Thermoelectric Properties of Arsenic Triphosphide (AsP₃) Monolayer: A First-Principles Study

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Recently, monolayer of triphosphides (e.g., InP₃, SnP₃, and GaP₃) attracts much attention due to their good thermoelectric performance. Herein, we predict a novel triphosphide monolayer AsP₃ and comprehensively investigate its thermoelectric properties by combining first-principles calculations and semiclassical Boltzmann transport theory. The results show that AsP₃ monolayer has an ultralow thermal conductivity of 0.36 and 0.55 Wm⁻¹K⁻¹ at room temperature along the armchair and zigzag direction. Surprisingly, its maximum Seebeck coefficient in the p-type doping reaches 2,860 µVK⁻¹. Because of the ultralow thermal conductivity and ultrahigh Seebeck coefficient, the thermoelectric performance of AsP₃ monolayer is excellent, and the maximum ZT of p-type can reach 3.36 at 500 K along the armchair direction, which is much higher than that of corresponding bulk AsP₃ at the same temperature. Our work indicates that the AsP₃ monolayer is the promising candidate in TE applications and will also stimulate experimental scientists’ interest in the preparation, characterization, and thermoelectric performance tuning.

Keywords: Seebeck coefficient, thermal conductivity, thermoelectric, first-principle calculations, transport

INTRODUCTION

Thermoelectric (TE) materials are regarded as potential candidates to alleviate the energy and environment crisis by recycling waste heat (Elsheikh et al., 2014; Champier, 2017; Gao et al., 2016). However, TE technology is currently facing two crucial issues: high production cost and low conversion efficiency (El Chaar et al., 2011). For the conversion efficiency of a TE material, it is characterized by the dimensionless figure of merit $ZT = S^2\sigma T/\kappa$ (Ding et al., 2016; Gandi and Schwingenschlögl, 2014), where $S$ is the Seebeck coefficient, $\sigma$ is the electronic conductivity, $T$ is the absolute temperature, and $\kappa$ is the thermal conductivity, respectively. Over the past few decades, great progress has been achieved in enhancing the $ZT$ values through certain strategies (Ouyang et al., 2019; Gayner and Kar, 2016), such as nanostructuring, quantum confinement, and the “phonon-glass electron-crystal” (Zhang et al., 2020; Hicks and Dresselhaus, 1993a; Hicks and Dresselhaus, 1993b). Therefore, searching “electronic crystal-phonon glass” thermoelectric materials has great significance (Jiang et al., 2019). Due to the development of nanotechnology, new thermoelectric materials are constantly being discovered in recent years. Phosphorene sheds light on two-dimensional (2D) layered materials in TE applications (Fei et al., 2014). However, the chemical degradation upon exposure to ambient conditions seriously limits its practical application (Wood et al., 2014). Scientists make great effort to find novel materials with puckered layered structure.
similar to phosphorene, which can not only retain the excellent electronic properties of phosphorene, but also overcome the chemical instability. Very recently, 2D triphosphides which include a combination of phosphorus and selective elements from Group III, IV, and V attract much attention because of their outstanding thermoelectric performance. For example, Ouyang et al. (2018) predicted the ZT value up to 2.06 along the armchair direction of InP3 monolayer at room temperature. Zhu et al. (2019) indicated that the ZT value of monolayer SnP3 was 3.46 along the armchair direction at 500 K. Single-layer SbP3 (Sun et al., 2020) and GeP3 (Jing et al., 2017) are also predicted as good TE materials.

In this work, utilizing first-principles calculations and the Boltzmann transport equation, we explore stability, phonon/electron, and TE properties of the AsP3 monolayer. Our calculated results show that the AsP3 monolayer exhibits ultrahigh Seebeck coefficient and ultralow thermal conductivity, and the maximum ZT of p-type AsP3 monolayer can reach 3.36 at 500 K along the armchair direction. This work reveals that AsP3 is a promising candidate for TE applications.

METHODS

The TE properties of single-layer AsP3 are calculated using the Boltzmann transport theory and rigid band approximation are used to evaluate the electronic transport properties, which are carried out in the BoltzTrap software with a dense k-mesh 40 × 40 × 1 (Madsen and Singh, 2006). This method has achieved good agreement between theoretical calculations and experiments for many TE materials (Bilc et al., 2006; Xu et al., 2010; Parker and Singh, 2010). For the phonon transport properties, it can be obtained by solving the Boltzmann transport equation in the ShengBTE packages with 50 × 50 × 1 k-points (Li et al., 2014). The phonon dispersions and the harmonic second-order interaction force constants (2nd IFCs) are calculated by using VASP and PHONOPY software (Togo and Tanaka, 2015), in which the 3 × 3 × 1 k-mesh within 4 × 4 × 1 supercell is adopted. The third-order IFCs (3rd IFCs) is obtained by using the 3 × 3 × 1 supercell with the finite-difference method (Li et al., 2012), which considers the interaction including the seventh nearest neighbor atoms.

RESULTS AND DISCUSSION

Atomic and Electronic Structures

Based on calculations of the first-principles, the AsP3 monolayer exhibits a hexagonal honeycomb configuration with space group P63m1 (No. 164), as shown in Figures 1A–C. A unit cell for AsP3 monolayer is constituted by two As and six P atoms, and the optimized lattice constants a = 6.62 Å. More calculated parameters are summarized in Table 1. Interestingly, the AsP3 monolayer has an obvious anisotropic structure, thus we will explore its TE performance in the armchair and zigzag direction.

We study the electrical band structures as well as the corresponding density of states (DOS) of AsP3 monolayer, as presented in Figure 2A. We find that the AsP3 monolayer is an indirect bandgap semiconductor, its valence band maximum (VBM) is locating at the Γ point, whereas the conduction band minimum (CBM) is located between the Γ and M points. The accurate bandgap of 2.28 eV is obtained by using the Herd–Scuseria–Emzerhof hybrid functional (HSE06) (Heyd et al., 2003). In the vicinity of Fermi level, the two highest valence bands (VBs) exhibit overlap at the Γ point, which benefits their electrical transport characteristics (Ding et al., 2018). The DOS further demonstrates that the edges of the VB and CB are mainly coming from the P atoms, which can also be observed in
Besides, the relaxation time \( \tau \) (ps) for electron and hole in AsP\(_3\) monolayer at 300 K.

### Table 2: Calculated elastic modulus \( C^{2D} \) (J m\(^{-2}\)), DP constant \( E_1 \) (eV), effective mass \( m^* \) (m\(_0\)), carrier mobility \( \mu \) (cm\(^2\) V\(^{-1}\) s\(^{-1}\)), and relaxation time \( \tau \) (ps) for AsP\(_3\) monolayer at 300 K.

| Direction | Type | \( C^{2D} \) | \( E_1 \) | \( m^* \) | \( \mu \) | \( \tau \) |
|-----------|------|-------------|---------|--------|-------|-------|
| Armchair  | Hole | 57.93       | 2.38    | 0.11   | 366.37| 0.13  |
|           | Electron | 57.93 | 2.99 | 1.11 | 75.09 | 0.05  |
| Zigzag   | Hole | 57.91       | 1.78    | 0.85   | 337.33| 0.16  |
|           | Electron | 57.91 | 3.83 | 0.56 | 167.96 | 0.05  |

### Electrical Transport Properties

Based on the deformation potential (DP) theory (Bardeen and Shockley, 1950), the carrier mobility of AsP\(_3\) monolayer can be calculated by the formula:

\[
\mu_{2D} = \frac{2e\hbar C^{2D}}{3\kappa_B T |m^*|^2 E_1^2},
\]

where \( m^* \), \( \kappa_B \), \( E_1 \) and \( C^{2D} \) are the effective mass, the Boltzmann constant, the DP constant, and the 2D elastic constants, respectively. These parameters and the relaxation time \( \tau = \mu m^*/e \) (s) are given in Table 2. One can see clearly that the hole mobility is significantly higher than the electron mobility. Besides, the flatter conduction bands provide a greater effective mass \( m^* \) of electron doping, which demonstrates a larger Seebeck coefficient \( S \) because it is proportional to \( m^* \) (Gao et al., 2018).

We obtain the electrical transport properties of AsP\(_3\) monolayer via calculating the semiclassical Boltzmann transport equation (May et al., 2009), involving Seebeck coefficient \( S \), electrical conductivity \( \sigma \), electrical thermal conductivity \( \kappa_e \), and power factor (PF), which are important parameters for evaluating the TE properties. The rigid band approximation theory is adopted to simulate the influence of doping on electron transport. It is assumed that the band structure of the n-type and p-type systems does not change in shape under light doping, whereas the Fermi level moves up and down (Singh, 2007; Parker and Singh, 2011). Positive and negative \( \mu \) correspond to the n-type and p-type doping. Here, the \( S, \sigma, \kappa_e \) and PF concerning chemical potential \( \mu \) can be computed by employing the Fermi–Dirac distribution function \( f_\mu \) (Parker and Singh, 2011) as:

\[
\sigma_{\alpha\beta}(T, \mu) = \frac{1}{eTV_{\alpha\beta}} \int \sum_{\phi} (\epsilon - \mu) \left[ \frac{\partial f_\mu(T, \epsilon)}{\partial \epsilon} \right] d\epsilon,
\]

\[
S_{\alpha\beta}(T, \mu) = \frac{1}{eTV_{\alpha\beta} \sigma_{\alpha\beta}(T, \mu)} \int \sum_{\phi} (\epsilon - \mu) \left[ \frac{\partial f_\mu(T, \epsilon)}{\partial \epsilon} \right] d\epsilon,
\]

where \( V \) is the volume of the primitive cell, and the transport distribution function \( \int \sum_{\phi} (\epsilon) \) is written as follows:

\[
\int \sum_{\phi} (\epsilon) = \frac{e^2}{N_q} \sum_i \sum_q \nu_{\phi}(i, q) v_{\phi}(i, q) \frac{\delta(\epsilon - \epsilon_{iq})}{\delta \epsilon},
\]

where \( N_q \) is the number of \( q \) points sampling, \( \tau \) is the electronic relaxation time, and \( v \) is electronic velocity.

**Figures 3A, B** are the Seebeck coefficient \( S \) of AsP\(_3\) monolayer as a function of \( \mu \). The downward trend of the \( S \) with the temperature gradually slows down as the temperature increases. Surprisingly, the AsP\(_3\) monolayer shows ultrahigh \( S \) compared to other triphosphates with high TE performance (InP\(_3\) (Ouyang et al., 2018), SnP\(_3\) (Zhu et al., 2019), and CaP\(_3\) (Zhu et al., 2020a)). At room temperature, the \( S \) of AsP\(_3\) monolayer reaches 2,860 \( \mu \)V K\(^{-1}\) along the zigzag direction and 2,800 \( \mu \)V K\(^{-1}\) along the armchair direction.
along the armchair direction. The double degeneracy of the valence band at the \( \Gamma \) point and the steep electronic density of states near the Fermi level effectively increase the \( S \).

The electrical conductivity \( \sigma \) vs. \( \mu \) is shown in Figures 3C,D. It is found that the p-type \( \sigma \) is visibly larger than that of the n-type for AsP\(_3\) monolayer, due to the higher mobility and relaxation time of hole. Since electrons submit the Fermi–Dirac distribution, the gradient of \( \sigma \) around VBM and CBM tends to be flat with increasing temperature. According to the Wiedemann–Franz law, the \( \kappa_e \) is proportional to the \( \sigma \): \( \kappa_e = L\sigma T \), where \( L \) is the Lorenz number (\( L = \pi^2 k_B^2/3e^2 \)) (Jonson and Mahan, 1980). As shown in Figures 3E,F, the \( \kappa_e \) of the AsP\(_3\) monolayer increases with rising temperature. The influence of p-type doping on the \( \kappa_e \) is greater than that of n-type doping, which is related to its larger p-type \( \sigma \).

Based on the obtained \( S \) and \( \sigma \), we calculate the PF as shown in Figures 3G,H. Similar to \( \sigma \), the PF of p-type AsP\(_3\) monolayer is significantly higher than that of n-type, which means that it is a potential p-type TE material.

**Phonon Transport Properties**

The phonon spectrum and projected density of state (PhDOS) of the AsP\(_3\) monolayer are illustrated in Figure 4A. No virtual phonon modes are observed in phonon dispersion, which indicates that the AsP\(_3\) monolayer is dynamically stable. The phonon spectrum of AsP\(_3\) contains three phonon branches (ZA, TA, and LA) and twenty-one optical branches. The low-frequency optical branch and the acoustic branch of the AsP\(_3\) monolayer are softened and overlapped, leading to the strong acoustic–optic interaction (Gao et al., 2018). Besides, the flat-frequency band over the entire frequency range can lead to smaller phonon group velocity (Ma et al., 2016; Ma et al., 2018). It can be seen from the corresponding PhDOS that the phonon mode mainly contains As atoms in the low-frequency region (below 3 THz), while the high-frequency region (over 12 THz) is contributed by the P atom.

Figure 4B depicts the corresponding vibration modes near the \( \Gamma \) point of the acoustic branch (ZA, TA, and LA) and the lowest optical branch (Opt\(_1\)) to display the characteristics of the phonon mode more intuitively. It can be seen that the vibration of the three-phonon branch occurs along the in-plane (TA and LA) or outside the plane (ZA), which is a property of natural vibration. Interestingly, it is observed that As atoms of the Opt\(_1\) branch have in-plane opposite motions relative to their adjacent As atoms, while P atoms have in-plane antiphase motions.
phenomenon can significantly block heat transport, thereby reducing the thermal conductivity of the lattice (Ding et al., 2015). Based on the 2nd and 3rd IFCs, the $\kappa_l$ is calculated by the self-consistent iterative method. The calculation formula of $\kappa_l$ is as follows:

$$\kappa_{\text{cal}} = \sum_{q,\lambda} C_{V}(q,\lambda) v_{\alpha}(q,\lambda) \phi^{\alpha}(q,\lambda) \tau_{q,\lambda},$$  \hspace{1cm} (5)

where $C_{V}$, $v$, and $\tau_{q,\lambda}$ are phonon model specific heat, group velocity, and relaxation time, respectively. As shown in Figure 5A, we plot the $\kappa_l$ of AsP$_3$ monolayer vs. temperature. The inherent $\kappa_l$ is obviously proportional to $1/T$, which is attributed to the inherent enhancement of phonon–phonon scattering (Liu et al., 2018). Excitingly, the AsP$_3$ monolayer shows ultralow thermal conductivity. At room temperature, $\kappa_l$ along the armchair direction ($0.36 \text{ Wm}^{-1} \text{ K}^{-1}$) is lower than that along the zigzag direction ($0.55 \text{ Wm}^{-1} \text{ K}^{-1}$). We explore the relationship between $\kappa_l$ and frequency to describe the contribution of different phonons. Figure 5B shows that acoustic branches (below 2 THz) along armchair (zigzag) direction contribute about 75% (86%) to $\kappa_l$. 

**FIGURE 5** | Lattice thermal conductivity of AsP$_3$ as a function of temperature (A) and frequency (B). The insets of (A) is lattice thermal conductivity as a function of $T^{-1}$.

**FIGURE 6** | (A) Phonon group velocity, (B) Grüneisen parameters, (C) phonon relaxation time, and (D) three-phonon scattering phase space as a function of frequency for AsP$_3$, respectively.
The phonon group velocity is an important coefficient to evaluate the heat transferability, which can be obtained by the following equation:

\[ v = \frac{d\omega(q)}{dq} \]  

(6)

The corresponding group velocity of AsP\textsubscript{3} monolayer is plotted in Figure 6A. We can see that the group velocity in the low-frequency area is distinctly larger than that of the high-frequency area. It exhibits a smaller average group velocity about 1.91 km s\textsuperscript{−1}, which is related to the flat phonon dispersions and low cutoff frequency.

To determine the other origin of ultralow $\kappa_l$ of AsP\textsubscript{3} monolayer, we calculate the Grüneisen parameter $\gamma$, which can be used to describe the anharmonic interaction of crystals. It can be described by the following equation:

\[ \gamma(q) \approx -\frac{V}{\omega(q)} \frac{\partial \omega(q)}{\partial V}. \]  

(7)

Generally, the larger $|\gamma|$ represents the stronger anharmonicity and the lower $\kappa_l$. As presented in Figure 6B, one can see a larger $|\gamma|$ in the low-frequency region, and the average of $|\gamma|$ is about 16.17, indicating the existence of strong phonon–phonon scattering.

Figure 6C is the phonon relaxation time vs. frequency of AsP\textsubscript{3} monolayer. At 300 K, our calculated phonon relaxation time of AsP\textsubscript{3} monolayer (4.3 ps) can be compared with the single-layer KAgS (4.05 ps) (Zhu et al., 2020b), which is an important factor for the low $\kappa_l$ of AsP\textsubscript{3} monolayer. The three-phonon scattering phase space ($P_3$) is the available space for the three-phonon scattering process (Li and Mingo, 2015), which can further analyze the source of lower $\kappa_l$. As shown in Figure 6D, the AsP\textsubscript{3} monolayer possesses a larger $P_3$ over the entire frequency region, which allows stronger phonon–phonon scattering and weaker heat transport.

**Thermoelectric Figure of Merit**

Combining the electrical transport coefficients and thermal conductivity, we can estimate the $ZT$ values of AsP\textsubscript{3}, as displayed in Figure 7. The p-type doped AsP\textsubscript{3} monolayer exhibits a higher $ZT$ than the n-type one, which is caused by larger PF of p-type. The maximum $ZT$ values of p-type doped AsP\textsubscript{3} monolayer at 500 K can reach 3.36 and 2.92 along the armchair and zigzag direction, while corresponding $ZT$ values at 300 K is 2.22 and 1.84, much higher than that of bulk AsP\textsubscript{3} (∼0.5 at 300 K) (Duan et al., 2019), which is mainly caused by the larger $S$ and lower $\kappa_l$ of AsP\textsubscript{3} single-layered structure by dimensionality reduction. The maximum $ZT$ value of AsP\textsubscript{3} monolayer at 500 K is comparable with other 2D triphosphides, such as n-type doped InP\textsubscript{3} ($ZT = 3.23$) (Ouyang et al., 2018), p-type doped SnP\textsubscript{3} ($ZT = 3.46$) (Zhu et al., 2019), and p-type doped SbP\textsubscript{3} ($ZT = 3.5$) (Sun et al., 2020). Besides, the maximum $ZT$ values can be achieved when the carrier concentration is between $1 \times 10^{10}$ and $10^{11}$ cm\textsuperscript{−2}. Generally speaking, if the $ZT$ value is close to 3, it is deemed a good TE material (Harman et al., 2002), therefore AsP\textsubscript{3} monolayer can be a potential candidate for TE applications.
CONCLUSION

In conclusion, we investigate the TE performance of AsP₃ monolayer by a highly precise first-principles method. The calculated results show that AsP₃ monolayer is an indirect bandgap semiconductor with a bandgap of 2.28 eV. It also possesses excellent Seebeck coefficients and electrical conductivity. Due to its lower values of phonon velocities (1.91 km s⁻¹), larger Grüneisen parameters |γ| (16.17), as well as shorter phonon relaxation time (4.30 ps), AsP₃ monolayer exhibits ultralow κₐ 0.36 Wm⁻¹ K⁻¹ (0.55 Wm⁻¹ K⁻¹) at room temperature in the armchair (zigzag) direction. At 500 K, the maximum ZT of the AsP₃ monolayer can reach up to 3.36 (armchair direction) and 3.08 (zigzag direction) by the optimal p-type doping. These results prove the huge advantages of AsP₃ single-layer film in high-efficiency conversion of heat energy.

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DATA AVAILABILITY STATEMENT

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

AUTHOR CONTRIBUTIONS

GX established the theoretical models and supervised the project, and LF and HY performed the calculations and data analysis.

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