I. INTRODUCTION

The one-atom-thick two-dimensional (OAT2D) materials have plenty of novel properties and have attracted intensive research interests in past decades. The size of this OAT2D material family is keeping on expansion currently, and contains following members; i.e., graphene, hexagonal boron nitride, 2D honeycomb silicon, layered transition metal dichalcogenides (MoS$_2$, WS$_2$, ...), black phosphorus, 2D ZnO, and etc. Graphene is best-known among all OAT2D family members, and has earned a Nobel prize in physics for Novoselov and Geim in 2010. From the above, we learn that, on the one hand, graphene attracts ongoing research interests from both academic and applied communities. Naturally, lots of review articles have been devoted to the summary of intense studies for graphene. On the other hand, more and more people start to examine possible applications in other OAT2D materials for their knowledge gained from graphene. In particular, MoS$_2$ has attracted considerable research interest. Many review articles have also been produced for MoS$_2$. The present review is characteristic for its focus on a detailed comparison for properties between graphene and SLMoS$_2$. This type of comparison makes us clear about positive/negative properties for graphene and MoS$_2$. Hence, we will be aware of possible advanced features or drawbacks for graphene/MoS$_2$ heterostructures which were expected to mitigate the negative properties of each individual constituent.

In this review, we comparatively introduce following properties for graphene and SLMoS$_2$; i.e., structure, interatomic potential, phonon dispersion, mechanical properties, nanomechanical resonator, thermal conductivity, electronic band structure, optical absorption, and the graphene/MoS$_2$ heterostructure. The article ends up with a summary table listing major results for all properties that have been compared in present article.
The interaction between carbon atoms in graphene can be calculated on four different computation cost levels. First, the first principles calculation is the most expensive approach to compute the interatomic energy for graphene. Many existing simulation packages can be used for such calculation, e.g. the commercial VASP software or the freely available SIESTA package. Second, to save computation cost, Brenner et al. developed an empirical potential for carbon based materials, including graphene. The bond-order Brenner potential takes the Tersoff potential form and is able to capture most linear properties and many nonlinear properties for graphene. For instance, it can describe the bond forming and breaking in graphene, besides its good description for the structural, mechanical, and thermal properties. Third, the Tersoff potential or SW potential can provide reasonable predictions for some nonlinear and linear properties of graphene. These two empirical potentials have less parameters than Brenner potential, so they are much faster than Brenner potential. Fourth, the linear portion of the C-C interaction in graphene can be captured by some valence force field models (VFFM). This type of linear model has the cheapest computation cost, and can be used to compute some linear properties in an efficient manner.

Potentials on these four computation levels can also be found for SLMoS$_2$. First, the first principles calculation can also be done properly for SLMoS$_2$. Second, in 2009, Liang et al. parameterized a bond-order potential for SLMoS$_2$ which is based on the bond order concept underlying the Brenner potential. This Brenner-like potential was recently further modified to study the nanoindentation of SLMoS$_2$ thin films using a molecular statics approach. Third, quite recently, we have parameterized a SW potential for SLMoS$_2$, where potential parameters were fitted to the phonon spectrum. This potential can be friendly used in some popular simulation packages, such as GULP or LAMMPS. Fourth, in 1975, Wakabayashi et al. developed a VFFM to calculate the phonon spectrum of the bulk MoS$_2$. This linear model has been applied to study the lattice dynamics properties of some MoS$_2$ based materials.

III. PHONON DISPERSION

Phonon is a quasi particle in the reciprocal space. Each phonon mode describes a particular kind of collective vibration of all atoms in the real lattice space. The symmetry of the vibration morphology follows an irreducible representation of the space group for the system. These irreducible representations are denoted by a wave vector $\vec{k}$. Phonon mode can be denoted by the wave vector $\vec{k}$ and a branch index $\tau$, where $\vec{k}$ is to distinguish the inter-cell degrees of freedom while $\tau$ corresponds to the intra-cell degrees of freedom. It has a specific angular frequency $\omega_{\vec{k}, \tau}$ and eigen vector $\vec{\xi}_{\vec{k}, \tau}$. For graphene or SLMoS$_2$, each degree of freedom can be indexed by $(l_1 l_2 s \alpha)$. $l_1$ and $l_2$ denote the position of the unit cell, $s$ describes different atoms inner the unit cell, and $\alpha = x, y, z$ is the axis direction. The frequency and eigen vector of the phonon mode can be obtained through the diagonalization of the
FIG. 2: (Color online) Phonon dispersion of graphene along the high symmetry ΓKM lines in the Brillouin zone. The interaction between carbon atoms is described by the Brenner potential. Inset shows the first Brillouin zone for the hexagonal lattice structure.

Following dynamical matrix,

$$D_{\alpha s\alpha' s'}(\vec{k}) = \frac{1}{\sqrt{m_s m_s'}} \sum_{l_1=1}^{N_1} \sum_{l_2=1}^{N_2} K_{00\alpha l_1l_2\alpha' s' \beta} e^{i \vec{k} \cdot \vec{R}_{l_1l_2}};$$

$$\sum_{s' \beta} D_{\alpha s s' \beta} \left( \vec{k} \right) \xi_{s \beta}^{(\tau')} (\vec{k}|00s') = \omega^{(\tau')} (\vec{k}) \xi_{\alpha \beta}^{(\tau')} (\vec{k}|00s').$$

The force constant matrix $K_{00\alpha l_1l_2\alpha' s' \beta}$ stores the interaction information between two degrees of freedom (00sα) and (l1l2s'β). $N_1 \times N_2$ gives the total number of unit cells. For short-range interactions, the summation over $(l_1, l_2)$ can be truncated to the summation over neighboring atoms.

FIG. 3: (Color online) Eigenvectors for the six phonon modes at the Γ point in graphene. Arrow attached to each atom represents the vibration component of the atom in the eigenvector. Numbers are the frequency of each phonon mode in the unit of cm$^{-1}$.

are six phonon branches in graphene, according to the two inequivalent carbon atoms in the unit cell. These branches (from bottom to top) are z-direction acoustic (ZA), transverse acoustic (TA), longitudinal acoustic (LA), z-direction optical (ZO), transverse optical (TO), and longitudinal optical (LO) branches. The three blue curves in lower frequency range correspond to the three acoustic branches, while the upper three red curves are with respect to optical branches. The eigen vector of the six phonon modes at Γ point is displayed in Fig. 3. In the top panel, the three acoustic phonons have zero frequency, as the interatomic potential does not vary during rigid translational motions. In the bottom panel, the two in-plane optical phonons have almost the same frequency, revealing an isotropic phonon property for the two in-plane directions in graphene.

FIG. 4: (Color online) Phonon dispersion of SLMoS$_2$ along the high symmetry ΓKM lines in the Brillouin zone. The interaction is described by the SW potential. Inset shows the first Brillouin zone for the hexagonal lattice structure.

Each unit cell has one Mo atom and two S atoms, so there are nine branches in the phonon spectrum. The three lower blue curves correspond to the three acoustic branches, while the other six upper curves are for optical branches. Fig. 4 shows eigen vectors for the nine phonons at Γ point. In particular, there are two interesting shearing-like phonons in panel (c) and two inter-layer breathing-like phonons in (d).

From phonon dispersions of graphene and SLMoS$_2$, it is hard for us to declare which material has better phonon property. Yet, we can tell two obvious differences in their phonon dispersions. First, the spectrum of graphene is overall higher than SLMoS$_2$ by about a factor of three. As a result, phonons in graphene can carry more energy than SLMoS$_2$ in the thermal transport phenomenon, leading to stronger thermal transport ability for graphene. Second, there is a distinct energy band gap between acoustic and optical branches in SLMoS$_2$. 
This band gap forbids many phonon-phonon scattering channels; thus protect acoustic phonons from being interrupted by high-frequency optical phonons for SiMoS$_2$.\cite{41} As a result, the SiMoS$_2$ nanoresonator has higher quality (Q)-factor than graphene, since SiMoS$_2$'s resonant oscillation (related to the ZA mode) has less possibility to be affected by thermal vibrations.

**IV. MECHANICAL PROPERTIES**

We are discussing several basic mechanical properties, including Young's modulus, bending modulus, and buckling phenomenon. These mechanical properties are fundamental for the application of graphene or SiMoS$_2$ in nano-devices. A good mechanical stability is essential in nanoscale devices, which are more sensitive than macroscopic devices to external perturbations due to their high surface to volume ratio.

**Young's modulus.** We talk about the in-plane/two-dimensional Young's modulus $E^{2D}$, which is thickness independent. The Young's modulus is related to this effective Young's modulus through $Y = E^{2D}/h$, with $h$ as the thickness. The nanoindentation experiment measured the effective Young's modulus of graphene to be around 335.0 Nm$^{-1}$.\cite{44} This value can be reproduced in a very simple approach, in which the nonlinear interaction is estimated from the Tersoff-Brenner potential.\cite{45}

For SiMoS$_2$, similar nanoindentation measurement found that the average value of the effective Young's modulus is 180 ± 60 Nm$^{-1}$ in the experiment by Bertolazzi et al.\cite{46} or 120 ± 30 Nm$^{-1}$ measured by Cooper et al.\cite{47} The nanoindentation set up has also been applied to study the Young's modulus of thicker MoS$_2$.\cite{48} The theoretical prediction for the in-plane Young's modulus is 139.5 Nm$^{-1}$ based on the SW potential.\cite{49} The trilayer structure of SiMoS$_2$ can bring some novel structure transitions,\cite{50,51} which cannot happen in graphene.

**Bending modulus.** Graphene is extremely soft in the out-of-plane direction, owing to its one-atomic-thick structure. It is so thin that it is natural for graphene to have an extremely small bending modulus, which can be inspired by the well-known relationship in the shell theorem, $D = E^{2D}h^2/(12(1-\nu^2))$, where $E^{2D}$ is the two-dimensional stiffness, $h$ is the thickness, and $\nu$ is Poisson's ratio. The bending modulus of graphene has been derived analytically from two equivalent approaches; i.e., 1.17 eV from the geometric approach with interaction described by a VFFM\cite{52} or 1.4 eV from the exponential Cauchy-Born rule using Brenner potential.\cite{53} Note that these two approaches are equivalent to each other, and the difference in bending modulus mainly comes from the different potentials used in these derivations.

Similar analytic approach has been applied to derive the bending modulus of SiMoS$_2$ using the SW potential.\cite{49} The bending modulus of SiMoS$_2$ is 9.61 eV, which is a factor of seven larger than graphene. The enhanced bending modulus for SiMoS$_2$ is due to its trilayer characteristic atomic structure, which results in more interaction terms against the bending motion. The bending modulus can be calculated by

$$D = \frac{\partial^2 W}{\partial \kappa^2},$$

(1)

where $W$ is the bending energy density, and $\kappa$ is the bending curvature. For the SiMoS$_2$, the bending energy can be written as\cite{54}

$$D = \sum_q \frac{\partial^2 W}{\partial r_q^2} \left( \frac{\partial r_q}{\partial \kappa} \right)^2 + \sum_q \frac{\partial^2 W}{\partial \theta_q^2} \left( \frac{\partial \theta_q}{\partial \kappa} \right)^2,$$

(2)

where $r_q$ and $\theta_q$ are geometrical parameters in the empirical potential expressions. This formula is substantially different from the bending modulus formula in graphene.\cite{50} Specifically, the first derivatives, $\frac{\partial r_q}{\partial \kappa}$ and $\frac{\partial \theta_q}{\partial \kappa}$, are nonzero owing to the trilayer structure of
SLMoS$_2$. As a result, the bending motion of SLMoS$_2$ will be counteracted by more cross-plane interactions.

**Buckling phenomenon.** The Euler buckling theorem states that the buckling critical strain is determined by the Young’s modulus and the bending modulus through following formula\(^\text{53}\)

$$
\epsilon_c = -\frac{4\pi^2D}{E^{2D}L^2},
$$

where \(L\) is the length of the system. For graphene, \(E^{2D} = 335\text{ Nm}^{-1}\) and \(D = 1.4\text{ eV}\) can be found from above discussions, so we get the explicit formula for the buckling critical strain,

$$
\epsilon_c = -\frac{2.64}{L^2}.\tag{4}
$$

The length \(L\) is in the unit of Å.

For SLMoS$_2$, \(E^{2D} = 139.5\text{ Nm}^{-1}\) and \(D = 9.61\text{ eV}\) can be found from above discussions, so we get the explicit formula for the buckling critical strain,

$$
\epsilon_c = -\frac{43.52}{L^2}.\tag{5}
$$

It is quite obvious that the buckling critical strain for SLMoS$_2$ is twenty times larger than graphene of the same length: i.e. SLMoS$_2$ is more difficult to be buckled under external compression. This phenomenon has been examined by both MD simulations and the phonon analysis\(^{45,54}\).

We have comparatively discussed in the above the mechanical properties for graphene and SLMoS$_2$. Graphene has larger Young’s modulus and is more flexible, while SLMoS$_2$ has higher bending modulus and is more difficult to be buckled under external compression. Hence, in terms of mechanical properties, it will be more productive for graphene and SLMoS$_2$ to collaborate with each other in a heterostructure form, so as to mitigate the negative mechanical properties of each other.

**V. NANOMECHANICAL RESONATOR**

Nanoresonators based on two-dimensional materials like graphene and SLMoS$_2$ are promising candidates for ultra sensitive mass sensing and detection due to their large surface area and small mass. For sensing applications, it is important that the nanoresonator exhibits a high Q-factor, since the sensitivity of the nanoresonator is inversely proportional to its Q-factor.\(^{\text{45,54}}\) Q-factor is a quantity that records the total oscillation cycles of the resonator before its resonant oscillation is considerably decayed. Hence, a weaker energy dissipation will lead to higher Q-factor.

For graphene nanoresonators, the Q-factor decreases exponentially with decreasing temperature \(^{\text{56,57}}\) \(T^{-\alpha}\). Zandie et al.\(^{\text{58}}\) found that the exponent \(\alpha = 0.35 \pm 0.05\) for temperature bellow 40 K. For temperature above 40 K, \(\alpha = 2.3 \pm 0.1\). Chen et al.\(^{\text{57}}\) observed similar transition in the Q-factor with different exponents. This continuous transition for the temperature dependence of the Q-factor is attributed to the out-of-plane diffusion of adsorbs on the graphene surface.\(^{\text{58,59}}\) MD simulations also predicted a discontinuous transition in the Q-factor at 7.0 K low temperature due to the in-plane diffusion of adsorbs on the graphene surface.\(^{\text{58}}\) Very high Q-factor can now be achieved in the laboratory at low temperatures. Bunch et al. observed Q-factor of 9000 for graphene nanoresonators at 10 K.\(^{\text{60}}\) Chen et al. also found that the Q-factor increases with decreasing temperature, and reaches \(10^4\) at 5 K.\(^{\text{56}}\) Eichler et al.\(^{\text{56}}\) found that Q-factors of graphene nanoresonators can reach values of \(10^5\) at 90 mK.

On the SLMoS$_2$ side, two recent experiments have demonstrated the nanomechanical resonator behavior for SLMoS$_2$ or few-layer MoS$_2$. In particular, Castellanos-Gomez et al. found the figure of merit i.e. frequency-Q-factor product \(f_0 \times Q \approx 2 \times 10^9\text{ Hz}\) for SLMoS$_2$.\(^{\text{61}}\) Lee et al. found that few-layer MoS$_2$ resonators exhibits a high figure of merit of \(f_0 \times Q \approx 2 \times 10^{10}\text{ Hz}\).\(^{\text{62}}\) This high Q-factor of SLMoS$_2$ is attributed to the energy band gap in the phonon dispersion of SLMoS$_2$, which protects the resonant oscillation from being scattered by thermal vibrations.\(^{\text{56,57}}\) As a result, SLMoS$_2$ was predicted to have a higher Q-factors by at least a factor of four than graphene.

Although MoS$_2$ has been predicted theoretically to have better mechanical resonant behavior than graphene, present experiments are quite limited for MoS$_2$ nanoresonators, so more measurements are in need to examine its properties, such as the mass sensitivity. Furthermore, MoS$_2$ has a finite electronic band gap, so it can have a good transistor behavior. This electronic property can be coupled with the mechanical resonant oscillation to provide an interesting electron-mechanical nanoresonator.

**VI. THERMAL CONDUCTIVITY**

Thermal transport phenomenon happens in materials with temperature gradients. The thermal energy can be carried by both phonons or electron. The electron thermal conductivity is important for metals. However, for graphene, the thermal conductivity is mainly contributed by the phonons, while electronic thermal conductivity is less than 1% of the overall thermal conductivity in graphene.\(^{\text{43,44}}\) We thus discuss only the phonon (lattice) thermal conductivity for graphene. The thermal conductivity \((\kappa)\) is related to the thermal current density \((J)\) and the temperature gradient \((\nabla T)\) through the Fourier law, \(\kappa = -\nabla T/J\).

In bulk materials, thermal conductivity is normally a constant that is size independent. However, it behaviors anomaly with the length in the OAT2D graphene; i.e., thermal conductivity is not a constant and keeps on increasing with increasing sample length.\(^{\text{45-49}}\) For
On the MoS$_2$ side, a recent experiment by Sahoo et al. found that few-layer MoS$_2$ as a thermal conductivity around 52 Wm$^{-1}$K$^{-1}$, which is much lower than thicker graphene layers (1000 Wm$^{-1}$K$^{-1}$). Although there is so far no measurement for the thermal conductivity of SLMoS$_2$, this topic has attracted increasing interest from the theoretical community. In 2010, Varshney et al. performed a force-field based MD simulation to study the thermal transport in SLMoS$_2$. In 2013, two first-principles calculations were performed to investigate the thermal transport in the SLMoS$_2$ in the ballistic transport regime. The predicted room temperature thermal conductivity in the ballistic regime is below 800 Wm$^{-1}$K$^{-1}$ for a SLMoS$_2$ of 1.0 µm in length. This value is considerably lower than the ballistic thermal conductivity of 5000 Wm$^{-1}$K$^{-1}$ for a graphene with the same length. The smaller thermal conductivity of SLMo is because the overall phonon spectrum of SLMo is lower than graphene by roughly a factor of three; i.e., each phonon mode in SLMo carries fewer thermal energy than graphene. In 2013, we performed MD simulations to predict the room temperature thermal conductivity of SLMoS$_2$ to be 6.0 Wm$^{-1}$K$^{-1}$ for a system with length 4.0 nm. In a more recent work, the size dependence for the thermal conductivity in SLMoS$_2$ is studied by MD simulations, and the obtained value is below 2.0 Wm$^{-1}$K$^{-1}$ for system length shorter than 120.0 nm.

Electrons in SLMoS$_2$ are normal fermions with parabolic energy dispersion, and it is a semiconductor with a direct band gap above 1.8 eV. This finite band gap endorses SLMoS$_2$ to work as a transistor. Similar as graphene, the band gap in SLMoS$_2$ can also be modulated by strain engineering. First principles calculations predict a semiconductor-to-metal transition in SLMoS$_2$ by both biaxial compression or tension. The experiment by Eknapiakul et al. shows that an uniaxial tensile mechanical strain of 1.5% can produce a direct-to-indirect band gap transition. With increasing number of layers, the electronic band gap for few-layer MoS$_2$ undergoes a direct-to-indirect transition, and decreases to a value of 1.2 eV for bulk MoS$_2$. From these comparisons, we find that SLMoS$_2$ possesses a finite band gap prior to any gap-opening engineering. Consequently, it may be more competitive than graphene for applications in transistor, optoelectronics, energy harvesting, and other nano-material fields.

The electronic band structure is fundamental for electronic processes, such as the transistor performance. In particular, the value of the electronic band gap determines whether the material is metallic (zero band gap), semiconductor (moderate band gap), or insulator (large band gap).
VIII. OPTICAL ABSORPTION

Optical properties of OAT2D materials are important for their applications in photodetector, phototransistor, or other photonic nanodevices. The photocarriers in these OAT2D materials may have quite different behavior from conventional semiconductors, due to their particular configuration.

Graphene has a Dirac cone electron band structure with zero band gap. Relating to this unique band structure, graphene can absorb about 2% of incident light over a broad wavelength, which is strong considering its one-atom-thick nature. Xia et al. demonstrated an ultrafast photodetector behavior for graphene, where the photoresponse did not degrade for optical intensity modulations up to 40 GHz, and the intrinsic band width was estimated to be above 500 GHz. However, the photoreponsivity for graphene is low due to zero bandgap.

SLMoS₂ has a direct band gap about 1.8 eV. This optical-range band gap lead to high absorption coefficient for incident light, so the SLMoS₂ have very high sensitivity in photon detection. Lopez-Sanchez et al. found that the photoresponsivity of the SLMoS₂ can be as high as 880 AW⁻¹ for an incident light at the wavelength of 561 nm, and the photoresponse is in the 400-680 nm. This high photoresponsivity together with its fast light emission enables SLMoS₂ to be an ultra sensitive phototransistors with good device mobility and large ON current. In phototransistors, the electron-hole pair can be efficiently generated by photoexcitation in doped SLMoS₂, which joins the doping-induced charges to form a bound states of two electrons and one hole. As a result, the carrier effective mass is considerably increased, and the photoconductivity can be decreased.

For optical properties, graphene is very fast in the photo detection, while SLMoS₂ is very sensitive in this photo detection application. Considering this complementary property, it may be fruitful for the cooperation of these two materials.

IX. GRAPHENE/MoS₂ HETEROSTRUCTURE

In the above, we have focused mainly on the comparison between graphene and MoS₂ in several properties. The rest of the article will be devoted to a close collaboration between these two materials. As long as graphene and MoS₂ have complementary physical properties, it is natural to combine graphene and MoS₂ in specific ways to create heterostructures that mitigate the negative properties of each individual constituent.

There have been some experiments investigating advanced properties of such graphene/MoS₂ heterostructures. Britnell et al. found that graphene/MoS₂ heterostructures have better photon absorption and electron-hole creation properties, because of the enhanced light-matter interactions by the SLMoS₂. Graphene has outstanding mechanical properties, and this nice property has been utilized to protect MoS₂ from radiation damage by coating graphene outside of the MoS₂. In a recent experiment, Larentis et al. measured the electron transport of the graphene/MoS₂ heterostructure and observed a negative compressibility in the MoS₂ component. This surprise phenomenon was interpreted based on the interplay between the Dirac and parabolic bands for graphene and MoS₂, respectively. Yu et al. have fabricated high-performance electronic circuits based on the graphene/MoS₂ heterostructure, with MoS₂ as the transistor channel and graphene as the contact electrodes and circuit interconnects.

Although experimentalists have shown great interest in various properties of graphene/MoS₂ heterostructures, the corresponding theoretical efforts have been quite limited until now, which mainly focus on the interaction between graphene and MoS₂ layers. The first-principle calculations predict the inter-layer space and the binding energy for the heterostructure to be around -21.0 meV and 3.66 Å in Ref. 106, or -23.0 meV and 3.32 Å in Ref. 110. Using these two quantities, a set of Lennard-Jones potential parameters are determined to be  ε=3.95 meV and σ=3.625 Å, with the cutoff 10.0 Å. These potential parameters are used to study the structure transition of the graphene/MoS₂/graphene heterostructure under mechanical tension. It was shown that the Young’s modulus (Y) of the graphene/MoS₂/graphene heterostructure can be predicted by the following rule of mixtures based on the arithmetic average.

\[ Y_{GMG} = Y_G f_G + Y_M f_M, \]  

where \( Y_{GMG} \), \( Y_G \), and \( Y_M \) are the Young’s modulus for the heterostructure, graphene, and SLMoS₂, respectively. \( f_G = 2V_G/(2V_G + V_M) = 0.524 \) is the volume fraction for the two outer graphene layers in the heterostructure, and \( f_M = V_M/(2V_G + V_M) = 0.476 \) is the volume fraction for the inner SLMoS₂ layer. The thickness is 3.35 Å and 6.09 Å for single-layer graphene and SLMoS₂, respectively. The room temperature Young’s modulus are 859.69 GPa for graphene and 128.75 GPa for SLMoS₂. From this mixing rule, the upper-bound Young’s modulus of the heterostructure is 511.76 GPa.

As another important mechanical property, the ultimate strain of the graphene/MoS₂/graphene heterostructure is about 0.26, which is much smaller than 0.40 for the MoS₂. Under large mechanical tension, the heterostructure collapses from the buckling of outer graphene layers. These graphene layers are compressed in the lateral direction by the Poisson effect induced stress, when the heterostructure is stretched in the longitudinal direction.

X. CONCLUSION

We have compared a series of physical properties for graphene and SLMoS₂, with the main results listed in Tab. [I]
TABLE I: Summary list for properties that have been compared for graphene and SLMoS in present review article.

| properties            | graphene                                      | SLMoS           |
|-----------------------|-----------------------------------------------|-----------------|
| structure             | $D_{ab}$: $a = 2.464\AA$; $b = 1.424\AA$ (Ref. 26) | $D_{ab}$: $a = 3.094\AA$; $b = 2.394\AA$ (Ref. 27) |
| interaction           | ab initio; Brenner; SW; VFFM                   | ab initio; Brenner; SW; VFFM |
| phonon dispersion     | \(\omega_{gap} \approx 1664.5\text{ cm}^{-1}\); \(\omega_{gap} = 0\) | \(\omega_{gap} \approx 478.8\text{ cm}^{-1}\); \(\omega_{gap} = 25.0\text{ cm}^{-1}\) |
| mechanical strength   | \(E^{2D} = 335.0\text{ Nm}^{-1}\) (Ref. 3)       | \(E^{2D} = 180 \pm 60\text{ Nm}^{-1}\) (Ref. 46) |
|                       | \(D = 1.17\text{ eV}\) (Ref. 5,6), 1.4 eV (Ref. 7,8) | \(D = 9.61\text{ eV}\) (Ref. 9) |
|                       | \(\epsilon_c = -2.64L^{-1}\)                    | \(\epsilon_c = -43.52L^{-2}\) |
| nanoresonator         | \(f_0 \times Q = 6.3 \times 10^{11}\text{ Hz} (10 \text{ K}, \text{Ref. 56})\) | \(f_0 \times Q \approx 2 \times 10^9\text{ Hz} (300 \text{ K}, \text{Ref. 61})\) |
|                       | \(f_0 \times Q = 1.82 \times 10^{12}\text{ Hz} (5 \text{ K}, \text{Ref. 57})\) | \(f_0 \times Q = 2.4T^{-1.3} \times 10^{11}\text{ THz} (\text{Ref. 44})\) |
|                       | \(f_0 \times Q = 1.56 \times 10^{13}\text{ Hz} (90 \text{ mK}, \text{Ref. 60})\) | \(f_0 \times Q = 5 \times 10^{10}\text{ Hz} (300 \text{ K}, \text{Ref. 61})\) |
| thermal conductivity  | 60 Wm$^{-1}$K$^{-1}$ \((L = 10 \text{ nm}, \text{Ref. 70})\) | 6 Wm$^{-1}$K$^{-1}$ \((L = 4 \text{ nm}, \text{Ref. 27})\) |
|                       | 250 Wm$^{-1}$K$^{-1}$ \((L = 300 \text{ nm}, \text{Ref. 69})\) | 2 Wm$^{-1}$K$^{-1}$ \((L = 120 \text{ nm}, \text{Ref. 81})\) |
|                       | \(\kappa > 1500 \text{ Wm}^{-1}\text{K}^{-1} (L > 4 \text{ \mu m}, \text{Refs. 69,71,73})\) | \(\kappa > 1500 \text{ Wm}^{-1}\text{K}^{-1} (L > 4 \text{ \mu m}, \text{Refs. 69,71,73})\) |
|                       | 1000 Wm$^{-1}$K$^{-1}$ \((\text{thick graphene layers, Ref. 76})\) | 52 Wm$^{-1}$K$^{-1}$ \((\text{thick MoS}_2 \text{ layers, Ref. 75})\) |
| electronic band       | Dirac cone; \(E_{gap} = 0\) (Refs. 82,83)       | parabolic; \(E_{gap} \approx 1.8\text{ eV}\) (direct, Refs. 90,91) |
| optical absorption    | fast photoresponse (Ref. 98)                   | high photoresponsivity \((0.5\text{ mAW}^{-1}\text{ Ref. 98})\) |
|                       | large band width (Ref. 98)                     | high photoresponsivity \((880\text{ AW}^{-1}\text{ Ref. 99})\) |

Acknowledgements The work is supported by the Recruitment Program of Global Youth Experts of China and the start-up funding from Shanghai University.

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