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Enhanced photocatalytic activity for water splitting of blue phase GeS and GeSe monolayers via biaxial straining

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Abstract: The structural, electronic, dipole-induced internal electric field, optical and photocatalytic properties of the monolayer GeS and GeSe under external biaxial strain have been investigated by using first principles calculations. The monolayer GeS and GeSe are indirect semiconductors with the band gaps of 3.265 eV and 2.993 eV, respectively. The band alignment of the monolayer GeS and GeSe manifests the photocatalytic activity for water splitting. Especially, it is effective to tune the properties, including structures, band gaps, surface potential difference, dipolmoment $P$, dipole-induced internal electric field, absorption and photocatalytic activity, of the monolayer GeS and GeSe via biaxial strain. Our results suggest that monolayer GeS and GeSe possesses photocatalytic properties for water splitting, and strain engineering, especially tensile strain, can enhance photocatalytic activity underultraviolet and visible light.

1. Introduction

Due to the serious environmental and energy problems, more and more fossil fuels should be replaced by clean and renewable energy. The conversion of solar energy into clean and renewable hydrogen by virtue of efficient and economical photocatalytic water splitting process, in which process only catalyst, water and solar energy are needed theoretically, is regarded as an efficient way.\textsuperscript{1-3} The photocatalytic water splitting process is that the solar energy is absorbed by the photocatalyst and the electron hole pairs are formed accordingly, and then the $H_2$ and $O_2$ are generated by the way of the $H_2O$ molecules are reduced by electrons and oxidized by holes respectively. In order to improve the efficiency of photocatalytic water splitting, a desirable photocatalyst should have the following properties: (1) Suitable band gap. (2) Wide adsorption range of solar energy. (3) The electron hole pairs can be effectively separated. (4) Proper position of band alignments. In addition, desirable photocatalyst should also be nontoxic, good chemical stability, inexpensive, earth abundant, and environment friendly. Traditional photocatalysts, such as TiO$_2$, have been reported to be active for photocatalytic water splitting under ultraviolet light.\textsuperscript{4-7} However, the photocatalytic performance of these bulk materials is unsatisfactory, due to the large band gap and low solar absorption.

Compare to the bulk materials, many studies showed that two dimensional (2D) materials have some excellent properties,\textsuperscript{8-10} such as advantageous optoelectronic and distinguished mechanical properties.\textsuperscript{11-14} Due to the ultrathin morphology features and quantum confinement, 2D materials have the unique superiority, such as high specific surface area, abundant surface active sites and low charge carrier diffusion distance,\textsuperscript{15-18} which are useful for photocatalytic water splitting. As a result, many 2D materials have been identified as promising photocatalysts.\textsuperscript{19-23} For example, Wang et al. experimentally reported that g-C$_3$N$_4$ can be used as a photocatalyst to generate hydrogen from water under visible-light irradiation in the presence of a sacrificial donor.\textsuperscript{20} Yang et al. experimentally reported that based on the Black Phosphorus anisotropic 2D layered structure with tunable bandgap in the range of 0.3–2.0 eV, the visible light photocatalytic hydrogen evolution rate of Black Phosphorus nanosheets reached 512 µmolh$^{-1}$g$^{-1}$ without using any noble metal cocatalyst, about 18 times higher than that of the bulk Black Phosphorus.\textsuperscript{24} Beyond black phosphorus, layered group-IV monochalcogenides MX (M=Ge, Sn; X=S, Se), which structures are similar to phosphorene, are a newly emerging class of 2D materials.\textsuperscript{25-29} Thanks to the properties, remarkable mechanical flexibility, high carrier mobility, high optical absorption, and high thermoelectric coefficient and dynamically stable as well as earth abundant and low toxic constituent elements, MX are regarded as promising materials for electronic and optoelectronic applications.\textsuperscript{30, 41, 42} For example, Xue et al. experimentally reported an in situ self-regulated process to
fabricate high quality polycrystalline GeSe film, which possessed a suitable band gap (1.14 eV), with high absorption coefficient (about 10^5 cm^-1) and showed p-type conductivity, for thin-film photovoltaic applications. Li et al. reported the GeS monolayer possessed a high carrier mobility about 3680 cm^2 V^-1 s^-1, which was much higher than that of MoS_2 monolayer. Dai et al. revealed that the MX based systems exhibit high photoresponsivity (Rph 0.16 AW^-1) and external quantum efficiency (EQE 30.3%) in the visible region. Similar to phosphorene which has black-phase (black phosphorus) and blue-phase (blue phosphorene) phases, the structures of layered group-IV monochalcogenides MX are predicted to have two phases, black-phase and blue-phase structures. Blue phase GeS and GeSe possess a large intrinsic dipole and introduce an internal electric field directing, which could prove useful for photocatalytic activity for water splitting. However, the band gaps of monolayer GeS and GeSe are about 3.00 eV, which are only suitable for ultraviolet light, for which the proportion is just about 5% of total solar energy. Therefore, it is of great importance to tune the properties, especially bandgap, internal electric field, energy alignment and light absorption spectrum of monolayer GeS and GeSe to enhance photocatalytic activity for water splitting in visible light spectrum. Strain engineering is a powerful and widely used strategy for boosting the performance of electronic, optoelectronic, and spintronic devices. Especially, strain engineering is convenient to achieve rapid and reversible tuning of the band gap. Therefore, it is essential to adopt strain engineering to tune the properties and enhance photocatalytic activity of monolayer GeS and GeSe for water splitting in visible light spectrum.

In this paper, the properties of blue phase monolayer GeS and GeSe and the effect of the external biaxial strain, including tensile and compressive strain, on the properties of blue phase monolayer GeS and GeSe were investigated by first principles calculations.

2. Computational methods

The present calculations were performed using the Vienna ab initio simulation package (VASP) in conjunction with the projector-augmented-wave (PAW) potential. The Perdew-Burke-Ernzerhof (PBE) functional of the generalized gradient approximation (GGA) was used to describe the exchange-correlation energy. The HSE06 hybrid functional was adopted to calculate more accurate band gaps. The energy cutoff for the plane-wave expansion of the wave function was set to 500 eV. All the structures were fully relaxed until satisfying an energy convergence of 10^-5 eV and the maximum Hellmann Feynman force convergence of 0.01 eV/Å. The Gamma center scheme was used for the first Brillouin zone integration with a fine grid of 8x8x1 and 11x11x1 for structure optimization and static calculation, respectively. The thickness of the vacuum region along the z direction was more than 20 Å to eliminate the artificial interactions due to the periodic image.

3. Results and discussion

As shown in Figure 1, the geometric configuration, including top view and side view, of monolayer GeS and GeSe, is similar to the blue phosphorene and silicene. The Ge atoms and X (X=S, Se) atoms bonded to each other and arranged alternately to form a hexagonal buckled lattice. After the structural relaxation, the optimized lattice constants and the Ge-X (X=S, Se) bond length of monolayer GeS and GeSe are 3.495 Å (3.676 Å) and 2.435 Å (2.570 Å), respectively, which are good agreement with the previous reported data. Apparently, the optimized lattice constants and the bond length of monolayer GeSe are both larger than those of monolayer GeS. The reason is that the increase of atomic radius of the element results in increase of the cell side and the bond length of monolayer accordingly. The phonon spectrum of monolayer GeS
and GeSe were calculated. As the figure S1 in the Supporting Information shown, there is no imaginary vibration mode for both GeS and GeSe structures, indicating the dynamical stability of these systems.

The electronic band structures of monolayer GeS and GeSe were calculated and shown in Figure 2 (HSE06) and Figure S2 (PBE). The electronic band structures between HSE06 method computation and PBE method computation are similar, except for the magnitude of band gaps. The band gaps based on PBE method computation are underestimated typically due to the improper treatment of the Coulomb repulsion, while based on the HSE06 hybrid functional will get more accurate band gaps. What is more, the electronic band structures between monolayer GeS and GeSe are similar, except for different band gaps, due to the same hexagonal buckled lattice with similar constituent element. As shown in the Figure 2(a) and Figure 2(b), both of the monolayer GeS and GeSe are an indirect gap semiconductor with the Conduction Band Minimum (CBM) located between the $\Gamma$ (0, 0, 0) and $M$ (0, 1/2, 0) points, as a comparison Valence Band Maximum (VBM) located between $K$ (-1/3, 2/3, 0) and $\Gamma$ (0, 0, 0) points. The band gaps of monolayer GeS (GeSe) are 3.265 eV (2.993 eV) based on HSE06 method and 2.486 eV (2.288 eV) based on PBE method, which are all agreed well with previous works. As shown in the Figure 2(c) and 2(d), the total and partial density of states (DOS) were

Figure 2. (a)(b) Band structures (HSE06), (c)(d) The total and partial density of states (HSE06) and (e)(f) The band gap (HSE06 and PBE) as a function of biaxial strain of monolayer GeS and GeSe.
calculated to shed light on the underlying mechanism of the orbital reconfiguration of the monolayer GeS and GeSe. For the monolayer GeS, it was $p$-orbitals of S and $s$-orbitals and $p$-orbitals of Ge that contributed mainly to the VBM below Fermi level, while above the Fermi level, $p$-orbitals of S and $s$-orbitals and $p$-orbitals of Ge that contributed mainly to the VBM below Fermi level, while above the Fermi level, $p$-orbitals of S and $p$-orbitals of Ge contributed mainly to the CBM. For the monolayer GeSe, similar to monolayer GeS, it was $p$-orbitals of S and $s$-orbitals and $p$-orbitals of Ge that contributed mainly to the VBM below Fermi level, while above the Fermi level, $p$-orbitals of S and $p$-orbitals of Ge contributed mainly to the CBM. As shown in Figure 2(e), Figure 2(f) and Figure S4, in-plane biaxial strain on the monolayer GeS and GeSe were applied by changing the lattice parameters. Here, compressing and stretching are represented by symbol "-" and "+", respectively. The magnitude of the monolayer GeS and GeSe, when the biaxial strain was tuned from 0% to ±10%, were calculated based on the HSE06 functionals and PBE functionals. Apparently, the trend of the band gaps based on HSE06 method and PBE method are very similar, except the magnitude. Considering the precision, the band gaps predicted from HSE06 functionals were taken for example to analyze the trend of monolayer GeS and GeSe as a function of biaxial strain. For the monolayer GeS, the band gap linearly decreased from 3.265 eV to 3.074 eV when the biaxial strain increased from 0 to +4%. The tendency of band gap decreased with a larger drop, when the biaxial strain increased from +4% to +10%. Moreover, when the biaxial strain decreased to -2%, the band gap reached the maximum ~ 3.342 eV. The band gap linearly decreased as the decrease of the biaxial strain from -2% to -10%. The band gaps are 1.732 eV and 2.202 eV at -10% and +10% biaxial strain, respectively. For the monolayer GeSe, when the biaxial strain was at the 0% point, the band gap reached the maximum ~ 2.993 eV. When the biaxial strain changed to -10% (+10%), the band gap decreased from 2.993 eV to 1.130 eV (1.756 eV). Apparently, strain engineering is an effective and promising method to modulate the band gap of 2D monolayer GeS and GeSe. Especially, the magnitude of the band gaps of the monolayer GeS (GeSe) could be modulated to about 1.732 eV (1.756 eV). Apparently, strain engineering is an effective and promising method to tune the orbital reconfiguration of the monolayer GeS and GeSe. For the monolayer GeS and GeSe, especially, the magnitude of the band gaps of the monolayer GeS (GeSe) could be modulated to about 1.732 eV (1.756 eV). Apparently, strain engineering is an effective and promising method to modulate the band gap of 2D monolayer GeS and GeSe. Hence, it is important and useful task.

As we known, the relationship between $E_{\text{eff}}$ and $\Delta \Phi$ according to the following equation

$$\Delta \Phi = e E_{\text{eff}} d$$  \hspace{1cm} (1)

in which, $e$ is the elementary charge and $d$ is the thickness of the junction. What is more, the monolayer GeS and GeSe with an internal effective electric field $E_{\text{eff}}$ is produced by its intrinsic dipole $P$ according to the following equation$^{52}$

$$E_{\text{eff}} = \frac{P}{\varepsilon Sd}$$  \hspace{1cm} (2)

in which, $\varepsilon$ is the dielectric constant and $S$ is the surface area. Therefore, from equation (1) and equation (2), we can get the equation between $E_{\text{eff}}$ and $\Delta \Phi$ according to the following formula$^{52}$

$$\Delta \Phi = \frac{eP}{\varepsilon S}$$  \hspace{1cm} (3)

From the equation (1), (2) and (3), there is a linear relationship between $\Delta \Phi$ and intrinsic dipole $P$ for the monolayer GeS and GeSe, due to $e$, $\varepsilon$ and $S$ are constant value, and the $\Delta \Phi$ or $P$ is in directly proportion to the $E_{\text{eff}}$ and $d$.

To shed further light on the underlying mechanism of the effect of strain engineering on the $\Delta \Phi$ and intrinsic dipole $P$, the schematic diagram of monolayer GeS and GeSe and the Ge-X (X=S, Se) bond length $L$, the Ge-X (X=S, Se) pucker distance $d$ and the Ge-X (X=S, Se) horizontal angle as a function of biaxial strain of monolayer GeS and GeSe was plot in the Figure S5. The monolayer GeS and GeSe, when the biaxial strain is 0%, is in the most stable state, yet the Ge-X (X=S, Se) bond length $L$ and the lattice constant $a$ of the monolayer GeS and GeSe decreases as the biaxial strain increases. And the atomic attractive force between Ge atom and X (X=S, Se) atom increases at the same time, which will lead to reduce of the $d$ to keep a stable state during the relaxation progress. In contrast, the Ge-X (X=S, Se) bond length $L$ and the lattice constant $a$ of the monolayer GeX (X=S, Se) decreases as the biaxial strain decreases. And the atomic repulsive force between Ge atom and X (X=S, Se) atom increases as the biaxial strain decreases at the same time, which will lead to enlargement of the $d$ to keep a stable state. As shown in the Figure 4S, the $L$ increases linearly as the strain increases and the $d$ decreases linearly as the strain increases confirming the relationship between $L$, $d$ and strain mentioned above. Moreover, the $d$ is in inversely proportion to the $E_{\text{eff}}$, due to the charge of 2D monolayer GeS and GeSe is constant. Therefore, the relationship between $E_{\text{eff}}$, $d$ and strain is comprehensible. When the strain increases, the $d$ decrease and $E_{\text{eff}}$ increases. When the strain decreases, the $d$ increase and $E_{\text{eff}}$ decreases. According to the relationship between $\Delta \Phi$, $P$, $E_{\text{eff}}$, $d$ and strain, it could be speculated that strain engineering would be a method to tune the $\Delta \Phi$ and $P$ of the monolayer GeS and GeSe.
Therefore, the planar average potential, the surface potential difference $\Delta \Phi$ and the dipolmoment $P$ of the monolayer GeS and GeSe within the strain range of -10%~+10% were calculated. As shown in Figure 3(a-f), the planar average potential of monolayer GeS and GeSe, when the biaxial strain was tuned from 0% to ±10%, were calculated. It is clearly to see that there is a $\Delta \Phi$ between Ge atomic surface and X (X=S, Se) atomic surface, such as, 0.484 eV (0.209 eV), 0.793 eV (0.574 eV) and 1.404 eV (1.189 eV) for the monolayer GeS (GeSe) at -10%, 0% and +10% biaxial strain, respectively. Especially, the potential of S or Se atomic surface are all higher than that of Ge atomic surface, which is opposite to that in the previous study, indicating that the Ge atomic surface with a smaller electronegativity value is positively charged and the S or Se atomic surface with a larger electronegativity is negatively charged, forming a dipole-induced internal electric field in monolayer GeS and GeSe. The direction pointing of the dipole-induced internal electric field is from Ge atomic surface to X (X=S, Se) atomic surface. Moreover, Figure 3(g) and 3(h) show that the magnitude of the $\Delta \Phi$ of the monolayer GeS and GeSe could be tuned effectively. Within the strain range of -10%~+10%, the magnitude of the $\Delta \Phi$ of the monolayer GeS linearly increases from 0.484 eV to 1.404 eV, due to the planar average potential of Ge atomic surface reduces from 1.556 eV to 0.531 eV, yet the planar average potential of S atomic surface is stable about 1.933 eV without obvious change. Similar to the monolayer GeS, the magnitude of the $\Delta \Phi$ of the monolayer GeSe increases from 0.209 eV to 1.189 eV, when the biaxial strain is tuned from -10% to +10%. As shown in the Figure 3(h) and Figure 3(i) the trend of dipolmoment $P$ is similar to the $\Delta \Phi$, indicating dipolmoment $P$ is linear to the $\Delta \Phi$. Moreover, the calculated dipolmoment $P$ as a function of $\Delta \Phi$ of monolayer GeS and GeSe is plot in the Figure 3(j), the straight lines indicate that our calculated data confirms the linear relationship between $\Delta \Phi$ and intrinsic dipole $P$ mentioned above.

It is obvious to find that the results from calculating data are well consistent with that predicted by theory, confirming that strain engineering would be an effective method to tune the $\Delta \Phi$ and $P$ of the monolayer GeS and GeSe by controlling the pucker distance $d$. Especially, under a tensile stain state, a larger electric field $E_{\text{eff}}$ and surface potential difference $\Delta \Phi$ were realized, which can effectively reduce recombination of photogenerated electron-hole pairs and enhance the photocatalytic activity.

A suitable photocatalyst material for water splitting should possess a suitable band alignment, especially, the VBM should be lower than the oxidation potential of $\text{O}_2/\text{H}_2\text{O}$ (−5.67 eV) and the CBM should be higher than the reduction potential of $\text{H}^+/{\text{H}_2}$ (−4.44 eV). As shown in the Figure 4(a) and 4(c), the CBM and VBM of monolayer GeS and GeSe straddle the water redox potentials.

Figure 3. The planar average potential of monolayer GeS and GeSe at (a) (d) -10%, (b) (e) 0% and (c) (f) +10% biaxial strain, respectively. (g) The planar average potential on the upper side (X (X=S, Se) atomic surface) and lower side (Ge atomic surface), (h) the surface potential difference ($\Delta \Phi$) and (i) the Dipolmoment of the monolayer GeS and GeSe within the strain range of -10%~+10%.
the Ge atom layer side, the CBM of monolayer GeS is higher than the reduction potential of \( \text{H}^+/\text{H}_2 \) (\(-4.44\) eV), and the energy difference \((\Delta E_c)\) between CBM level and the reduction potential level of \( \text{H}^+/\text{H}_2 \) is 1.496 eV. On the S atom layer side, the VBM of monolayer GeS is lower than the oxidation potential of \( \text{O}_2/\text{H}_2\text{O} \) (\(-5.67\) eV), and the energy difference \((\Delta E_v)\) between VBM level and the oxidation potential level is 1.332 eV. Similar to the monolayer GeS, the \( \Delta E_c \) and \( \Delta E_v \) of monolayer GeS and GeSe are large enough for water splitting into \( \text{H}_2 \) and \( \text{O}_2 \), indicating monolayer GeS and GeSe would be a suitable photocatalyst material for water splitting.

As mentioned above (Figure 2(e) and 2(f)), the magnitude of the band gaps of the monolayer GeS (GeSe) could be modulated from \(3.265\) eV (2.993 eV) to \(1.732\) eV (1.130 eV) within the strain range of \(-10\%\sim+10\%\), which is useful to broad light spectrum from ultraviolet light to visible light. To further evaluate the photocatalytic potential of the monolayer GeS and GeSe under different biaxial strain, the energy alignment as a function of biaxial strain of monolayer GeS and GeSe was calculated by HSE06 method. As shown in the Figure 4(b), Figure 4(d), Figure S6 and Figure S7, it is observed that, on the Ge atom layer side, all the CBM of monolayer GeS are higher than the reduction potential of \( \text{H}^+/\text{H}_2 \), as a contrast, on the S atom layer side, all the VBM of monolayer GeS are lower than the oxidation potential of \( \text{O}_2/\text{H}_2\text{O} \). Within the strain range of \(-10\%\sim-2\%\), the CBM increases slightly as the biaxial strain increases, yet the VBM decreases obviously as the biaxial strain increases. Especially, within the strain range of \(-4\%\sim+10\%\), the change of CBM and VBM aren’t obvious when the biaxial strain changes, indicating the monolayer GeS could keep a suitable band alignment for water splitting under different biaxial strain. Similar to the monolayer GeS, on the Ge atom layer side, all the CBM of monolayer GeSe are higher than the reduction potential of \( \text{H}^+/\text{H}_2 \), and on the Se atom layer side, the VBM of monolayer GeSe are higher than the oxidation potential of \( \text{O}_2/\text{H}_2\text{O} \) within the strain range of \(-10\%\sim-6\%\), yet the VBM are lower than the oxidation potential within the strain range of \(-4\%\sim+10\%\), indicating the monolayer GeSe possessed a suitable band alignment for water splitting within the strain range of \(-4\%\sim+10\%\).

![Figure 4.](image-url) The energy alignment of monolayer (a) GeS and (c) GeSe at 0\% biaxial strain. The energy alignment as a function of biaxial strain of monolayer (b) GeS and (d) GeSe.

The optical absorption property is an important factor for efficient photocatalysts in water splitting. The perfect photocatalysts should absorb as much visible light and UV light as possible due to the visible light accounts for more than 50% of solar energy, yet traditional photocatalysts have low solar absorption performance due to the large band gap. As shown in the Figure 5(a) and 5(b), the monolayer GeS and GeSe exhibit strong light absorption and the absorption coefficients are about \(10^5\) cm\(^{-1}\), which agrees well with the previous experimentally\(^{34, 35}\) and theoretically\(^{36}\) reported. Besides, the absorption edges lie in the visible light region. Especially, the absorption edges have red shift, indicating a wider light absorption range in the visible light region, due to the smaller band gap tuned by biaxial strain. The above results indicate that the monolayer GeS and GeSe possess strong
absorption performance and it is effective to expand the absorption range to absorb as much visible light as possible via biaxial strain, which can enhance the photocatalytic activity of monolayer GeS and GeSe for water splitting.

![Figure 5. Absorption coefficients of monolayer (a) GeS and (b) GeSe.](image)

### 4. Conclusions

We systematically investigated the structural, electronic, dipole-induced internal electric field, optical and photocatalytic properties of the monolayer GeS and GeSe under external biaxial strain, both tensile and compressive, by using first principles calculations. The band gaps of monolayer GeS and GeSe are, respectively, 3.265 eV and 2.993 eV based on HSE06 method. Besides, the direction pointing of the dipole-induced internal electric field is from Ge atomic surface to S or Se atomic surface. There is a surface potential difference $\Delta \Phi$ between Ge atomic surface and X (X=S, Se) atomic surface. The monolayer GeS and GeSe have a suitable band alignment for water splitting, in which the CBM of monolayer GeS and GeSe are higher than the reduction potential and the VBM of monolayer GeS and GeSe are lower than the oxidation potential. Our results indicate that monolayer GeS and GeSe possesses suitable photocatalytic properties for water splitting. Especially, it is effective to tune the electronic and optical properties, including structures, band gaps, surface potential difference $\Delta \Phi$, dipolmoment $P$, dipole-induced internal electric field, absorption and photocatalytic activity, of the monolayer GeS and GeSe via biaxial strain. For example, the magnitude of the band gaps of the monolayer GeS (GeSe) could be modulated to 1.732 eV (1.130 eV) and red shift has taken place at its absorption edge as the biaxial strain increased, which is useful to expand and enhance absorption for visible light. A larger electric field ($E_{\text{eff}}$) and surface potential difference $\Delta \Phi$ were realized in the monolayer GeS (GeSe) by a tensile strain, which can effectively reduce recombination of photogenerated electron-hole pairs. Furthermore, the monolayer GeS could keep a suitable band alignment for water splitting under different biaxial strain and the monolayer GeSe could possess a suitable band alignment within the strain range of -4%~+10%. In view of the band gap, absorption, surface potential difference $\Delta \Phi$ and band alignment of the monolayer GeS (GeSe) within the strain range of -10%~+10%, it is obvious to find that strain engineering, especially tensile strain, can enhance photocatalytic activity of the monolayer GeS (GeSe) under ultraviolet and visible light.

### Conflicts of interest

There are no conflicts to declare.

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