Anisotropic phonon transport and lattice thermal conductivities in tin dichalcogenides SnS\(_2\) and SnSe\(_2\)

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In recent years, layered semiconductor tin dichalcogenides, SnX\(_2\) (X = S and Se), have received great attention owing to their wide applications in numerous fields. However, theoretical studies on their phonon transport properties and lattice thermal conductivities are very rare. Herein, we carry out comprehensive investigations on the phonon transport properties and heat transfer phenomena in tin dichalcogenides using first-principles calculations combined with the Boltzmann transport theory, and compare them with the recent popular thermoelectric materials SnS (SnSe) and widely studied typical TMD MoS\(_2\) (MoSe\(_2\)). The obtained total thermal conductivities of SnS\(_2\) and SnSe\(_2\) agree well with the experimental measured values. The ultralow out-of-plane thermal conductivities of both materials may be useful for thermoelectric applications. The contributions of different phonon branches to the total lattice thermal conductivities are evaluated, and the results suggest that it would be difficult for alloying to reduce \(\kappa\) because the contribution of the optical branches is rather small compared with SnS and SnSe. Subsequently, we investigated the size dependence of the thermal conductivities and found that nanostructuring may be efficient to further reduce \(\kappa\) since the mean free paths of the dominant phonon modes are relatively long. This conclusion is consistent with recent experimental findings, where the \(\kappa\) of SnS\(_2\) was found to evidently decrease with a decrease in the thickness of SnS\(_2\) films. We believe that this phenomenon may also exist in SnSe\(_2\), which may demonstrate a much better thermoelectric performance than that of SnS\(_2\) because of its higher anharmonicity than that of SnS\(_2\), leading to much lower thermal conductivity.

1. Introduction

Transition metal dichalcogenides (TMDs) (MX\(_2\), where M denotes a transition metal and X denotes a chalcogen) are currently attracting increasing interest as a group of mostly semiconducting two-dimensional (2D) and few-layer materials that complement other 2D systems, such as graphene\(^{1-2}\) or h-BN.\(^{3,4}\) Among all the TMDs, tin dichalcogenides (SnS\(_2\) and SnSe\(_2\)) (hereafter denoted as SnX\(_2\)) are more earth-abundant and environmentally-friendly. Recently, they have attracted much attention due to their great potential in a wide spectrum of applications, e.g., thin film solar cells, optoelectronic devices, field-effect transistors (FETs), lithium-ion batteries and portable electronic information storage devices.\(^{5-12}\) In spite of the large amount of research on their structural, electronic and optical properties,\(^{11-16}\) only limited information is now available concerning the thermoelectric performances of SnS\(_2\) and SnSe\(_2\).\(^{17-19}\) In the recent theoretical study by B. Sun et al.,\(^{19}\) it was shown that the peak ZT can reach as high as 0.96 for SnS\(_2\) and 0.88 for SnSe\(_2\) at room temperature, which shows their potential for TE applications. Moreover, in another recent experimental study,\(^{19}\) the authors suggest that SnS\(_2\) nanosheets are negatively correlated thermoelectric materials with a negative correlation between electrical and thermal conductivity, that is, as the thickness of SnS\(_2\) decreases, \(s\) increases, whereas \(\kappa\) decreases. Naturally, this is an important finding since most TE materials demonstrate decreased thermal conductivity when their electrical conductivity increases. Although the lattice thermal conductivity is crucial to the thermoelectric performance of TE materials, to date, theoretical reports that discuss the lattice thermal conductivity of SnX\(_2\) are still lacking, with the exception of one recent study\(^{18}\) that considered the theoretically minimum lattice thermal conductivity (\(\kappa_{\text{min}}\)). On the other hand, several of the experimentally measured values of thermal conductivity differ enormously.\(^{19-21}\) Furthermore, a complete and comparative prediction and understanding of the underlying phonon transport properties of SnS\(_2\) and SnSe\(_2\) are key to expanding the range of their application in nanoelectronics, optoelectronics and thermoelectrics; however, thus far, the phonon transport properties of these two dichalcogenides are still less known. Therefore, it is necessary to give a detailed study of their

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phonon transport and accurately predict their intrinsic thermal conductivity. Another fact that should be noted is that the present materials have several similarities with SnS and SnSe, which have been recently found to display high thermoelectric efficiencies with great potential for the conversion of heat to electricity.\textsuperscript{7,14,25} For example, they are all constituted of Sn and S (Se) that tend to form weak atomic bonds and usually lead to strong anharmonicity. In addition, they all have anisotropic (orthorhombic) layered structures and the interplanar van der Waals forces usually bring ultralow out-of-plane thermal conductivity. Then, the question arises of whether SnX\textsubscript{2} could perform well as thermal insulators similar to SnS and SnSe.

Herein, we conduct comprehensive investigations into the anisotropic phonon transport properties and intrinsic thermal conductivities of SnX\textsubscript{2} based on first-principles calculations. A systematic study of the lattice dynamics are performed and related properties, including Born effective charge (BEC), dielectric constant (DC) and frequencies of optical modes, together with their irreducible representation are given. Then, the lattice thermal transports of both materials are calculated by solving the phonon Boltzmann transport equation. The obtained thermal conductivities of SnS\textsubscript{2} and SnSe\textsubscript{2} are close to the experimental measured values. The contributions of each phonon branch to the total thermal conductivities, phonon lifetimes and the dependence of thermal conductivities for both materials are evaluated, and the underlying mechanism governing their diverse thermal transport behavior are analyzed and discussed in detail.

2. Computational details

First-principles calculations were performed using the density functional theory as implemented in the Vienna \textit{ab initio} simulation package (VASP)\textsuperscript{26–28} with a plane wave energy of up to 500 eV in the expansion of the electronic wave function. The local density approximation (LDA),\textsuperscript{29} which is typically used for layered structures where van der Waals interactions are important, was chosen as the exchange–correlation functional of DFT. The valence electron configurations considered in this calculation are Sn (4d\textsuperscript{10}5s\textsuperscript{2}5p\textsuperscript{2}), S (3s\textsuperscript{2}3p\textsuperscript{4}), and Se (4s\textsuperscript{2}4p\textsuperscript{4}). The internal coordinates and lattice constants were optimized until the Hellmann–Feynman forces acting on each atom became less than 10\textsuperscript{–3} eV Å\textsuperscript{–1}. The convergence for energy was chosen as 10\textsuperscript{–6} eV between two steps, and a Monkhorst–Pack \textit{k}-mesh of 7 × 7 × 5 was used to sample the Brillouin zone in the structure optimization. Phonon frequencies and the corresponding thermodynamic properties were obtained using the PHONOPY\textsuperscript{30} program. Moreover, an iterative self-consistent method was used for solving the phonon Boltzmann transport equation to calculate the lattice thermal conductivity with the ShengBTE\textsuperscript{31} code, which is based on the second-order (harmonic) and third-order (anharmonic) interatomic force constants (IFCs) combined with an iterative self-consistent algorithm to solve the BTE, and has also successfully predicted the thermal conductivities of many materials.\textsuperscript{25–38} We used 4 × 4 × 2 supercells containing 96 atoms with 3 × 3 × 3 \textit{k}-mesh for calculations of second-order and third-order IFCs for both SnS\textsubscript{2} and SnSe\textsubscript{2}. In the calculations of the third-order IFCs, we considered third-order interatomic force constants up to the fourth shell of neighbors. Well-converged 20 × 20 × 11 \textit{q}-meshes were used in the calculation of the lattice thermal conductivity of SnX\textsubscript{2}.

3. Results and discussion

Tin dichalcogenides (SnS\textsubscript{2} and SnSe\textsubscript{2}) crystallize in the hexagonal closed packed CdI\textsubscript{2}-type structure with \textit{P}6\textit{3}\textit{m}1 symmetry (space group 164). They have three atoms in the unit cell, which extends over only one sandwich layer as seen in Fig. 1. The intralayer metal (Sn)–chalcogenide (S or Se) bonds are predominantly covalent in nature, whereas the layers themselves are coupled by weak van der Waals bonds. The Sn atoms provide four electrons to fill the bonding states of SnX\textsubscript{2} such that the oxidation states of the Sn and S (or Se) atoms are +4 and −2, respectively. Our relaxed lattice constants resulting from LDA are \(a = 3.63\) Å and \(c = 5.71\) Å for SnS\textsubscript{2}, and \(a = 3.80\) Å and \(c = 5.90\) Å for SnSe\textsubscript{2}, which agree well with previous \textit{ab initio} calculations\textsuperscript{31} but are slightly underestimated compared with the experimental results.\textsuperscript{39} This is reasonable because of the overbinding effect of LDA.

3.1 Lattice dynamics properties

The harmonic phonon dispersions of SnX\textsubscript{2} as obtained from the force constants and considering the longitudinal optical–transverse optical (LO–TO) splitting are shown in Fig. 2. The LO–TO splitting is predicted by incorporating the effects of long-range Coulomb interactions based on the Born effective charges and high-frequency dielectric constants calculated by first-principles. Our calculated Born effective charges and dielectric constants are illustrated in Table 1. It is worth noting that the ionic contribution to the dielectric constant of SnS\textsubscript{2} along the out-of-plane (\(c\) axis) direction is very small (0.69), which indicates that SnS\textsubscript{2} holds more two-dimensional characteristics than SnSe\textsubscript{2}. This is consistent with the fact that the out-of-plane thermal conductivity of SnS\textsubscript{2} is much lower than that of SnSe\textsubscript{2}, which will be discussed later.

![Fig. 1 Crystal structures of SnX\textsubscript{2} (X = S and Se).](image-url)
There exists an evident phonon gap (about 30 cm⁻¹ higher, which is mainly due to the smaller atomic mass of S. (2) for SnSe₂. Larger cation/anion mass ratio, whereas there is no similar gap for SnS₂. In fact, as revealed by Babu Ram et al, which can be attributed to ultra weak interactions between the layers. In particular, the interlayer (vdW) interactions being much weaker than the much smaller group velocities in the out-of-plane direction. This is the result of the interlayer (vdW) interactions being much weaker than the intralayer Sn-X covalent bonding. The average lattice thermal conductivity of both materials are extremely anisotropic; for example, the ratio of \( \frac{\kappa_{\text{in-plane}}}{\kappa_{\text{out-plane}}} \) for SnSe₂ at 300 K is as large as 7.1, which is much higher than that of MoSe₂ (~5.0)²⁰ and SnSe (~2.5),²⁴ showing much larger anisotropy of the present materials. The large anisotropy between the in-plane and out-of-plane thermal conductivity is largely due to the much smaller group velocities in the c direction. This is the result of the interlayer (vdW) interactions being much weaker than the intralayer Sn-X covalent bonding. The average lattice thermal conductivity of both materials are extremely anisotropic; for example, the ratio of \( \frac{\kappa_{\text{in-plane}}}{\kappa_{\text{out-plane}}} \) for SnSe₂ at 300 K is as large as 7.1, which is much higher than that of MoSe₂ (~5.0)²⁰ and SnSe (~2.5),²⁴ showing much larger anisotropy of the present materials. The large anisotropy between the in-plane and out-of-plane thermal conductivity is largely due to the much smaller group velocities in the c direction. This is the result of the interlayer (vdW) interactions being much weaker than the intralayer Sn-X covalent bonding. The average lattice thermal conductivity of both materials are extremely anisotropic; for example, the ratio of \( \frac{\kappa_{\text{in-plane}}}{\kappa_{\text{out-plane}}} \) for SnSe₂ at 300 K is as large as 7.1, which is much higher than that of MoSe₂ (~5.0)²⁰ and SnSe (~2.5),²⁴ showing much larger anisotropy of the present materials. The large anisotropy between the in-plane and out-of-plane thermal conductivity is largely due to the much smaller group velocities in the c direction. This is the result of the interlayer (vdW) interactions being much weaker than the intralayer Sn-X covalent bonding.
thermal conductivity of bulk SnS₂ and SnSe₂ can be evaluated as \( \frac{2}{3}k_{\text{in-plane}} + \frac{1}{3}k_{\text{out-plane}} \). Our calculated average \( k_L \) values at room temperature (8.2 W m K\(^{-1}\) for SnS₂ and 5.6 W m K\(^{-1}\) for SnSe₂) are close to the historically measured \( k_L \) of bulk single crystals (10 W m K\(^{-1}\) (ref. 20) for SnS₂ and 7.29 W m K\(^{-1}\) (ref. 21) for SnSe₂ at 300 K). Although the calculated thermal conductivity for SnS₂ is much larger than the experimental value for 22 nm-thick nanosheets (4.63 W m K\(^{-1}\))\(^{19}\), it is perfectly reasonable since in 2D SnS₂, the surface phonon scattering may be greatly enhanced and thus possibly decrease the lattice thermal conductivity. In comparison with other typical layer materials, the lattice thermal conductivities of SnX₂ are much larger than that of SnS (~1.6 W m K\(^{-1}\))\(^{19}\) and SnSe (~1.5 W m K\(^{-1}\))\(^{19}\) at 300 K calculated using the same iterative self-consistent method with the ShengBTE code and the experimental value of ~1.7 W m K\(^{-1}\) (ref. 43)) and SnSe (~1.5 W m K\(^{-1}\))\(^{19}\) at 300 K calculated with the ShengBTE code and the experimental value of ~0.67 W m K\(^{-1}\) (ref. 43)), but greatly lower than that of MoS₂ (~67 W m K\(^{-1}\))\(^{19}\) at 300 K calculated with the ShengBTE code and the experimental value of 110 ± 20 W m K\(^{-1}\) (ref. 44)) and MoSe₂ (~60 W m K\(^{-1}\))\(^{19}\) at 300 K calculated using the ShengBTE code.

What is even more important is that the out-of-plane thermal conductivities for both materials are found to be unexpectedly low; for example, the calculated room-temperature \( k_L \) of SnS₂ along the out-of-plane direction is 0.78 W m K\(^{-1}\), which approaches the predicted amorphous limit (0.47 W m K\(^{-1}\))\(^{18}\) and is even lower than that of SnS (0.8 W m K\(^{-1}\) along the out-of-plane direction at room temperature).\(^{18}\) Furthermore, these values are remarkably low among most of the TMDs; for example, the calculated out-of-plane thermal conductivity using the same method for MoS₂ is 2.3 W m K\(^{-1}\) (ref. 36) (the experimental out-of-plane thermal conductivity of bulk MoS₂ at 300 K is 1.05 W m K\(^{-1}\) (ref. 43)) and that of WTe₂ is 1.04 W m K\(^{-1}\)\(^{38}\). This implies that the thermoelectric performance of SnX₂ along the out-of-plane direction may be as good as that of SnS. In fact, it is difficult to definitely say how its thermoelectric performance would be because the thermoelectric figure of merit is determined by several strongly coupled quantities and the lattice thermal conductivity is only one of them, but at least, we can conclude that the present material is a good thermal insulator in the out-of-plane direction. Unfortunately, the experimentally measured thermal conductivity values of the out-of-plane direction are not yet available in the literature.

Using the obtained thermal conductivity values of SnX₂, its thermal diffusivity can be derived from the formula \( \alpha = \frac{k_L}{C_p \rho} \) (\( k_L \) is thermal conductivity, \( C_p \) is heat capacity and \( \rho \) is density).

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**Fig. 4** Calculated temperature dependent lattice thermal conductivities of (a) SnS₂ and (b) SnSe₂ along the a axis and c axis, in comparison with the experimental data at 300 K.
Thermal diffusivity is one of the crucial parameters to investigate the thermal transportation process, which indicates that the rate of temperature changes and reflects the correlation between thermal conductivity and heat capacity. The TAPP software gives heat capacity values of $C_p = 252$ J kg$^{-1}$ K$^{-1}$ for SnS$_2$ and $C_p = 261$ J kg$^{-1}$ K$^{-1}$ for SnSe$_2$ at room temperature. The density of SnS$_2$ is easily calculated as $\rho_{\text{SnS}_2} = 4700$ kg m$^{-3}$ for SnS$_2$ and $\rho_{\text{SnSe}_2} = 6200$ kg m$^{-3}$, then, we derive the thermal diffusivity $\alpha_{\text{SnS}_2} = 6.9 \times 10^{-6}$ m$^2$ s$^{-1}$ for SnS$_2$ and $\alpha_{\text{SnSe}_2} = 3.4 \times 10^{-6}$ m$^2$ s$^{-1}$ for SnSe$_2$. Clearly, the thermal diffusivity of SnS$_2$ is much larger than that of SnSe$_2$ mainly due to its larger thermal conductivity and smaller mass density. Our calculated thermal diffusivity for SnSe$_2$ is close to the historically calculated value ($\alpha_{\text{SnSe}_2} = 5.4 \times 10^{-6}$ m$^2$ s$^{-1}$ at 300 K), however, the thermal diffusivity of bulk SnS$_2$ was not found in the literature.

We then determined the contribution of the different phonon modes to the total lattice thermal conductivities for the two materials, as illustrated in Table 3. It is found that along the in-plane direction, the contribution of the optical branches to the total thermal conductivity at room temperature for both SnS$_2$ and SnSe$_2$ is small, whereas along the out-of-plane direction, the contribution of the optical branches is relatively large, particularly for SnS$_2$, where the contribution of the optical branches is as large as 22%. This may be one of the reasons for the ultralow out-of-plane thermal conductivity since the optical branches usually possess much smaller group velocities and much shorter phonon lifetimes than those of the acoustic branches. The small contributions of the optical phonons of SnX$_2$ is an obvious difference with SnX, for instance, the optical phonon branches contribute ~60% to the total thermal conductivity of SnSe$_2$. Therefore, alloying may not be an effective strategy for further reducing the $\kappa_L$ of SnX$_2$.

Furthermore, the temperature dependence of contributions from the phonon branches is plotted in Fig. 5 using SnSe$_2$ as an example. One can see that the contributions of all the phonon modes along the in-plane direction are very insensitive to temperature, where the percentage contributions of the acoustic phonon branches slightly decrease with an increase in temperature, and at the same time, the contribution of the optical phonon branches slightly increases with an increase in temperature. While along the out-of-plane direction, the increase tendency of the contributions of the optical branches becomes evident and reaches 16.5% at 800 K, indicating that higher frequency optical phonons are excited at higher temperatures.

Considering the significant difference in the contribution of different phonon branches to the total thermal conductivity in SnX$_2$, it is worthwhile to examine the relaxation times of the phonon modes as functions of phonon frequency, as displayed in Fig. 6. It is found that the relaxation times of the phonon modes for SnS$_2$ and SnSe$_2$ are very close to each other. Otherwise, the relaxation times of the acoustic branch are one order of magnitude bigger than that of the optical branches, which indicates small contributions of optical phonons to the total $\kappa_L$. In comparison with SnX and MoX$_2$, the relaxation times of SnX$_2$ are much shorter than that of MoX$_2$, although slightly longer than that of SnX. For example, the calculated longest relaxation time of acoustic phonons for SnS$_2$ is about 160 ps, whilst that of MoS$_2$ is as large as $10^5$ ps, and that of SnS is only about 28 ps.

Since the phonon lifetimes of these two materials are comparable, what is the main mechanism that leads to the higher $\kappa_L$ in SnS$_2$? We next calculated the phonon group velocities of SnX$_2$ around the $\Gamma$ point. Our calculated sound velocity in the long-wavelength limit of SnS$_2$ is about 5060 m s$^{-1}$ along the in-plane direction, and that of SnSe$_2$ is only 4050 m s$^{-1}$. Thus, the conclusion is clear that it is just the relatively larger phonon group velocities combined with the higher phonon frequencies of SnS$_2$ that induce the much higher $\kappa_L$ than SnSe$_2$. We also evaluated the anharmonic phase space volume $P_3$, that is, the number of allowed three-phonon processes of the present two compounds, which is usually used to quantify the anharmonicity of a certain material. The obtained $P_3$ of SnS$_2$ is $0.54 \times 10^{-2}$ eV$^{-1}$, and that of SnSe$_2$ is
0.83 × 10⁻² eV⁻¹; therefore it is clear that the anharmonicity of SnSe₂ is higher than that of SnS₂. In comparison with other low-conductivity compounds, the anharmonic phase space volume $P_3$ is slightly larger than that of Si (0.47 × 10⁻² eV⁻¹), but much smaller than that of SnSe (1.9 × 10⁻² eV⁻¹). Furthermore, the mode Grüneisen parameters are calculated as 1.18 for SnS₂ and 1.21 for SnSe₂, which also indicates that the anharmonicity of SnSe₂ is higher than that of SnS₂.

Finally, we investigate the size effect of the present materials by studying the cumulative thermal conductivity $k(l)$ as a function of phonon mean free path, which is defined as the thermal conductivity contributed by phonons whose mean free path $l$ is smaller than a given value $l_{\text{max}}$. Fig. 7 shows the cumulative thermal conductivity along the $a$ and $c$ directions with respect to the phonon MPFs at room temperature, 300 K. It can be seen that the cumulative thermal conductivity of both materials continuously increases as MFP increases, until reaching the limit length $L$, which represents the longest mean free path of the heat carriers. We derived the limit lengths of $L_a \sim 585$ nm and $L_c \sim 400$ nm for SnS₂, and $L_a \sim 575$ nm and $L_c \sim 1100$ nm for SnSe₂. It should be noted that the limit lengths $L$ of the present compounds are much larger than that of SnS and SnSe.

Then, we fitted the cumulative $k(l)$ for SnX₂ along the in-plane and out-of-plane directions at 300 K to a single parametric function, $\kappa(l < l_{\text{max}}) = \frac{\kappa_{\text{max}}}{1 + l/l_{\text{max}}}$, where, $\kappa_{\text{max}}$ is the ultimate cumulated $\kappa$, $l_{\text{max}}$ is the maximal MFP concerned, and $l_0$ is the parameter to be evaluated by the fitting. The fitted curves are plotted in Fig. 7, which reproduce the calculated data well and yield the parameter $l_0$ for the two materials along the in-plane and out-of-plane directions, which could be interpreted as the representative MFP (rMFP). The rMFP is helpful to study the size effect on ballistic or diffusive phonon transport, which is important for thermal design with nanostructuring. Our fitted rMFPs ($l_0$) for SnS₂ are 30 nm along the in-plane direction and 20 nm along the out-of-plane direction, and for SnSe₂, they are 24 nm along the in-plane direction and 38 nm along the out-of-plane direction. These values are quite larger than that of SnSe (4.30 nm along the armchair direction and 6.86 nm along the zigzag direction). Such large representative rMFPs suggest that there are strong size effects in the phonon transport of micro-/nano-sized materials based on these two materials. Our results suggest that to reduce the lattice thermal conductivities of both materials, nanostructuring will be an effective way. This suggestion is consistent with recent experimental findings, where the $k_L$ of SnS₂ was found to evidently decrease with a decrease in the thickness of SnS₂ films. Moreover, we believe that such a phenomenon may also exist in SnSe₂, that is, this material may also be a negatively correlated thermoelectric material just like SnS₂ with a negative correlation between electrical and thermal conductivity. In addition, SnSe₂ may demonstrate a much better thermoelectric performance than that of SnS₂ because of its higher anharmonicity than that of SnS₂, leading to much lower thermal conductivity.

Fig. 6 Frequency-dependent phonon relaxation times of the acoustic (AP) and optical phonons (OP) for (a) SnS₂ and (b) SnSe₂ at 300 K.

Fig. 7 Cumulative lattice thermal conductivity of SnX₂ along the (a) in-plane and (b) out-of-plane directions as a function of phonon MFP at room temperature. The fitted curves are plotted with dotted lines.
4. Conclusion

In summary, we have systematically investigated the anisotropic phonon transport properties and intrinsic lattice thermal conductivities for tin dichalcogenides (SnS$_2$ and SnSe$_2$) from first principles calculations. The calculated in-plane lattice thermal conductivity of SnS$_2$ is 12.10 W mK$^{-1}$, whereas that of SnSe$_2$ is much lower (7.76 W mK$^{-1}$), which mainly originates from its relatively smaller phonon group velocities combined with lower phonon frequencies. The out-of-plane thermal conductivities of both materials are found to be remarkably low (0.78 W mK$^{-1}$ for SnS$_2$ and 1.12 W mK$^{-1}$ for SnSe$_2$) due to very weak interlayer forces, which indicates their significance in thermoelectric applications. The obtained total thermal conductivities of SnS$_2$ and SnSe$_2$ agree well with experimental measured values. The phonon lifetimes of all branches are found to be much shorter in comparison with that of MoS$_2$ (MoSe$_2$) but slightly longer than that of SnS (SnSe). The contributions of the optical phonon branches to the total thermal conductivities are found to be rather small, which suggests that it would be difficult for the strategy of alloying to reduce $\kappa_L$. However, nanosstructuring may be effective to further reduce $\kappa_L$ since the mean free paths of the dominant phonon modes are relatively long. This conclusion is consistent with recent experiment findings, where the $\kappa_L$ of SnS$_2$ thin films were found to be much lower than that of bulk SnS$_2$. Our study not only presents comprehensive investigations on the phonon transport properties of SnS$_2$ and SnSe$_2$, but also provides discussions and analyses on the origins of the diverse heat transfer phenomena, which would be of significance for further studies and applications based on these two TMDs.

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