., 2012). The large group velocity and MFP lead to a high lattice thermal conductivity, thus limiting the TE performance of 2D GeS$_2$.

### Electronic Transport Properties

The Seebeck coefficient of the GeS$_2$ monolayer is given in Figure 5A. It is noted that with the carrier concentration increasing from $10^{11}$ to $10^{14}$ cm$^{-2}$, the absolute value of the Seebeck coefficient $|S|$ of n- and p-type GeS$_2$ decreases at the temperatures of 300 and 500 K, which can be explained by the following equation (Guo, Hu et al., 2013):

$$S = \frac{8\pi^2k_B^2}{3\hbar^2m^*}T\left(\frac{n}{3m}\right)^{2/3},$$

(4)

where $k_B$, $e$, $h$, $m^*$, and $n$ are the Boltzmann constant, electron charge, Planck constant, effective mass, and carrier concentration, respectively. In addition, it can be seen that the absolute value of the Seebeck coefficient $|S|$ of n- and p-type GeS$_2$ increases as the temperature increases from 300 to 500 K with the carrier concentration at the range of $10^{11}$–$10^{14}$ cm$^{-2}$. Besides, the $|S|$ for p-type GeS$_2$ is larger than that for n-type GeS$_2$ at a given carrier concentration under 300 and 500 K due to the larger effective mass. For example, the Seebeck coefficient of 696 $\mu$VK$^{-1}$ for the p-type system is larger than that of 620 $\mu$VK$^{-1}$ for the n-type system along the x-axis at 500 K with a carrier concentration of $1 \times 10^{11}$ cm$^{-2}$. The $|S|$ is comparable with that of another FeOCl-type monolayer, Al$_2$I$_2$Se$_2$, which was reported as a promising TE material (Qi et al., 2021). In addition, the comparison of calculated thermoelectric parameters at 300 K between GeS$_2$ and Al$_2$I$_2$Se$_2$ monolayers has been made in Table 1.

The relaxation time, mobility, and effective mass are shown in Table 2. Based on the calculated relaxation time, the $\sigma$ as $\sigma/\tau$ within the constant RTA is obtained, as shown in Figure 5B. It can be seen that the $\sigma$ of both n- and p-type systems increases with the increase in carrier concentration at a given temperature, which can be explained with the following formula (Snyder et al., 2020):

$$\sigma = ne\mu,$$

(5)

where $n$ is the carrier concentration and $\mu$ is the mobility of the charge carrier. In addition, $\sigma$ decreases with the increasing temperature because of more frequent scattering of electrons and lower relaxation time at a higher temperature. As can be clearly noticed, the $\sigma$ of the n-type system is larger than that of the p-type system due to the larger effective mass for n-type GeS$_2$ at a given temperature and carrier concentration. For example, the value of $\sigma$ for n-type GeS$_2$ is 287 S/m, which is larger than that for p-type GeS$_2$ (210 S/m) at 500 K with a carrier concentration of $1 \times 10^{11}$ cm$^{-2}$.

The power factor $PF = (S^2\sigma)$ of the GeS$_2$ monolayer is calculated combined with the Seebeck coefficient and electrical conductivity, as shown in Figure 5C. Due to the opposite changes of $S$ and $\sigma$ with the carrier concentration, the $PF$ value increases first and then decreases as the carrier concentration increases in all cases. In addition, the $PF$ value of p-type GeS$_2$ is higher than that of n-type GeS$_2$, suggesting that better TE performance can be
obtained from the p-type system. The maximum PF value occurs at the temperature of 300 K for the p-type system, which is 3.4 mW m\(^{-1}\) K\(^{-2}\) at the carrier concentration of 2.64 \times 10^{13} \text{ cm}^{-2}. This value is higher than those of other typical TE materials, such as PbTe (3.0 mW m\(^{-1}\) K\(^{-2}\)) (Pei et al., 2011) and LaCuOSe (2.1 mW m\(^{-1}\) K\(^{-2}\)) (Wang et al., 2020). Consequently, the prediction of EFF values for electronic transport properties is reliable.

### Dimensionless Figure of Merit (ZT)

Combining the thermoelectric transport parameters obtained above, the ZT values of n- and p-type GeS\(_2\) monolayers are estimated, as plotted in Figure 5D. It can be found that the maximum ZT values for the p-type system are larger than those for the n-type system at 300 and 500 K due to the higher PF values of p-type GeS\(_2\). At the temperature of 500 K, an optimal ZT value of 0.23 for the p-type system can be reached, which is almost twice the value of 0.13 for the n-type system. The maximum ZT value is smaller than those of most TE materials, like SnSe (2.6 at 923 K) (Zhao et al., 2014) and GeAs\(_2\) (2.78 at 800 K) (Wang et al., 2017), suggesting that the TE performance of the GeS\(_2\) monolayer is not as good as the prediction with high-throughput computations indicated, which is attributed to its high lattice thermal conductivity. Therefore, only considering the EFF values without thermal transport properties for predicting the TE performance of materials is incomplete.

### CONCLUSION

Motivated by the prediction with high-throughput computations, we systematically study the TE performance of the GeS\(_2\) monolayer via first-principles calculations combined with Boltzmann transport theory. Our results show that the electronic transport properties exhibit great performance, consistent with the prediction of high EFF. Specifically, the largest PF value of the GeS\(_2\) monolayer reaches 3.4 mW m\(^{-1}\) K\(^{-2}\) at 300 K because of its high electrical conductivity. However, we also find that its lattice thermal conductivity is as high as 9.52 Wm\(^{-1}\) K\(^{-1}\) at 300 K, resulting in an unsatisfactory ZT value (0.1) for the p-type system. Additionally, the highest ZT value is only 0.23 at 500 K. This work suggests that the GeS\(_2\) monolayer is not suitable for TE applications; thus, the prediction of EFF values by high-throughput computations is incomplete.

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**DATA AVAILABILITY STATEMENT**

The original contributions presented in the study are included in the article/Supplementary Material; further inquiries can be directed to the corresponding author.

**AUTHOR CONTRIBUTIONS**

XW conceived the idea. XW conducted the simulation and analysis. All authors participated in the writing and correction of the manuscript.
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**Conflict of Interest:** The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.