1 Introduction

Thermoelectric (TE) materials, providing a promising route for converting waste heat into electricity directly, 1–4 have been extensively used in space satellites, automobiles, and solar TE generators. 5,6 In recent years, layered two-dimensional (2D) materials, such as graphene, transition metal dichalcogenides, IVA–VIA compounds and black phosphorus, have attracted much attention as high-performance TE materials. 7–10 These unique 2D geometric structures and their excellent physical properties foreshow the great potential for integration into new energy storage and conversion devices. 11 The conversion efficiency of TE materials is usually determined by a dimensionless figure of merit (ZT), ZT = S2σT/(κl + κe), which depends on the Seebeck coefficient (S), electrical conductivity (σ), absolute temperature (T), lattice thermal conductivity (κl), and electronic thermal conductivity (κe). 12,13 During the last few decades, the ZT of a commercial material has been limited to about 1 in a wide temperature range. 2 A high ZT demands high S and σ, and low κe and κl. Hence, the concurrent increase in the power factor (PF = S2σ) and decrease in thermal conductivity (κ) (κ = κl + κe) are key factors to achieve high ZT in a particular material system. Due to the complex inter-relation and dependence on the material’s band and crystal structure among these three parameters, S, σ, and κ, it is difficult to optimize one parameter without negative effects on the other parameters. 2 In fact, the electrical conductivity and electron thermal conductivity are limited by the Wiedemann–Franz law (κe = LσT). S, σ, and κ should be rationally selected to obtain the maximum ZT value. It is still a challenge to improve their conversion efficiency in an economic way so as to extend their application range.

As potential TE materials, the bulk Sn(S, Se, Te), Ge(S, Se, Te), Pb(S, Se, Te), and Sn(Se, S)2 compounds which belong to group IVA–VIA materials have been widely studied in the TE field. 2,10,14 However, the maximum PF of bulk compounds is determined by the nature of the material itself, and the improvement of the ZT value is limited. Hicks and Dresselhaus et al. 15–17 theoretically proposed that low-dimensional materials have excellent TE properties. The reduction in the dimensionality of these materials has been proved as one of the most efficient methods to enhance their ZT values. 18,19 For example, both the theoretical research on 2D CaP3 20 and KAgX (X = S, Se) 21
and the experimental study on phosphorene-like SnSe materials\textsuperscript{22} have shown that reducing the dimensionality can not only avoid the poor TE performance along certain crystal orientations, but also effectively reduce the thermal conductivity. In particular, Sa et al.\textsuperscript{23} introduced a series of two dimensional (2D) group IV chalcogenides (AX\textsubscript{2}), with the building block X–A–A–X (A = Si, Ge, Sn, and Pb, and X = Se and Te), which showed remarkable stability, narrow gapped semiconducting nature and potential applications in nanoscale electronics and optoelectronics. Besides, the quantum size effect induced in the 2D nanostructure materials can increase the Seebeck coefficient.\textsuperscript{10,24} Both the n- and p-type 2D bilayer \( \text{XGeTe} \) systems displayed high \( ZT \) values in the range of 0.8–0.95 and showed superior TE properties.\textsuperscript{25}

In this work, we have systematically studied the TE properties of the new hexagonal QL XTe (X = Ge, Sn, Pb) based on DFT calculations and Boltzmann transport methods. The present results indicate that 2D GeTe, SnTe and PbTe have extremely low lattice thermal conductivities. In particular, QL PbTe exhibits high-performance mid-temperature TE characteristics; the \( ZT \) values of both the p- and n-types can reach 2.39 and 2.44 at 700 K. Our results could motivate further experimental efforts to synthesize remarkable 2D group-IV telluride materials and also can stimulate theoretical works in finding new 2D systems for applications in the TE field.

## 2 Materials and methods

Our first-principles calculations are performed by using the Vienna ab initio simulation package (VASP)\textsuperscript{26} based on DFT.\textsuperscript{27} The projector augmented wave (PAW) pseudopotentials are employed to represent the ion–electron interactions.\textsuperscript{28,29} The exchange–correlation functional for describing the interactions is the generalized gradient approximation from Perdew, Burke, and Ernzerhof (GGA–PBE). In addition, geometry convergence is achieved with a cut-off energy of 500 eV, and the relaxation convergence for ions and electrons is \( 1 \times 10^{-6} \) eV. For the electronic property calculation, \( k \)-mesh of \( 35 \times 35 \times 1 \) is automatically generated with the \( \Gamma \) symmetry based on the Monkhorst–Pack scheme in the Brillouin zone. Both GGA–PBE and Heyd–Scuseria–Ernzerhof (HSE06) exchange–correlation functionals\textsuperscript{30} are used for calculating the electronic band structure of XTe to obtain a more accurate band gap. A vacuum layer of 20 Å is added in the nonperiodic direction (\( z \) axis) to avoid interactions between the neighboring layers. The electrical transport properties are calculated using the semiclassical Boltzmann transport theory within the BoltzTraP code.\textsuperscript{31}

Lattice thermal conductivity is evaluated with phonon lifetime which is self-consistently calculated using the ShengBTE package.\textsuperscript{32} The harmonic second-order interaction force constants (2nd IFCs) and the anharmonic third-order IFCs (3rd IFCs) are calculated using Phonopy package.\textsuperscript{33} A \( 3 \times 3 \times 1 \) supercell and \( 3 \times 3 \times 1 \) \( \kappa \)-mesh are adopted to calculate the 2nd IFCs. The thirdorder.py is used to compute the 3rd IFCs with the \( 3 \times 3 \times 1 \) supercells. Here, the 6th nearest neighbor is considered. Phonon dispersion relation is also calculated using Phonopy\textsuperscript{34} interfaced to VASP.

## 3 Results and discussion

### 3.1 Crystal and electronic structures

The 2D one QL materials XTe (X = Ge, Sn, Pb) studied by us could be obtained by isovalent substitutions of germanium and selenium in experimentally reported layered materials of \( \text{Ge,Se}_{0.5} \text{Te} \).\textsuperscript{23,34,35} The optimal geometric structures of QL XTe are shown in Fig. 1. From the top view, it is clear that QL XTe has a hexagonal structure (space group \( P\bar{3}m1 \)), which is consistent with the previously calculated stable structure of SnM (M = Te, Se, and S).\textsuperscript{36} There are four atoms (two X and two Te) in unit cell of the 2D XTe (X = Ge, Sn, Pb) monolayer, in the stacking order of \( \text{Te–X–Te} \) (with hexagonal sites of A–B–C–A). Each X is surrounded by three neighboring Te atoms and three neighboring X atoms. The optimized lattice structure parameters and bond lengths are shown in Table 1. The lattice constants of \( a = b = 4.032, 4.092 \) and 4.372 Å for GeTe, SnTe and PbTe, respectively, which are consistent with previous calculations.\textsuperscript{23} The lattice constant increases with the increase of the X atomic number. The bond lengths of X–Te are 2.766, 2.907, 3.016 Å and those of X–X are 2.988, 3.295, 3.599 Å for GeTe, SnTe and PbTe, respectively.

The electronic band structures calculated by using PBE and HSE06 hybrid functional as well as the corresponding density of states (TDOS and PDOS) of one QL (a) GeTe, (b) SnTe, and (c) PbTe are presented in Fig. 2. It can be seen that the two approaches exhibit analogous band structures. Our calculated results show that these 2D XTe are indirect band gap semiconductors with gaps of \( \sim 0.71, 0.25 \) and 0.76 eV for GeTe, SnTe and PbTe, respectively. To accurately predict the electronic properties of 2D XTe, the band structures are also calculated using HSE06, as listed in Table 1. The bandgaps are \( \sim 0.90, 0.48, \) and 1.71 eV for GeTe, SnTe and PbTe, respectively, which are comparable to those of the polymorph SnSe monolayer (0.91 eV)\textsuperscript{37} and PbSe monolayer (0.96 eV).\textsuperscript{38} It can be seen from the comparison that the bandgaps calculated using the HSE06

![Fig. 1. The structure sketch of QL XTe (X = Ge, Sn, Pb).](image-url)
Table 1  Lattice constants (LC), the degrees of α, β and γ angles, bond lengths of X–Te (lX–Te), X–X (lX–X) and band gaps (based on PBE and HSE06 methods) of 2D XTe (X = Ge, Sn, Pb)

<table>
<thead>
<tr>
<th></th>
<th>LC</th>
<th>α</th>
<th>β</th>
<th>γ</th>
<th>lX–Te</th>
<th>lX–X</th>
<th>PBE</th>
<th>HSE06</th>
</tr>
</thead>
<tbody>
<tr>
<td>GeTe</td>
<td>4.032</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td>2.766</td>
<td>2.988</td>
<td>0.71</td>
<td>0.90</td>
</tr>
<tr>
<td>SnTe</td>
<td>4.092</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td>2.907</td>
<td>3.295</td>
<td>0.25</td>
<td>0.48</td>
</tr>
<tr>
<td>PbTe</td>
<td>4.372</td>
<td>90</td>
<td>90</td>
<td>120</td>
<td>3.016</td>
<td>3.599</td>
<td>0.76</td>
<td>1.17</td>
</tr>
</tbody>
</table>

Fig. 2  The electronic band structures calculated by using PBE (dashed red lines), HSE06 hybrid functional (solid black lines) and density of states (DOS) of QL (a) GeTe, (b) SnTe, and (c) PbTe.

method are larger than that from using the PBE method, especially for PbTe. Even then, the band gaps are still in the ideal narrow band gap range for good TE materials.39 Both the valence band maximum (VBM) locate along the Γ–M line for the GeTe and SnTe semiconductors, but along the K–Γ line for PbTe. From DOS distribution of different elements (X and Te), it can be seen that the valence band (−1 to −3 eV) is mainly contributed by Te atoms, which belong to the group VI atoms, while the conduction band (0−2 eV) is mainly contributed by X atoms, which belong to the group IV atoms. This is similar to the (PbTe), layer40 and SnTe alloy.41 It should be directly connected with the electronic structure of each type of material, because the four electrons (s²p²) for X and six electrons (s²p⁴) for Te are used as the valence electrons in the XTe system. Meanwhile, we also find that there exist stair-like-shaped DOSs for all three 2D XTe, which imply a large Seebeck coefficient.

3.2 Electrical transport properties

On the basis of the above calculated electronic structures, the corresponding electrical transport properties can be obtained by using the Boltzmann transport theory with a constant scattering time approximation. The transport coefficients $\sigma / \tau$, and $\kappa _{e} / \tau$ with respect to $T$ and $\mu$ can be calculated as follows:

$$S_{\sigma \beta}(T, \mu) = \frac{1}{e TV \sigma_{\sigma \beta}(T, \mu)} \sum_{\mathbf{q}} \langle \varepsilon \rangle \left( \varepsilon - \mu \right) \left[ \frac{\partial f_{\beta}(T, \varepsilon)}{\partial \varepsilon} \right] d\varepsilon,$$

$$\sigma_{\sigma \beta}(T, \mu) = \frac{1}{V} \sum_{\mathbf{q}} \langle \varepsilon \rangle \left[ \frac{\partial f_{\beta}(T, \varepsilon)}{\partial \varepsilon} \right] d\varepsilon,$$

where $\alpha, \beta$ are Cartesian indices, $\varepsilon$ and $V$ are the energy and volume of the primitive cell. $\sum_{\mathbf{q}} \langle \varepsilon \rangle$ is the transport distribution function and can be defined as

$$\sum_{\mathbf{q}} \langle \varepsilon \rangle = \frac{e^2}{N_0} \sum_{i,k} \tau_{e\nu_2}(i,k) \nu_{\beta}(i,k) \delta(\varepsilon - \varepsilon_{i,k})$$

After the calculation, we find that the electrical transport properties of XTe are isotropic within the $x$-$y$ plane, which results from their perfect lattice symmetry. It is consistent with the results of 2D one QL SnTe reported in the literature.36 The electrical transport coefficients as functions of the $\mu$ and $T$ at 300, 500 and 700 K are shown in Fig. 3. The negative and positive $\mu$ imply the p- and n-type doping of QL XTe, respectively. It can be observed in Fig. 3(a)–(c) that $S$ is inversely proportional to temperature. We can clearly find that the absolute value of $S$ for SnTe and PbTe decreases with increase in temperature. Meanwhile, the p- and n-type doping of QL GeTe and PbTe surprisingly possess very large absolute values of $S$, up to 1420 and 1966 $\mu$V K$^{-1}$ at 700 K, respectively. The calculated large $S$ of QL XTe can be benefited from the DOS, and the maximum value of $S$ is usually linearly related to the energy bandgap.42

The calculated electrical conductivity ($\sigma$) at different temperatures is shown in Fig. 3(d)–(f). It can be found that $\sigma$ is almost independent of temperature, which is different from the trends of $S$. The temperature effect is not significant because it depends on the edge reconstruction of the atomic structure.43

The electronic thermal conductivity ($\kappa _{e}$) can be calculated by the Wiedemann–Franz law:

$$\kappa _{e} = L\sigma T$$

(4)
where \( L = \frac{\pi^2 k_B^2}{3e^2} \) is the Lorenz number. Fig. 3(g)–(i) show the changes of \( \kappa_e \) with a chemical potential \( \mu \) at different temperatures (300, 500, and 700 K). We can find that the change rule of \( \kappa_e \) is similar to \( \sigma \), which is contributed by the proportional relationship between them. However, the effect of temperature on \( \kappa_e \) is significantly greater than \( \sigma \). An increase in temperature leads to evident increase in electron thermal conductivity.

### 3.3 Thermal transport properties

Fig. 4 shows the phonon dispersion curve and phonon state density (PhDOS) obtained from 2nd IFCs calculated using the Phonopy software. As is known to all, the phonon dispersion is a common way to verify the stability of a structure. The real frequencies of all modes in the Brillouin zone (see Fig. 4) indicate that the three 2D crystals are all kinetically stable. As shown in Fig. 4, the two transverse (TA and TA’0) and one longitudinal acoustic (LA) branches of monolayers cross each other in the Brillouin zone, which are same as that of the single-layer XSe (X = Ge, Se and Pb).\(^{35}\) In addition, since acoustic branches play an important role in heat transfer, we label the three acoustic branches as TA, TA’0, and LA, respectively. It is conspicuous that the three acoustic branches of the GeTe and PbTe sheets are linear near the \( G \) points, while the acoustic branches of SnTe show complex trends. This is similar to the group-IV selenides.\(^{35}\) In addition, the lowest optical frequency at \( G \) point of QL PbTe is 0.8 THz, which is smaller than those of QL GeTe (1.40 THz) and SnTe (1.38 THz). For the optical branches, it can be clearly seen that wide phonon gaps of 1.24, 1.41, and 1.45 THz for GeTe, SnTe, and PbTe separate the optical phonon modes into high-energy and low-energy areas. The low-energy optical branches below the phonon gaps are overlapping with the acoustic branches in XTe, leading to strong acoustic-optical interactions. The frequency range of phonon gap in GeTe and SnTe is 2.3–3.9 THz, while that of PbTe is between 1.7 THz and 3.2 THz. PbTe exhibits relatively low acoustic branches, which means that PbTe may have low phonon group velocities and low lattice thermal conductivity.

Concerning the phonon dispersions and density of states, separation of the phonon branches into two parts is more pronounced in the presence of heavier metals. In the low-frequency region of the PhDOS, Te mainly contributes to PbTe while Pb dominates the PhDOS in GeTe. This is reverse in the high-frequency regions for the two crystals. In both regions, the contributions of Sn and Te atoms to the PhDOS in SnTe are approximately the same. These features are mainly from the atomic number of Ge (72.6 g mol\(^{-1}\)), Sn (118.7 g mol\(^{-1}\)), Te (127.6 g mol\(^{-1}\)) and Pb (207.2 g mol\(^{-1}\)).\(^{44}\) Clearly, the heavier the nuclei, the lower the frequency. In addition, from the PhDOS, one can see that all the Ge, Sn, Te and Pb vibrations contribute in the full-energy region. The Sn
and Te atoms make significant contributions in all the phonon modes, while Ge and Pb atoms mainly contribute to the high-energy and low-energy regions, respectively, which may be due to the weakening of the covalent bonding characteristic when going from GeTe, SnTe to PbTe with the increase in mass and bond lengths. This is similar to the (PbTe)₂ layer,⁴⁰ MoS₂/MoS₂ bilayer heterostructure,⁵⁵ and group-IV selenides MSe (M = Ge, Sn, and Pb) compounds.⁵⁶

As an important factor for evaluating the TE properties, the lattice thermal conductivity ($k_l$) of QL XTe can be computed based on Boltzmann transport theory:²²

$$k_l = \frac{1}{V} \sum \frac{C_v v_i^2 \tau_i}{\nu}$$

(5)

where $V$, $C_v$, $v_i$, and $\tau_i$ are the crystal volume of the primitive cell, the heat capacity, phonon group velocity and phonon relaxation time, respectively. $k_l$ as a function of temperature between 300 and 800 K is presented in Fig. 5(a). It is clearly seen that $k_l$ of QL XTe gradually reduce with increase in temperature. At room temperature, the $k_l$ values of QL GeTe, SnTe and PbTe are 5.36, 0.67 and 0.33 W m⁻¹ K⁻¹, respectively. When the temperature rises to mid-temperature (700 K), the corresponding $k_l$ values are reduced to 2.29, 0.29 and 0.15 W m⁻¹ K⁻¹, respectively. That being said, the lattice thermal conductivity is reduced by almost half from 300 to 700 K. Notably, QL SnTe and PbTe show lower $k_l$ values (<1 W m⁻¹ K⁻¹) at room temperature than most 2D materials, such as phosphene (83.5 W m⁻¹ K⁻¹)⁴⁶ and layered MoS₂ (23.2 W m⁻¹ K⁻¹).⁴⁷ In addition, the $k_l$ values of QL XTe are lower than those of the other bulk GeTe (~7.9 W m⁻¹ K⁻¹)⁴⁸ SnTe (~3.6 W m⁻¹ K⁻¹)⁹,²⁰ and PbTe (~2.14 W m⁻¹ K⁻¹)⁵¹ which means that the thermal conductivity can be reduced by decreasing the dimensions.²²

These extremely low thermal conductivities strongly suggest that XTe (X = Ge, Sn and Pb) could be promising candidates for mid-temperature TE materials. Besides, $k_l$ of a crystalline material can also be simply evaluated using Slack theory:²³

$$k_l = \frac{A M \Theta^2 \delta n^{1/3}}{\gamma T}$$

(6)

where $A$ is a physical constant, $M$ is the average mass per atom in the crystal, $\Theta$ is the Debye temperature, $\delta$ is the cube root of the average volume per atom, $n$ is the number of atoms in the primitive unit cell, and $\gamma$ is the Grüneisen parameter. Obviously, developing materials with a large average atomic mass and small Grüneisen parameter is crucial for ideal TE candidates.

To further understand low thermal conductivity, we extract the phonon group velocities ($v$), Grüneisen parameters ($\gamma$), and phonon relaxation time ($\tau$) with respect to frequency as shown in Fig. 5(b)-(d). Phonon group velocity $v$ is an important physical quantity in determining $k_l$. The phonon velocity can be calculated using:²⁴

$$v_i(q) = \frac{d\omega_i(q)}{dq}$$

(7)

where $\omega_i(q)$ is the phonon frequency of the phonon mode $\lambda$.

The calculated phonon group velocity at 300 K is shown in Fig. 5(b). We also calculate the average phonon group velocities using $\bar{v} = \sum \frac{v_i(q)^2}{\sum q}$. The $\bar{v}$ values are 0.66, 0.63 and 0.42 km s⁻¹ for 2D GeTe, SnTe, and PbTe, respectively. These low phonon group velocities are mainly due to their lower and flat phonon branches, which imply an extremely low lattice thermal conductivity.⁵⁵ Among the three 2D XTe, the average phonon group velocity of PbTe was the smallest. According to the formula (5), these results adequately indicate that a low phonon group velocity correlates with a low thermal conductivity. For PbTe, the low phonon velocity appears both in low-frequency and high-frequency regions. As for GeTe, the low phonon velocity only appears in the high-frequency region. Therefore, it can be concluded that the decrease in group velocity, coupled with the enhancement of phonon–phonon scattering, leads to the decrease of phonon thermal conductivity for 2D hexagonal PbTe.

The Grüneisen parameters ($\gamma$) of one QL XTe with respect to frequency, which can be calculated using

$$\gamma(q) = -\frac{V}{\omega(q)} \frac{\partial \omega(q)}{\partial V}$$

(8)

where $V$ is the volume, is calculated and presented in Fig. 5(c). Generally, large $|\gamma|$ implies strong anharmonicity, which accordingly gives rise to low $k_l$. As shown in Fig. 5(c), we can clearly see that large Grüneisen parameters exist mainly in the low-frequency region. We can find that QL XTe possesses a very high maximum $|\gamma|$ at a low frequency (~0.8 THz), corresponding to 2, 7 and 9 for GeTe, SnTe and PbTe, respectively. Obviously, the $|\gamma|$ of single-layer PbTe is much larger than those of GeTe and SnTe. This indicates that QL PbTe has a large non-harmonic interaction, resulting in the smallest $k_l$ in the three group-IV tellurides compounds, especially at the mid-temperature region. These large-mode Grüneneisen parameters at low frequencies are

![Fig. 5](a) Lattice thermal conductivity, (b) phonon group velocities, (c) Grüneisen parameters, and (d) phonon relaxation time with respect to frequency for XTe.
crucial to the phonon transport in materials, because most of the heat is carried by acoustic phonons.\textsuperscript{56} The average values of the acoustic Grüneisen parameters $\bar{\gamma}$ for these 2D XTe are calculated as,
\begin{equation}
\bar{\gamma} = \sum \frac{\sqrt{H_{ij}}}{q_i}
\end{equation}
As shown in Fig. 5c, we can clearly see that large Grüneisen parameters exist mainly in the low-frequency region. For PbTe, the calculated $\bar{\gamma}$ value is 2.03, which is larger than those of GeTe (1.09) and SnTe (1.29). These values are comparable with the reported results of GeSe (0.71), SnSe (0.96) and PbSe (2.05).\textsuperscript{38} Such inherent properties, low phonon velocities and large Grüneisen parameters, can lead to an ultralow $k_l$ for QL PbTe.

The phonon relaxation time is another key contributor to phonon thermal conductivity. Here, we calculate it from the anharmonic 3rd IFCs and the plot is shown in Fig. 5(d). We find that the phonon relaxation time of PbTe is distinctly lower than that of GeTe. This indicates that PbTe has stronger phonon scattering than GeTe. Similar to group velocity, a substantial reduction of phonon relaxation time is also observed in the whole frequency region for PbTe, especially for the acoustic phonons (less than 2 THz). These lead to the low values of phonon thermal conductivity for PbTe.

### 3.4 Thermoelectric figure of merit (ZT)

Combined with the obtained lattice thermal conductivity and electrical transport coefficients, we further calculate the ZT values of one QL XTe at 300, 500 and 700 K, as shown in Fig. 6. The ZT values of XTe increase with increase in temperature. The ZT values near the Fermi surface have the largest variation amplitude. Besides, the variation amplitude for n-type PbTe is the most evident one. We can see that the n-type ZT values are significantly larger than the corresponding p-type ZT values for GeTe and SnTe. The calculated ZT values of the n-type XTe (X = Ge, Sn and Pb) monolayer are 0.69, 1.89, and 2.44 at 700 K, respectively. In particular, both n- and p-types QL PbTe materials have large ZT values of 2.44 and 2.38 at 700 K, which are significantly larger than that of other bulk structures of 0.25,\textsuperscript{57} and also larger than the best conventional p-type PbTe-based alloys, such as 0.71 for Na\textsubscript{0.01}Pb\textsubscript{0.99}Te\textsubscript{57} 1.5 for Tl\textsubscript{0.02}Pb\textsubscript{0.98}Te at 773 K\textsuperscript{58} and 1.65 for PbTe/7% PbTe@C:Ag\textsuperscript{59} at 723 K. Such a high ZT is comparable to those of several famous TE materials. Thus, we can conclude that once synthesized the hexagonal QL PbTe can be used as an ideal TE material.

## 4 Conclusions

In summary, we studied the TE properties of 2D one QL of GeTe, SnTe and PbTe using DFT and Boltzmann transport theory. The results indicate that the crystal structure of one QL of XTe is dynamically stable. The n-type 2D PbTe possesses a large Seebeck coefficient of $\sim$1996 $\mu$V K$^{-1}$ and a large PF value of 6.10 $\times$ 10$^{11}$ W K$^{-2}$ m$^{-1}$ s$^{-1}$ at 700 K. Subsequently, the phonon spectrum, lattice thermal conductivity, phonon group velocity, and Grüneisen parameters were analyzed in detail. The small average group velocity of 0.42 km s$^{-1}$ and the large Grüneisen parameter of 9 for PbTe promote the generation of a minimum lattice thermal conductivity of about 0.15 W m$^{-1}$ K$^{-1}$ at medium temperature (700 K). The 2D PbTe shows extraordinary mid-temperature TE performance with high ZT in both p-type (2.39) and n-type (2.44) systems at 700 K. Based on all these merits, we propose to consider our studied hexagonal QL PbTe as a high-performance mid-temperature TE material.

## Author contributions


Conflicts of interest

There are no conflicts to declare.

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