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Structural stabilities, electronic structures, photocatalysis and optical properties of $\gamma$-GeN and $\alpha$-SnP monolayers: a first-principles study

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Abstract

Exploring two-dimensional materials with excellent photoelectricity properties is of great theoretical significance and practical value for developing new photocatalysts, electronics and photonic devices. Here, using first-principle calculations, we designed and analyzed systematically a series of $\alpha$, $\beta$ and $\gamma$ phase structures of two-dimensional group IV-V monolayers (IV-V, IV $=$ C, Si, Ge, Sn, Pb; V $=$ N, P, As, Sb, Bi), most of them are semiconductors. Among them, $\gamma$-GeN and $\alpha$-SnP monolayers with thermodynamic and kinetic stability (at 300 K) have been further studied due to their wide range of energy band gaps ($\gamma$-GeN: 2.54 eV, $\alpha$-SnP: 1.34 eV). The two band gaps are greater than the free energy for water splitting (1.23 eV), which are crucial for photocatalytic decomposition of water. The $\gamma$-GeN and $\alpha$-SnP monolayers present excellent photocatalystics properties in pH $= 0$ and 10 environments, respectively. Moreover, both of the monolayers show strong light absorption coefficients greater than $10^5$ cm$^{-1}$ in the visible and ultraviolet regions. In addition, it is found that the band edge positions and band gap sizes of $\gamma$-GeN and $\alpha$-SnP monolayers can be regulated by biaxial strain. Benefitting from the wide selection of energy band gaps and high absorption coefficients, the $\gamma$-GeN and $\alpha$-SnP monolayers are the next generation of promising candidate materials for photocatalysts, nanoelectronics and optoelectronics.

1. Introduction

Two-dimensional semiconductor materials show their extraordinary and superior transport properties due to their unique atomic layer structure, which makes them have great application potential in shaping the future generation of electronic and optoelectronic devices [1–8]. To manufacture high-performance miniaturized devices, such as ultra-thin channel field effect transistors (FETs) or realize the photolysis of water and efficient conversion of solar energy, it is necessary to find two-dimensional semiconductor materials with high stability and appropriate band gap width. So far, MX$_2$ compounds semiconductors have been deeply studied [9–13] to explore their potential applications in photocatalysis and photolysis of water. It is found that the band gap range of the MX$_2$ compounds are small (0.50–1.82 eV), and most of the band edge energy positions do not meet the conditions for photocatalytic decomposition of water. Although the two-dimensional semiconductor black phosphorus with appropriate direct band gap has excellent electronic properties, it is easily oxidized in air, limiting its application in optoelectronic devices field [14, 15]. The monolayer materials of GaX (X $=$ S, Se, Te) and InSe with the excellent mechanical, electronic and photovoltaic properties have been synthesized experimentally [16–22]. The two-dimensional compounds of group IV-V elements with the same space group as GaX (X $=$ S, Se, Te) have been theoretically predicted to be semiconductors with moderate band gaps and
suitable band edge energy position for photodegradation of water [21, 23–36]. The theoretical studies have brought group IV-V monolayers into the family of 2D semiconductors as promising candidates for nanoelectronics and nanophotonic device.

It is generally known that the properties of materials are not only determined by their chemical elements, but also closely related to the arrangement of atoms in the lattice [37, 38]. The monolayer SiP and SiAs with different arrangement (IV-V-V-IV, V-IV-IV-V, IV-V-IV-V) have various band gaps and band edge energy positions [39, 40]. Group IV-V monolayers with different phase structure have been rarely studied and it is worth exploration through theoretical calculation.

In this paper, we carried out a systematical investigation of group IV-V monolayers (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) with three different arrangement $\alpha$-(IV-V-V-IV), $\beta$-(V-IV-IV-V), $\gamma$-(IV-V-IV-V)/(V-IV-V-IV) according to first-principles calculations. From 75 different allotropes of group IV-V monolayers, we first proposed the structures of $\gamma$-GeN, $\gamma$-SnN, $\alpha$-SnP, $\alpha$-PbN, $\alpha$-PbP, $\alpha$-PbAs, $\alpha$-PbSb, $\alpha$-PbBi, which are more energetically favorable than their corresponding $\beta$ phase. By comparing their electronic properties and photocatalytic properties, we furtherly studied the $\gamma$-GeN, $\alpha$-SnP monolayers due to their appropriate band edge position and found that they are excellent in absorbing visible light and can decompose water at appropriate pH environment. Then we verified the structural stability of $\gamma$-GeN, $\alpha$-SnP monolayers and the effects of strain on their band gap, band edge position and absorption spectrum.

2. Computational methods

The calculations were performed based on first-principles in this work using the Vienna $ab$-initio simulation package (VASP) [41–43]. The generalized gradient approximation (GGA) for exchange correlation functional was employed, and the monolayer structures were optimized with the Perdew–Burke–Ernzerhof (PBE) exchange correlation functional [44]. Heyd–Scuseria–Ernzerhof (HSE06) hybrid functionals was also employed to predict the energy band gaps correctly [45]. All of the structures were relaxed fully, so that the forces became smaller than 0.02 eV Å and the tolerances of the energy were fewer than $10^{-6}$ eV per atom. The energy cutoff for plane-wave basis sets were taken to be 500 eV. A vacuum of 20 Å was used between these monolayer structures. The research employed the Monkhorst–Pack scheme for sampling k-point of the Brillouin zone with $11 \times 11 \times 1$ for structure optimization and $27 \times 27 \times 1$ k-point mesh for static self-consistent calculation. The phonon dispersion relationship was calculated based on the finite displacement method in the PHONOPY code [46] combined with the VASP. The evaluation of the optical properties (absorption coefficient) was accessed using the HSE06 approach found in the VASP code.

3. Results and discussion

Here, we report three possible allotropes of group IV-V (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) monolayers with the same space group as GaX (X = S, Se, Te) as shown in figures 1 (a)–(c). All phases are stacked in the form of IV-V-V-IV, V-IV-IV-V, IV-V-IV-V/IV-V-IV, which are labeled $\alpha$-, $\beta$-, and $\gamma$-phase, respectively. The dotted black line represents the lowest repeating unit with lattice constant a. The lattice constants $\alpha$, bond lengths $d_1, d_2, d_3$, and the bond angles $\theta$ of the group IV-V monolayers (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) optimized are detailed in table S1 in the Electronic Supplementary Material (ESM). The difference in interlayer height $d_1$ and $d_2$ and bond angle are caused by the different positions of IV and V atoms and the chemical environment. For $\gamma$ Phase, bond angle $\theta_2/\theta_2'$ corresponds to the IV-V-IV/V-IV-V-IV arrangement.

A comparison of the energies between the 75 group IV-V monolayers (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) with three allotropes is shown in figure S1 (available online at stacks.iop.org/MRX/8/125010/mmedia). And the most energetically favorable phase distribution are presented in figure 1(e). It is found that the $\alpha$ phase structures are the most energetically favorable for lead containing compounds and SnP monolayers. For GeN and SnN, the lowest-energy configurations are $\gamma$ phase, while it is the $\beta$ phase for the other IV-V monolayers. The $\beta$ phase of 25 group IV-V monolayers (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) have been intensely studied in previous work [35–38, 47]. Here, our calculations on the $\beta$ phases coincide with the previous calculation results, which implies that the calculation method is reliable. Then we turned our attention to deep study the properties of $\gamma$-GeN, $\gamma$-SnN, $\alpha$-SnP, $\alpha$-PbN, $\alpha$-PbP, $\alpha$-PbAs, $\alpha$-PbSb, $\alpha$-PbBi monolayers which have not been studied.

The band structures and band edge positions of group IV-V monolayers were calculated on the HSE06 level. As shown in figure 2, $\alpha$-PbN, $\alpha$-PbP, $\alpha$-PbAs, $\alpha$-PbSb and $\alpha$-PbBi are direct band-gap semiconductors with band gaps of 0.49, 0.89, 0.76, 0.81 and 0.47 eV at the $\gamma$ point, respectively. $\gamma$-GeN, $\gamma$-SnN and $\alpha$-SnP are indirect band-gap semiconductors with band gaps of 2.54, 1.02 and 1.34 eV, respectively. Band structures of other group
IV-V monolayers with lowest energy phase are shown in figure S2 in the ESM. We found that the most of metastable group IV-V monolayers with different phase states are semiconductors, and their detailed structure parameters and band gaps are shown in tables S2–S4.

Photocatalytic decomposition of water [48, 49] is a popular field, which aims to decompose water into hydrogen and oxygen by visible light. For effective water splitting, there are some basic requirements for photocatalysts. The band edge potentials must straddle the water redox potentials, which is that the energy level of conduction band minimum (CBM) must be higher than the reduction potential of H\(^+\) to H\(_2\) and the energy level of valence band maximum (VBM) must be lower than the oxidation potential of OH\(^-\) to O\(_2\). To assess the suitability of \(\gamma\)-GeN, \(\gamma\)-SnN, \(\alpha\)-SnP, \(\alpha\)-PbN, \(\alpha\)-PbP, \(\alpha\)-PbAs, \(\alpha\)-PbSb, \(\alpha\)-PbBi monolayers as a photocatalyst for splitting water under visible-light irradiation, the relationship between the band edge positions and redox potential of water has been studied.

The potential reduction for H\(^+\)/H\(_2\) and the potential of oxidation for O\(_2\)/H\(_2\)O depend on the pH value and are described by the following formula [50, 51].

\[
\begin{align*}
E_{\text{H}^+/\text{H}_2}^{\text{red}} &= -4.44 \text{ eV} + \text{pH} \times 0.059 \text{ eV} \\
E_{\text{H}_2\text{O}}^{\text{ox}} &= -5.67 \text{ eV} + \text{pH} \times 0.059 \text{ eV}
\end{align*}
\]

In figure 2 (i), the oxidation-reduction potentials of the water decomposition under various pH conditions have been compared with the CBM and VBM energy levels. For \(\gamma\)-GeN, the band edge crosses the water redox potential under pH = 0 and 7, which implies that the band edge positions of the \(\gamma\)-GeN monolayer are favorable for full water splitting at pH = 0 and 7. It is found that the CBM and VBM of \(\alpha\)-SnP monolayer are just above the reduction potential of H\(^+\) to H\(_2\) and just below the oxidation potential of OH\(^-\) to O\(_2\) at pH = 10, respectively. In this case (pH = 10), \(\alpha\)-SnP monolayer can also decompose water into hydrogen and oxygen. The band gap of \(\gamma\)-SnN, \(\alpha\)-PbN, \(\alpha\)-PbP, \(\alpha\)-PbAs, \(\alpha\)-PbSb and \(\alpha\)-PbBi monolayers are too small to straddle the water redox potentials. Therefore, they cannot be used as photocatalyst for visible light decomposition of water.

To examine the stability of the \(\gamma\)-GeN and \(\alpha\)-SnP monolayers, we calculated the cohesive energy \((E_{\text{coh}})\) from the equation:

\[
E_{\text{coh}} = \left[ E_{\text{tot}} - (n_{\text{IV}}E_{\text{IV}} + n_{\text{V}}E_{\text{V}}) \right] / (n_{\text{IV}} + n_{\text{V}})
\]

where \(E_{\text{tot}}, E_{\text{IV}}\) and \(E_{\text{V}}\) are the total energy of the system, the energies belonging to group IV and V neutral atoms, respectively. \(n_{\text{IV}}\) (\(n_{\text{V}}\)) is the number of group IV (V) atoms in each unit cell. The cohesive energies of \(\gamma\)-GeN and \(\alpha\)-SnP monolayers are 6.23 eV and 4.53 eV, respectively. Due to the stronger binding ability of electrons in nitrogen atoms, the cohesive energies of the monolayers containing nitrogen elements are relatively higher than...
the monolayers containing phosphorus elements. In addition, the high enough cohesive energies of $\gamma$-GeN and $\alpha$-SnP prove that they may be highly stable.

Then the phonon dispersions of $\gamma$-GeN and $\alpha$-SnP monolayers were calculated to investigate the dynamical stability as shown in figures 3(a)–(b). It is seen that there are no virtual frequencies in the phonon spectra, indicating the $\gamma$-GeN and $\alpha$-SnP monolayers are dynamically stable. Additionally, we also performed ab initio molecular dynamic calculations at 300 K using a supercell of $6 \times 6 \times 1$ unit cells as shown in figures 3(c)–(d). The molecular dynamics simulation in the NVT canonical ensemble was performed for 10 ps with a time step of 1.0 fs based on the previous studies [52–56]. The integrity of the original configurations with time evolution confirms their good thermal stability.

The above three stability calculations can be used as evidence of the high stability of $\gamma$-GeN and $\alpha$-SnP monolayers. Due to the explosive growth of experimental techniques for producing and fabricating 2D materials over the course of the last few years, it is possible that IV-V monolayers are fabricated as actual materials for experiments in the foreseeable future. Since they are non-layer bulking phases, it is advised that they can be synthesized through molecular beam epitaxy (MBE) or chemical vapor deposition (CVD) methods. These have been proven and are regularly utilized for research of new 2D materials [57, 58].

Strain engineering is considered to be a useful method to adjust the electronic structure for two-dimensional monolayers [35, 40, 59–63]. This turned our attention to explore the influence of biaxial strain on the band gap and band edge potentials of the $\gamma$-GeN and $\alpha$-SnP monolayers. The biaxial strain $\eta$ can be defined as

$$\eta = \frac{(a - a_0)}{a_0}$$

(4)
where $a_0$ and $a$ represent the lattice optimized constants in the original and the lattice length along the strain direction. The strain has been introduced in the range of ±5% and ±3% by changing the lattice constant of the γ-GeN and α-SnP monolayers respectively. Here, the negative values and positive values express compressive strain and tensile strain, respectively. In figure 4 (a), it’s clearly seen that the strain could effectively regulate the band gap of γ-GeN, and the value decreases from 2.59 eV to 1.65 eV under biaxial strain from $-1\%$ to 5%. The band gap reduces monotonously when the compression strain continues to increase from $-1\%$ to $-5\%$. When the strain reaches 1%, the band gap of α-SnP monolayer reaches the maximum (1.37 eV) as shown in figure 4 (b).

We calculated the corresponding CBM and VBM of γ-GeN and α-SnP monolayers under different biaxial strain values, as shown in figures 4 (c) and (d). When the biaxial strain $\eta$ is in the range of compression $-5\%$ to tension $3\%$, the γ-GeN monolayer is still suitable for photocatalytic water splitting at pH $\phi H = 0$. When γ-GeN is applied in the range of $-2\% < \eta < 0\%$ biaxial strain, its CBM increases, which meets the standard of photocatalytic water decomposition at pH $\phi H = 0$, 7. For α-SnP, the band edge potentials can straddle the water redox potentials at pH $\phi H = 10$ without strain. The standard of photocatalytic decomposition of water is also met when the tensile strain is 1% at pH $\phi H = 14$ as shown in figure 4(d). Figure 4 supplies us with useful feedback for making adjustments to the VBM, CBM and the band gaps of the group IV-V monolayers in order to draw out their max efficiency in solar energy conversion.

The absorption spectrum of γ-GeN and α-SnP monolayers were calculated to study their utilization of sunlight. Based on the dielectric constant from HSE06, the absorption coefficients can be formulated as

$$\alpha(\omega) = \sqrt{2} \omega \sqrt{\varepsilon_1^2(\omega) + \varepsilon_{\alpha\beta}^2(\omega) - \varepsilon_1(\omega)}^{1/2}$$

where $\omega$, $\varepsilon_1$, and $\varepsilon_{\alpha\beta}$ are referring to the frequency of the incident light, the real part, and imaginary part of the dielectric constants, respectively. Considering that the good photocatalytic performance of γ-GeN/α-SnP monolayer under strain $= -1\%/1\%$, we studied the light absorption coefficient (in-plane direction) of γ-GeN/α-SnP monolayer without strain and with $-1\%/1\%$ biaxial strain. The results are shown in figure 5. Both of the monolayers have obvious absorption peaks in the visible region (1.6 ~ 3.1 eV), whose absorption coefficients achieve more than $2 \times 10^5 \text{cm}^{-1}$ no matter if it is with biaxial strain or without strain. They are slightly lower than the one of single-layer MoS$_2$ ($4.7 \times 10^5 \text{cm}^{-1}$) [53, 54], much higher than the ones of single-layer BP [64],...
b-AsP [64] and GeP [65]. Thus, it is indicating that they have effective solar energy conversion rate, and the biaxial strain has little effect on the light absorption range of the $\gamma$-GeN/\alpha-SnP monolayer with $-1\%/1\%$ biaxial strain. The highest absorption peaks of both monolayers appear in the ultraviolet region. Especially for \alpha-SnP, an obvious optical absorption appears from the infrared to ultraviolet region with the highest absorption peak (being close to $10^6$ cm$^{-1}$) in the ultraviolet region. It is worth noting that $\gamma$-GeN does not absorb in the red-

**Figure 4.** (a) and (b) The change of bandgaps for $\gamma$-GeN and \alpha-SnP monolayers with biaxial strain. (c) and (d) Biaxial strain effects on band edge positions of the $\gamma$-GeN and \alpha-SnP monolayers, respectively.

**Figure 5.** The absorption spectra of (a) $\gamma$-GeN and (b) \alpha-SnP monolayers. The black lines stand for their absorption without strain, and the red line represents the absorption spectrum when biaxial strain most conducive to photocatalytic decomposition of water is applied.
light region, it indicates that it will be a promising filter device. The $\gamma$-GeN and $\alpha$-SnP monolayers offer an appealing alternative platform for realizing optoelectronic applications.

4. Conclusions

In this paper, we designed the group IV-V monolayers (IV-V, IV = C, Si, Ge, Sn, Pb; V = N, P, As, Sb, Bi) with three different arrangements $\alpha$(IV-V-V-IV), $\beta$(V-IV-IV-V), $\gamma$(IV-V-IV-V)/(V-IV-IV-V) based on first-principles calculations. Within the various allotropes of group IV-V monolayers, we first proposed $\gamma$-GeN, $\gamma$-SnN, $\alpha$-SnP, $\alpha$-PbN, $\alpha$-PbP, $\alpha$-PbAs, $\alpha$-PbSb, $\alpha$-PbBi, which are more energetically favorable than their corresponding $\beta$ phase. It is worth noting that $\gamma$-GeN, and $\alpha$-SnP have suitable band gaps and band edge positions, which make them excellent in photocatalytic decomposition of water under pH = 0, 7 and pH = 10 environments, respectively. Moreover, both of the monolayers show strong light absorption coefficients, which are greater than $10^5$ cm$^{-1}$ in the visible and ultraviolet regions. In addition, it is found that the band edge positions and band gap sizes of $\gamma$-GeN and $\alpha$-SnP monolayers can be regulated by biaxial strain. The study is helpful for the application of $\gamma$-GeN and $\alpha$-SnP monolayers in photocatalysts, nanoelectronics and optoelectronics fields. With the gradual maturity of experimental fabrication technology, we believe that the series of IV-V monolayers with the most stable energy and appropriate band gap predicted by us will provide good groundwork for experimental researchers to expand two-dimensional semiconductor materials to the predicted IV-V monolayers.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Author contributions

Liming Liu; Cuixia Yan; Lei Gao; Jianqing Dai; Jinming Cai contributed to the conception of the study;
Liming Liu performed the calculation and the data analyses and wrote the manuscript;
Cuixia Yan performed the analysis with constructive discussions and wrote the manuscript; Wei Shangguan contributed significantly to analysis and manuscript preparation; Lei Gao helped perform the analysis with constructive discussions.

Notes

The authors declare no competing financial interests.

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