High intrinsic $ZT$ in InP$_3$ monolayer at room temperature

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Abstract

Two-dimensional thermoelectric (TE) materials which have the figure of merit $ZT$ that is greater than 1.5 at room temperature would be highly desirable in energy conversion since the efficiency is competitive to conventional energy conversion techniques. Here, we report that the indium triphosphide (InP$_3$) monolayer shows a large $ZT$ of 1.92 at 300 K, based on the quantum calculations within the ballistic thermal transport region. A remarkably low and isotropic phononic thermal conductivity is found due to the flat lattice vibration modes, which takes a major responsibility for the impressively high $ZT$ at room temperature. Moreover, a large $ZT$ of 1.67 can still be achieved even under a 1% mechanical tension on the lattice. These results suggest that the InP$_3$ monolayer is a promising candidate for low dimensional TE applications.

Keywords: indium triphosphide, thermoelectric properties, NEGF-DFT

(Some figures may appear in colour only in the online journal)

1. Introduction

Thermoelectric (TE) materials can directly convert between thermal and electrical energy, and therefore have important applications such as in power generation and heat pumping [1]. The efficiency of TE materials is determined by the dimensionless figure of merit, $ZT = \frac{\sigma S^2 T}{\kappa_e + \kappa_p}$, where $\sigma$ is the electrical conductivity, $S$ the seebeck coefficient, $T$ the absolute temperature and $\kappa_p(e)$ the phononic (electronic) thermal conductivity [2]. Great efforts have been put into finding TE materials with the high $ZT$ value. A remarkable $ZT$ of 2.6 has been reported for the single-crystal SnSe [3], and it can be improved to 2.8 in the $n$-type SnSe crystal [4]. At the nanoscale, quantum confinement can reduce substantially the phononic thermal conductivity, and thus leads to a considerable enhancement of the TE efficiency in nanostructures. The TE properties of the low-dimensional materials have attracted great research interest since the ground-breaking experiment which demonstrated that the rough silicon nanowires were efficient TE materials [5].

Currently, there is intense focus on the thermoelectricity of the 2D materials, such as graphene, silicene, black phosphorus and transition-metal dichalcogenides, for their attractive electrical and thermal transport properties [6–14]. For example,
theoretical calculations have shown that the $ZT$ of the silicene nanoribbons is close to 2.5 at 90 K [9], and also a large $ZT$ of 2.8 at 800 K has been predicted for the monolayer SnS [15]. In reality, a high $ZT$ at room temperature will largely facilitate the utilization of the 2D TE materials in various fields, including electricity generation and cooling. Unfortunately, most of the pristine 2D materials show a poor TE efficiency at room temperature, which results essentially from their limited electrical transport properties, while the relatively high thermal conductivity. For instance, graphene has a small $ZT$ about 0.01 [16], and the 2D black phosphorene and blue phosphorene show the $ZT$ around 0.2 and 1.0, respectively [8]. Besides, the 2D MX$_2$ (M = Mo, W; X = S, Se) monolayers have the $ZT < 2$ at 300 K, as predicted by the theoretical calculations [7].

Recently, the high $ZT$ at room temperature has been predicted for several 2D materials. For example, the buckled antimonene [17] has a $ZT$ of 2.15, and moreover the TiS$_3$ calculations [7].

ZT of the mechanical strain on the structure with the phonon blocking materials [21]. Besides, the 2D MX$_2$ (M = Mo, W; X = S, Se) monolayers show a small $ZT$ about 0.01 [16], and the 2D black phosphorene and blue phosphorene show the $ZT$ around 0.2 and 1.0, respectively [8].

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For instance, the $ZT$ of graphene was enhanced impressively by strain engineering, chemical doping and heterostructuring [20]. Specifically, there are several bands including both the heavy-hole and light-hole bands located at the $\Gamma$ point near the Fermi energy. The light bands contribute to the high mobility, and the heavy bands indicate the large effective masses, which leads to a high Seebeck coefficient since the $S$ is proportional to the effective mass. Besides, there are several heavy-hole bands with similar energy value at the $\Gamma$, M and K points, which exhibits converged characteristics and multi-valley transport behavior. Moreover, the top valance bands close to the Fermi energy ($\mu = 0$) are very flat and intensive, which means a high density of states and thus a large transmission coefficient. All these features indicate a high $ZT$, and therefore motivate us to study the TE performance of the InP$_3$ monolayer.

On the other hand, the TE performance of the 2D materials can be effectively improved by various methods, including strain engineering, chemical doping and heterostructuring [20]. For instance, the $ZT$ of graphene was enhanced impressively to around 3.2 at room temperature by constructing a layered structure with the phonon blocking materials [21]. Besides, the $ZT$ of the antimonene was improved largely from less than 0.1 to about 0.6 at room temperature by n-type doping [22]. Therefore, it is also of importance to investigate the influence of the mechanical strain on the $ZT$ of InP$_3$ monolayer.

In this work, we investigated the TE properties of the InP$_3$ monolayer, by using first-principles calculations combined with the non-equilibrium Green’s functional formalisms (NEGF-DFT) [23]. A large $ZT$ of 1.92 at 300 K is achieved, which benefits from the unique electronic properties and also the low thermal conductivity of the InP$_3$ monolayer.

2. Model and methods

The primitive cell of the InP$_3$ monolayer is presented in figures 1(a) and (b), which has a hexagonal structure and is composed of two In atoms bonded with six P atoms via the covalent interactions. The lattice constant of the InP$_3$ monolayer is 7.55 Å optimized by VASP code [24], which agrees well with the previous theoretical result [19]. Using this primitive cell, we calculated both the electronic and thermal transport properties of the InP$_3$ monolayer, based on which the TE properties is then obtained. The details of the simulation methods are described in the following.

The lattice constant is optimized and the force-constant were calculated using VASP code [24] to construct the dynamic matrix for the phonon spectrum calculation. During the optimization, the atoms were fully relaxed until the maximum force is less than 0.005 eV Å$^{-1}$. The plane wave was used for wave function expansion with a cutoff energy of 550 eV. The projector augmented-wave method [25] was used for describing core electrons. The PW91 version of the generalized gradient approximation (GGA) was used for the electron exchange and correlation functional [26]. In structure relaxing, a $9 \times 9 \times 1$ k sampling was used. For calculating the force-constant, a $3 \times 3 \times 1$ supercell was used with a $3 \times 3 \times 1$ k sampling. Both the electronic and thermal transport properties were carried out using Nanodcad code [27] within the NEGF-DFT theoretical method. In the calculation, 150 $\times$ 150 $\times$ 1 k points were adopted for electronic transmissions. A double-zeta polarized (DZP) atomic orbital basis was implemented to expand all physical quantities, and the GGA-PW91 exchanges and correlation functional was used, and the atomic cores were defined using the standard norm-conserving nonlocal pseudopotentials. After self-consistent calculation was finished, a scissor correction [28, 29] was applied to eliminate the underestimation of energy gap for GGA functional. These calculation details were verified to provide the accurate results.

Within the linear response limit, the electrical current and electrical thermal current can be defined by

$$ I = \frac{2e}{h} \int T_\varepsilon(E)(f_L(E) - f_K(E))dE, $$

where $T_\varepsilon(E)$ is the electronic transmission function, which can be calculated by the standard nonequilibrium Green’s function method, and $f(E, \mu) = \frac{1}{\exp[(E - \mu)/k_B T] + 1}$ is the Fermi–Dirac distribution function at the chemical potential $\mu$.

For ballistic electronic transport, the electronic transmission function $T_\varepsilon(E)$ can be calculated as

$$ T_\varepsilon(E) = \text{Tr}(G_\varepsilon^L \Gamma_{\varepsilon} G_\varepsilon^R \Gamma_{\varepsilon}), $$

where $G_\varepsilon^L$ and $G_\varepsilon^R$ are the left and right Green’s functions, respectively.
\[ \Gamma_L = i(\Sigma'_L - \Sigma''_L), \Gamma_R = i(\Sigma'_R - \Sigma''_R), \]  

(4) 

\[ \Gamma_L = i(\Sigma'_L - \Sigma''_L), \Gamma_R = i(\Sigma'_R - \Sigma''_R), \]  

(11) 

\[ G''_e = [ES - H - \Sigma'_L - \Sigma'_R]^{-1}. \]  

(5) 

Here, \( G''_e \) is the retarded Green’s function, \( H \) and \( S \) are the hamiltonian and overlap matrix, \( \Sigma'_L \) and \( \Sigma'_R \) are self-energy from left and right semi-infinite leads, respectively.

From the above equations, we can obtain the electrical conductivity \( \sigma \), Seebeck coefficient \( S \) and the thermal conductivity \( \kappa_e \) \cite{2, 30}:

\[ \sigma = e^2L_0/l, \]  

(6) 

\[ S = -\frac{L_1}{eTL_0}, \]  

(7) 

\[ \kappa_e(T) = \frac{1}{T_L} \left( L_2 - \frac{L_1^2}{L_0} \right), \]  

(8) 

where \( l \) is the device length, and \( L_{mn}(\mu) \) is given by

\[ L_{mn}(\mu) = \frac{2}{\hbar} \int_{-\infty}^{\infty} d\varepsilon T_e(\varepsilon)(\varepsilon - \mu)^m \left( \frac{\partial f(\varepsilon, \mu)}{\partial \varepsilon} \right). \]  

(9)

For the ballistic thermal transport, the phonon transmission \( T_p(\omega) \) is obtained using the similar methods, except that the \( T_p(\omega) \) is calculated from the dynamic matrix \( D \) instead of the Hamiltonian matrix. Specifically,

\[ T_p(\omega) = \text{Tr}(G''_p\Gamma_L G''_p\Gamma_R). \]  

(10)

The phononic thermal conductivity can then be achieved by \cite{2, 30}

\[ \kappa_p(T) = \frac{\hbar^2}{2\pi K_B T^2} \int_0^\infty d\omega \omega^2 T_p(\omega) \frac{e^{\hbar\omega/k_B T}}{(e^{\hbar\omega/k_B T} - 1)^2}. \]  

(13)

In the simulation, the unit of electronic conductivity is \( \text{kAV}^{-1}\text{M}^{-1} \), the unit of Seebeck coefficient is \( \text{mVK}^{-1} \), the unit of thermal conductivity is \( \text{WV}^{-1}\text{M}^{-1} \), and \( A \) is ampere, \( V \) is volt, \( W \) is watt, \( K \) is kelvin, \( M \) is meter.

3. Results and discussion

The origin energy gap for GGA functional is 0.73 eV, and the energy gap for HSE functional is 1.21 eV. So we apply a scissor correction on hamiltonian to revise the energy gap.

The electronic band structure of the InP3 monolayer is given in figure 1(c). It can be seen that the valence band maximum (VBM) \( E_{\text{vbm}} \) is \(-0.62\) eV, and the conduction band minimum (CBM) \( E_{\text{cbm}} \) is 0.59 eV. The corresponding electronic transmission spectrum along the zigzag direction is shown in figure 1(d). Moreover, the transmission coefficient for the valence bands (\( \mu < 0 \)) is evidently higher than that for the conduction bands (\( \mu > 0 \)), which should be attributed to the flatter
shape and denser energy bands near the VBM, as compared to that around the CBM.

The electrical conductivity $\sigma$ vanishes in the bandgap at the zero temperature. As the temperature is sufficiently high, transport is mediated by activated electrons and/or holes. Therefore, the nonzero conductivity appears inside the bandgap due to the finite temperature. The electrical conductivity $\sigma$ varying with the chemical potential $\mu$ is shown in figure 2(a) at 200 K, 300 K and 350 K, respectively. The $\sigma$ below the Fermi energy is evidently larger than above the Fermi energy, and shows several peaks corresponding to the peaks in the transmission spectrum (figure 1(d)). Figure 2(b) gives the Seebeck effect $S$ as a function of the chemical potential $\mu$, which increases with increasing temperature.

Having known the electronic transport properties of the InP$_3$ monolayer, we now investigate its thermal transport properties. The phonon dispersion curves are shown in figure 3(a), which are symmetrical with respect to the $\Gamma$ point for the $\Gamma \rightarrow K$ and $\Gamma \rightarrow M$ directions, suggesting an approximately isotropic thermal properties between the zigzag and armchair directions. There are twenty four curves in the phonon band structure, which are contributed by the vibration modes of the two In atoms and six P atoms in the primitive cell. The three lowest curves correspond to the three acoustic branches, which are the z-direction acoustic (ZA) mode, in-plane transverse acoustic (TA) mode, and the longitudinal acoustic (LA) mode, respectively. These three types of the acoustic phonon modes have the highest group velocities among all the phonon modes, and therefore contribute most importantly to the thermal conductivity. The group velocities can be calculated by $\frac{\partial \omega}{\partial k}$, which are $0.93 \text{ K ms}^{-1}$, $0.45 \text{ K ms}^{-1}$ and $0.16 \text{ K ms}^{-1}$ for the LA, TA, and ZA phonon modes, respectively. These group velocities are about one order lower than those of the monolayer black phosphorous [31]. Moreover, the whole phonon dispersions are very flat and exhibit highly localized properties, as shown in figure 3(a), which indicates the low group velocities for most of the band branches. Since a low
phonon group velocity leads to a weak thermal transport capability and thus a lower thermal conductivity, a higher $ZT$ is then to be expected.

The phonon transport spectrum is given in figure 3(b). The thermal transmission has a larger value for the modes with the energy lower than 0.02 eV. Importantly, these low energy phonon modes will give the major contribution to the $\kappa_p$ for the temperature below 300 K. The thermal conductivity contributed from the electrons ($\kappa_e$) is also given in the figure. The $\kappa_p$ is approximately 3.1 times larger than the $\kappa_e$ at 300 K, indicating that the phonon thermal conductivity has a larger influence on the TE properties than the $\kappa_e$. Figure 3(d) gives the figure of merit $ZT$ at 200 K, 300 K and 350 K, as a function of the chemical potential.

We now investigate the influence of the mechanical strain on the figure of merit $ZT$ of the InP$_3$ monolayer, as shown in figure 5(a). Under the compression, large imaginary frequency appears and hence the system is unstable, whereas upon the mechanical tension no imaginary frequency exists, indicating a stable structure, as shown in figure 5(b). However, the $ZT$ drops evidently with the increased mechanical tension, and is reduced to 1.67 at 300 K for the 1% tension strain, as shown in figure 5(a). This can be understood from the variation in both the thermal conductivity and the power factor $\sigma_S^2$. Figure 5(c) shows that under the 1% tension strain the power factor decreases significantly, whereas the thermal conductivity increases instead (figure 5(d)). Such behaviors thus lead to a decreased $ZT$.

It should be noted that the thermal properties are calculated within the ballistic transport region. This means that the phonon–phonon scattering effects and electron–phonon scattering effects, which have a critical influence on the thermal transport at a higher temperature (>300 K) are not considered. These factors can be safely eliminated below the Debye temperature $\Theta_D(T)$. The $\Theta_D$ is about 380 K, which is obtained by fitting the Debye formula [34],

$$C_v = 9Nk_B \left( \frac{T}{\Theta_D} \right)^3 \int_0^{\Theta_D/T} \frac{x^4e^x}{(e^x-1)^2}dx,$$  \hspace{1cm} (14)$$

where $x = \hbar\omega/k_B T$. The isometric heat capacity $C_v$ can be obtained by
where $\hbar$ is the reduced Planck constant, $k_B$ is Boltzmann constant, $T$ is temperature, and $\omega_n(q)$ is phonon frequency of the $n$th branch with the wave vector $q$. By solving the equation (14) numerically, we obtained the $\Theta_D$ at the $T$ where the heat capacity is equal to the half of Dulong and Petit value.

Above the $\Theta_D$, all the phonon modes are activated, and the phonon–phonon scattering plays a major role in determining the thermal conductivity. This effect however can now be safely neglected at room temperature due to the high $\Theta_D$ of 380 K. More importantly, in the 2D system the phonon-surface scattering is dominant in decreasing the thermal conductivity instead of the phonon–phonon scattering [35]. This means that the anharmonic effects are of the limited importance, and thus the ballistic transport is reasonable in describing the

![Figure 4](image-url)  
**Figure 4.** The variation of the maximum $ZT$ with temperature for the zigzag and armchair directions, respectively.

![Figure 5](image-url)  
**Figure 5.** The $ZT$ (a), phonon bands (b), power factor (c), and the thermal conductivity $\kappa_e + \kappa_p$ (d) for the mechanical tension of 0% and 1%, respectively.
behavior of thermal conductivity of the InP$_3$ monolayer at room temperature.

4. Conclusions

In summary, we have studied the intrinsic TE properties of the InP$_3$ monolayer by using the quantum transport calculations within the ballistic transport region. A large ZT of 1.92 is obtained at room temperature, which is contributed significantly by the lower thermal conductivity and also the larger power factor. Moreover, even if a mechanical tension of 1% is applied on the lattice, a large ZT of 1.67 can also be obtained at room temperature. Such remarkable TE performance of the InP$_3$ monolayer benefits largely from its unique electronic band structure, which has the multi-valley and flat shape around the VBM. Our results show that the InP$_3$ monolayer is a promising TE material, and moreover give an insight to the thermoelectric performance of rough silicon nanowires (31 J. Phys.: Condens. Matter 124710 140).

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