Phonon transport of Janus monolayer MoSSe: a first-principles study

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Transition Metal Dichalcogenide (TMD) monolayers have most widely studied due to their unique physical properties. Recently, Janus TMD Monolayer MoSSe with sandwiched S-Mo-Se structure has been synthesized by replacing the top S atomic layer in MoS₂ with Se atoms. In this work, we systematically investigate the phonon transport and lattice thermal conductivity ($\kappa_L$) of MoSSe monolayer by first-principles calculations and linearized phonon Boltzmann equation within the single-mode relaxation time approximation (RTA). Calculated results show that the $\kappa_L$ of MoSSe monolayer is very lower than that of MoS₂ monolayer, and higher than that of MoSe₂ monolayer. The corresponding sheet thermal conductance of MoSSe monolayer is 342.50 W K$^{-1}$ m$^{-2}$ at room temperature. These can be understood by phonon group velocities and lifetimes. Compared with MoS₂ monolayer, the smaller group velocities and shorter phonon lifetimes of MoSSe monolayer give rise to lower $\kappa_L$. The elastic properties of MoS₂, MoSSe and MoSe₂ monolayers are also calculated, and the order of Young’s modulus is identical with that of $\kappa_L$. Calculated results show that MoSSe monolayer is more than 5.8% reduce of $\kappa_L$. The size effects on the $\kappa_L$ are also considered, which is usually used in the device implementation. When the characteristic length of MoSSe monolayer is about 110 nm, the $\kappa_L$ reduces to half. These results may offer perspectives on thermal management of MoSSe monolayer for applications of thermoelectrics, thermal circuits and nanoelectronics, and motivate further theoretical or experimental efforts to investigate thermal transports of Janus TMD monolayers.

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I. INTRODUCTION

Due to many novel properties, two-dimensional (2D) materials have been attracting increasing attention since the discovery of graphene. The TMD, group-VA, group IV-VI and group-IV monolayers have been predicted theoretically or synthesized experimentally, which have potential applications in electronic, thermoelectric, quantum and optoelectronic devices. Recently, Janus monolayer MoSSe has been synthesized, based on MoS₂ monolayer by breaking the out-of-plane structural symmetry. The existence of vertical dipoles has been proved by second harmonic generation and piezoresponse force microscopy measurements. The strong piezoelectric effects have been predicted in monolayer and multilayer Janus TMD MX₂ (M = Mo and W; X/Y = S, Se and Te) by first-principles calculations, which has potential applications in energy harvesting and sensors. Electronic and optical properties have been studied in pristine Janus MoSSe and WSes monolayers and their vertical and lateral heterostructures. The ZrSSe monolayer has also been predicted with the 1T phase, which is different from MoSSe monolayer with 2H phase. It is proved that ZrSSe monolayer has better n-type thermoelectric properties than monolayer ZrSe₂.

The thermal property of 2D materials is quite worth studying due to its importance on the performance and reliability on the nano-devices. As is well known, a high thermal conductivity can effectively remove the accumulated heat, while a low thermal conductivity is beneficial to thermoelectric applications. In theory, thermal transports of many 2D materials have been widely studied, such as TMD, group-VA, ATeI (A=Sb or Bi), group IV-VI and group-IV monolayers. It is found that strain can effectively tune $\kappa_L$ for various kinds of 2D materials, such as group-IV monolayers, antimonene and Penta-Structures monolayers. With strain increasing, the $\kappa_L$ shows monotonous increase/decrease and up-and-down behavior, and tensile strain can induce strong size effects on $\kappa_L$. The phonon transports of TMD MX₂ (M=Mo, W, Zr and Hf; X=S and Se) monolayers have been systematically studied by phonon Boltzmann transport equation approach. The $\kappa_L$ of 2H-type TMD monolayers are generally higher than those of 1T-type ones, which can be attributed to the large acoustic-optical frequency gap. In this work, the phonon transport of Janus TMD MoSSe monolayer is performed from a combination of first-principles calculations and linearized phonon Boltzmann equation. It is found that the $\kappa_L$ of MoSSe monolayer is very lower than that of MoS₂ monolayer, but higher than one of MoSe₂ monolayer. The order of their...
κL is explored by phonon group velocities and lifetimes. It is found that the order of Young’s modulus (MoS2 > MoSSe > MoSe2) is identical with that of κL, which accords with the relation: κL ∼ √E28. The isotope and size effects on κL are also studied, which can provide valuable information for designing MoSSe-based nanoelectronics devices.

The rest of the paper is organized as follows. In the next section, the computational details about phonon transport calculations are given. In the third section, the phonon transport and elastic properties of MoSSe monolayers, together with ones of MoS2 and MoSe2 monolayers for a comparison, are shown. Finally, we shall give some discussions and conclusions in the fourth section.

II. COMPUTATIONAL DETAIL

Within projector augmented-wave method, we perform the first-principles calculations using the VASP code29–32 by adopting generalized gradient approximation of Perdew-Burke-Ernzerhof (PBE-GGA) as exchange-correlation functional32. During structural relaxation, a 20 × 20 × 1 k-mesh is used with a Hellman-Feynman force convergence threshold of 10−4 eV/Å. A plane-wave basis set is employed with kinetic energy cutoff of 450 eV, and the electronic stopping criterion is 10−8 eV. The 5s and 4d electrons of Mo, and 3/4s and 3/4p electrons of S/Se are treated as valence electrons. The lattice thermal conductivity is performed by using Phono3py+VASP codes20–31,33. By solving linearized phonon Boltzmann equation, the κL is calculated with single-mode RTA, as implemented in the Phono3py code33. The κL can be expressed as:

\[ \kappa = \frac{1}{NV_0} \sum_{\lambda} \kappa_\lambda = \frac{1}{NV_0} \sum_{\lambda} C_\lambda \nu_\lambda \otimes \nu_\lambda \tau_\lambda \]  

in which λ, N and V0 are phonon mode, the total number of q points sampling Brillouin zone (BZ) and the volume of a unit cell, and Cλ, νλ, τλ is the specific heat, phonon velocity, phonon lifetime. The phonon lifetime τλ can be attained by phonon linewidth 2Γλ(ωλ) of the phonon mode λ:

\[ \tau_\lambda = \frac{1}{2\Gamma_\lambda(\omega_\lambda)} \]  

The Γλ(ω) takes the form analogous to the Fermi golden rule:

\[ \Gamma_\lambda(\omega) = \frac{18\pi}{h^2} \sum_{\lambda' \lambda''} |\Phi_{-\lambda \lambda' \lambda''}|^2 [(f_\lambda + f_\lambda'' + 1)\delta(\omega - \omega_\lambda - \omega_\lambda' - \omega_\lambda'') + (f_\lambda - f_\lambda'')\delta(\omega + \omega_\lambda - \omega_\lambda') - \delta(\omega - \omega_\lambda + \omega_\lambda'')] \]  

in which fλ and Φ−λλ′λ′′ are the phonon equilibrium occupation and the strength of interaction among the three phonons λ, λ’, and λ” involved in the scattering. Based on the supercell approach with finite atomic displacement of 0.03 Å, the second-order interatomic force constants (IFCs) can be attained by using a 5 × 5 × 1 supercell with k-point meshes of 2 × 2 × 1. According to second-order harmonic IFCs, phonon dispersions can be calculated by Phonopy package34. The third-order IFCs can be attained by using a 3 × 3 × 1 supercell with k-point meshes of 3 × 3 × 1. To compute accurately lattice thermal conductivity, the reciprocal spaces of the primitive cells are sampled by 100 × 100 × 1 meshes.

![FIG. 2. Phonon dispersion curves of MoS2, MoSSe and MoSe2 monolayers.](image-url)
TABLE II. The calculated optical phonon frequencies (THz) of MoS$_2$, MoSSe and MoSe$_2$ monolayers at the $\Gamma$ point with experimental results given in parentheses.

| Name   | $E'$  | $E''$ | $A_1$  | $A_2$  |
|--------|-------|-------|--------|--------|
| MoS$_2$| 8.29  | 11.20 | 11.91  | 13.73  |
| MoSSe  | 6.00  | 10.24 | 8.50   | 12.83  |
| MoSe$_2$| 4.88  | 8.35  | 7.06   | 10.34  |

For 2D material, the calculated lattice thermal conductivity depends on the length of unit cell along $z$ direction\textsuperscript{36}. They should be normalized by multiplying $L_z/d$, where $L_z$ and $d$ are the length of unit cell along $z$ direction and the thickness of 2D material. However, the $d$ is not well defined, for example graphene. In this work, the $L_z=24.64$ Å is used as $d$. By $\kappa \times d$, the thermal sheet conductance can be attained.

III. MAIN CALCULATED RESULTS AND ANALYSIS

The structure of Janus MoSSe monolayer is similar to MoS$_2$/MoSe$_2$ monolayer with the 2H phase, containing three atomic sublayers with Mo layer sandwiched between S and Se layers. The Janus monolayer MoSSe can be constructed by replacing one of two S (Se) layers with Se (S) atoms in MoS$_2$ (MoSe$_2$) monolayer. The schematic crystal structure of MoSSe monolayer is plotted in Figure 1. It is clearly seen that the Janus MoSSe monolayer loses the reflection symmetry with respect to the central metal Mo atoms compared with MoS$_2$/MoSe$_2$ monolayer. Therefore, the MoSSe monolayer (No.156) has lower symmetry compared with MoS$_2$/MoSe$_2$ monolayer (No.187). To avoid spurious interaction between neighboring layers, the unit cell of Janus MoSSe monolayer, containing one Mo, one S and one Se atoms, is constructed with the vacuum region of more than 18 Å. The optimized lattice constants (other theoretical values\textsuperscript{7}) and bond lengths of MoS$_2$, MoSSe and MoSe$_2$ monolayers are listed in Table I. It is expected that $a$ of MoSSe monolayer is between ones of MoS$_2$ and MoSe$_2$ monolayers, which is about 2.2% higher than that of MoS$_2$ monolayer, and 1.5% lower than that of MoSe$_2$ monolayer. It is noted that the bond length of Mo-S/Se between MoSSe and MoS$_2$/Se$_2$ monolayers is almost the same. The bond length of S-Se of MoSSe monolayer is between ones of S-S (MoS$_2$) and Se-Se (MoSe$_2$).

Figure 2 shows the phonon dispersions of MoS$_2$, MoSSe and MoSe$_2$ monolayers along high symmetry path, which agree well with previous results\textsuperscript{7,11,16}. The 3 acoustic and 6 optical phonon branches are observed due to three
atoms in the unit cell. The longitudinal acoustic (LA) and transversal acoustic (TA) branches are linear near the Γ point, while out-of-plane acoustic (ZA) branch deviates from linearity. Similar behavior can be found in many 2D materials. Due to $D_{1h}$ symmetry for MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers, the optical lattice-vibration modes at Γ point can be defined as:

$$\Gamma_{optical} = A_2'(IR) + A_1'(R) + E'(IR + R) + E'(R)$$ (4)

in which IR and R mean infrared- and Raman-active mode, respectively. The optical phonon frequencies of MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers are in agreement with the experimental results. From MoS$_2$ to MoSe$_2$ to MoS$_2$ monolayer, acoustic modes become softened, and the optical branches overall move toward lower energy, which mean reduced group velocities. A frequency gap between the acoustic and optical phonon branches can be observed, which is due to mass differences between the constituent atoms. The frequency gap is 1.36 THz for MoS$_2$, 0.63 THz for MoSe$_2$ and 0.15 THz for MoS$_2$. The frequency gap along with the width of acoustic branches are listed in Table III. The phonon frequencies are very close to previous ones. It is noted that the frequency gap can produce important influence on acoustic + acoustic $\rightarrow$ optical (aa) scattering. The large gap induces ineffective aa scattering due to the requirement on energy conservation, while small gap results in much more frequent aa scattering. These have important effects on phonon transports of both bulk and 2D materials.

Within RTA method, Figure 3 shows the intrinsic lattice thermal conductivities of MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers from harmonic and anharmonic IFCs. With the same thickness $d$ (24.64 Å), the room-temperature lattice thermal conductivity is 23.15 Wm$^{-1}$K$^{-1}$, 13.90 Wm$^{-1}$K$^{-1}$ and 11.54 Wm$^{-1}$K$^{-1}$, respectively. Their thermal sheet conductance is 570.42 WK$^{-1}$, 342.50 WK$^{-1}$ and 284.35 WK$^{-1}$, respectively. The thermal conductance values of MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers are listed in Table III, together with reported theoretical values using similar RTA method, which have been converted into thermal sheet conductances. Our calculated values of MoS$_2$ and MoS$_2$ monolayers are very close to previous ones. It is expected that the lattice thermal conductivity of MoS$_2$ monolayer is between ones of MoS$_2$ and MoS$_2$ monolayers. In the considered temperature range, the $\kappa_L$ of MoS$_2$ monolayer is about 60% of one of MoS$_2$ monolayer, and around 121% of $\kappa_L$ of MoSe$_2$. For MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers, the ratio between accumulated and total lattice thermal conductivity with respect to frequency are plotted in Figure 4 at room temperature. It is clearly seen that acoustic branches of MoS$_2$, MoSe$_2$ and MoS$_2$ monolayers dominate lattice thermal conductivity, providing a contribution of 97.3%, 97.6% and 96.9%, respectively. The relative contribution of every phonon mode of acoustic branches to the total lattice thermal conductivity (300 K) also are shown in Figure 4.
To further understand phonon transports of MoS$_2$, MoSSe and MoSe$_2$ monolayers, phonon mode group velocities and lifetimes are calculated. Due to dominant contribution to total $\kappa_L$ from acoustic phonon branches, we only show acoustic phonon mode group velocities and lifetimes in Figure 5 and Figure 6. From MoS$_2$ to MoSSe to MoSe$_2$ monolayer, most of group velocities become small due to softened acoustic phonon modes, which results in the decrease of the lattice thermal conductivity. The largest phonon group velocity at the $\Gamma$ point of the LA/TA modes decreases from 6.60/4.11 km/s to 5.62/3.55 km/s to 5.06/3.22 km/s from MoS$_2$ to MoSSe to MoSe$_2$ monolayer. For ZA branch, the largest phonon group velocity changes from 4.18 km/s to 3.56 km/s to 3.29 km/s. Therefore, the group velocity reduction may be partial reason for the thermal conductivity reduction from MoS$_2$ to MoSSe to MoSe$_2$ monolayer. It is straightforward to find that most of phonon lifetimes of MoSSe and MoSe$_2$ monolayers are shorter than ones of MoS$_2$ monolayer, which may be due to larger acoustic and optical phonon gap. However, the phonon lifetimes between MoSSe and MoSe$_2$ monolayers are comparative. The lower $\kappa_L$ for MoSSe/MoSe$_2$ than MoS$_2$ monolayer is due to lower group velocities and shorter lifetimes. The $\kappa_L$ of MoSe$_2$ is lower than that of MoSSe, which is mainly due to lower group velocities.

Based on the formula proposed by Shin-ichiro Tamura\textsuperscript{42}, phonon-isotope scattering is included, and the mass variance parameters are read from database of the natural abundance data for elements. The room temperature “isotope effect” can be measured by $P = (\kappa_{\text{pure}}/\kappa_{\text{iso}} − 1)$. The calculated value is 6.2%, which means that phonon-isotope scattering has little effects on $\kappa_L$. With increasing temperature, isotopic effect on $\kappa_L$ gradually becomes weak due to enhancement of phonon-phonon scattering. In reality, finite-size sample is usually used in the device implementation. By adopting a most simple boundary scattering model, the boundary scattering rate can be obtained by $v_g/L$, in which $v_g$, $L$ are the group velocity and boundary mean free path (MFP), respectively. The lattice thermal conductivities of infinite and finite-size (0.6, 0.3, 0.1, 0.06 and 0.03 µm) MoSSe monolayer as a function of temperature are plotted in Figure 7. It is apparent that the thermal conductivity decreases with length decreasing, which is due to enhanced boundary scattering. For the 0.6, 0.3, 0.1, 0.06 and 0.03 µm cases, the room-temperature $\kappa_L$ of MoSSe monolayer is about 81.5%, 70.2%, 47.6%, 37.1% and 24.8% of one of infinite (Pure) case.

The MFP distributions over a wide range of length scales can be measured by thermal conductivity spectroscopy technique\textsuperscript{43}. At 300 K, the ratio between cumulative and total lattice thermal conductivity of MoS$_2$, MoSSe and MoSe$_2$ monolayers as a function of phonon MFP are shown in Figure 7, which measures how phonons with different MFP contribute to the total lattice thermal conductivity. With MFP increasing, the ratio approaches one. When the ratio reaches 99%, the corresponding MFP is 728 nm, 502 nm and 748 nm from MoS$_2$ to MoSSe to MoSe$_2$ monolayer. The critical MFP of MoSSe is smaller than that of MoS$_2$ or MoSe$_2$ monolayer, which is because MoSSe monolayer contains more element types. It is noted that critical MFP significantly depends on strain, which has been found in antimonene, silicene, germanene, and stanene\textsuperscript{25,27}. With $\kappa_L$ reducing to half by nanostructures, the characteristic length changes from 121 nm to 111 nm to 129 nm from MoS$_2$ to MoSSe to MoSe$_2$ monolayer.

The $\kappa_L$ is connected with Young’s modulus by the simple relation $\kappa_L \sim \sqrt{E}$\textsuperscript{28}, and the Young’s modulus can be attained from elastic constants. Due to $D_{3h}$ symmetry, two independent elastic constants $C_{11} = C_{22}$ and $C_{12}$ can be calculated, and the $C_{66} = (C_{11}−C_{12})/2$. Table IV lists the elastic constants $C_{ij}$ of MoS$_2$, MoSSe and MoSe$_2$ monolayers, and they all satisfy the Born criteria of mechanical stability, namely

$$C_{ij} > 0, \quad C_{66} > 0$$

The 2D Youngs moduli $Y_{2D}$ in the Cartesian [10] and
TABLE IV. For MoS$_2$, MoSSe and MoSe$_2$ monolayers, the elastic constants $C_{ij}$, shear modulus $G^{2D}$, Young’s modulus $Y^{2D}$ in Nm$^{-1}$, and Poisson’s ratio $\nu$ dimensionless.

| Name    | $C_{11} = C_{22}$ | $C_{12}$ | $C_{66} = G^{2D}$ | $Y^{2D}_{[01]}$ | $Y^{2D}_{[10]}$ | $\nu_{[10]}$ | $\nu_{[01]}$ |
|---------|-----------------|---------|------------------|----------------|----------------|-------------|-------------|
| MoS$_2$ | 131.7 (138.5$^a$, 130$^{15}$, 130.3$^{46}$) | 31.2 (31.7$^a$, 32$^{15}$, 31.0$^{46}$) | 59.3 | 124.3 | 0.24 |
| MoSSe   | 119.3 (126.8$^a$) | 27.5 (27.4$^a$) | 45.9 | 113.0 | 0.23 |
| MoSe$_2$ | 115.6 (115.9$^a$, 108$^{15}$, 110.1$^{46}$) | 26.5 (24.0$^a$, 25$^{15}$, 26.0$^{46}$) | 44.6 | 109.5 | 0.23 |

![FIG. 8. Phonon dispersion curves of ZrSSe and MoSSe monolayers.](image)

Strain effects on $\kappa_L$ of various 2D materials have been investigated$^{19,24,26,27}$. For penta-SiN$_2$, a planar structure can be achieved from a buckled structure by tensile strain, and the $\kappa_L$ jumps up by 1 order of magnitude$^{24}$, which is because the reflection symmetry selection rule strongly restricts anharmonic phonon scattering. For penta-SiC$_2$, the $\kappa_L$ exhibits an unusual nonmonotonic up-and-down behavior$^{24}$. For MoTe$_2$, the $\kappa_L$ shows monotonic reduction due to the reduction in phonon group velocities and phonon lifetime$^{19}$. Therefore, it is very interesting to investigate the strain influence on $\kappa_L$ of MoSSe monolayer.

In summary, based on phonon Boltzmann equation within the single-mode RTA, the $\kappa_L$ of MoSSe monolayer is investigated together with MoS$_2$ and MoSe$_2$ monolayers. Calculated results show that the $\kappa_L$ of MoSSe monolayer is very lower than that of MoS$_2$ monolayer, which is due to the smaller group velocities and shorter phonon lifetimes for MoSSe than MoS$_2$ monolayer. However, the $\kappa_L$ of MoSSe monolayer is higher than that of MoSe$_2$ monolayer, which is mainly due to larger group velocities. It is expected that the order of Young’s modulus is MoS$_2 >$ MoSSe > MoSe$_2$, which is identical with that of $\kappa_L$. The isotope effect and size dependence of $\kappa_L$ of MoSSe monolayer are also investigated, which is useful for designing nanostructures. This work presents comprehensive investigations on the phonon transport of Janus monolayer MoSSe, which is useful for further study in TMD Janus monolayers.
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