A novel two-dimensional transition metal dichalcogenide as water splitting photocatalyst with excellent performances

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With the rising demand for renewable energy, photocatalysts are considered the most promising solution to harness solar energy, and the search for photocatalysts with excellent performances remains an urgent task. Here, based on density functional theory (DFT), the photocatalytic properties of MoWS₄ are systematically investigated. The MoWS₂ monolayer and bilayer are demonstrated as semiconductors with indirect band gaps of 2.01 and 1.48 eV. Moreover, they exhibit high and anisotropic light absorption coefficients of up to ~10⁵ cm⁻¹ in the visible-ultraviolet region. The intrinsic band edge positions could fully satisfy the redox potentials of water without any external adjustment. The electron mobility of MoWS₂ monolayer is 557 cm² V⁻¹s⁻¹, which is seven times higher than MoS₂ monolayer. Hence, MoWS₄ can be regarded as a promising 2D photocatalyst candidate for water splitting.

KEYWORDS
two-dimensional materials, transition metal dichalcogenides, water splitting photocatalyst, high mobility, density functional theory

Introduction

With the depletion of fossil energy and the increasing pollution of the natural environment, the demands for renewable energy become critical and urgent for sustainable development of global economy. In 1972, Fujishima and Honda discovered that TiO₂ can split water to produce hydrogen and oxygen in the presence of sunlight, making photocatalysis one of the most noteworthy solutions to harness solar energy (Fujishima and Honda, 1972). Afterwards, great efforts have been made to develop effective photocatalysts, including transition metal oxides, sulfides, nitrides, and so forth (Tsuji et al., 2005; Suntivich et al., 2011; Han et al., 2018). However, the low quantum efficiency derived from charge recombination on the surface and in the bulk of these
photocatalysts could not meet the criteria of favorable photocatalyst for sunlight driven water splitting (Fujishima et al., 2000).

Due to the interesting structures and corresponding electronic properties, two-dimensional (2D) materials have been widely used in various fields and also provide new research directions for efficient photocatalysis (Singh et al., 2015). In recent years, 2D photocatalysts showed the greater advantages over their bulk phase counterparts in terms of photocatalytic performance. For example, Both SnS2 monolayer and ZnSe nanosheet exhibited higher photocurrent density than their bulk materials (Sun et al., 2012a; Sun et al., 2012b). In addition, various 2D materials have also been theoretically and experimentally demonstrated to be used as photocatalysts for water splitting, such as 2D transition metal dichalcogenides, g-C3N4, phosphorene, and so on (Wang et al., 2009; Zhuang and Hennig, 2013a; Rahman et al., 2016; Phuc et al., 2018; Zhang et al., 2022). However, few of these photocatalysts can simultaneously satisfy high visible light absorption, high carrier mobility and perfect band edge positions. For instance, MoS2 monolayer showed lower carrier mobility, and MoTe2 monolayer can’t perfectly meet the redox potential of water (Wang et al., 2009; Zhuang and Hennig, 2013a; Cai et al., 2014; Rahman et al., 2016; Zhang et al., 2022). Both GaS and GaSe monolayers demonstrated low visible light absorption due to the large band gaps (Zhuang and Hennig, 2013b). Therefore, it is still a challenge to develop water splitting photocatalysts with excellent performances.

In this work, based on the first-principles calculations, we propose a novel 2D transition metal dichalcogenide namely MoWS4 and systematically investigate its photocatalytic properties. Firstly, the stability of MoWS4 monolayer is confirmed by calculating its phonon spectra and ab initio molecular dynamics (AIMD) simulations. Secondly, we calculate the band structures of MoWS4 monolayer and bilayer, and show their semiconductive characteristic. Then, relevant photocatalytic properties are systematically investigated. It is found that MoWS4 monolayer and bilayer can nicely meet the redox potentials without strain engineering, and their light absorption coefficients reach ~$10^5$ cm$^{-1}$ in the visible-ultraviolet region. Moreover, the electronic mobility of MoWS4 monolayer is as high as 557 cm$^2$ V$^{-1}$s$^{-1}$.

**Computational details**

For geometric and electronic structures, all calculations are performed by using the Vienna ab initio simulation package (VASP) based on density functional theory (DFT) (Kresse and Furthmuller, 1996). We choose the generalized gradient approximation (GGA) to perform the calculations. The exchange-correlation potential is described by the Perdew-Burke-Ernzerhof (PBE) functional. The Brillouin zone of the unit cell is sampled using a Monkhorst-Pack mesh of $2	imes2	imes1$ k-points. The cutoff energy for the plane-wave basis set is set to 400 eV. The lattice constants and atomic positions are relaxed until the forces on the atoms are below 0.01 eV/Å and the Hellmann-Feynman forces are below 0.01 eV/Å. The self-consistent field (SCF) convergence criterion is 1.0×10$^{-5}$ eV. The phonon calculations are done using the PAW method and the Perdew-Zunger (PZ) scheme. The Hellmann-Feynman forces on the atoms are relaxed until they are below 0.01 eV/Å. The self-consistent field (SCF) convergence criterion is 1.0×10$^{-5}$ eV.
approximation (GGA) of the Perdew–Burke–Ernzerhof (PBE) functional as the exchange-correlation functional to perform these calculations (Perdew et al., 1996). For the 2D monolayer structure, the vacuum layer thickness is set as about 20 Å to avoid layer-to-layer effects. The kinetic energy cutoff is set as 500 eV. The Brillouin zone is regulated with 10 × 6 × 1. During the calculations, the DFT-D2 method with Grimme correction is used to describe the long-range van der Waals interactions (Grimme, 2006). Besides, all atoms are fully relaxed, and the energy and force convergence criteria are set as 10−6 eV and 0.01 eV Å−1, respectively. Except for PBE functional, to obtain the more accurate results, the HSE06 functional is also adopted to calculate the band structures and the band edge positions (Desai et al., 2010). To identify structural stability of MoWS₄ monolayer, its phonon spectra are calculated by using the PHONOPY code (Gonze and Lee, 1997). A 6 × 3 supercell structure of MoWS₄ is used in ab initio molecular dynamics (AIMD) simulations (NVT ensemble), which is carried out for 3 ps with a time step of 1 fs at 500 K (Cimas et al., 2014).

The optical properties can be defined by the complex dielectric function (frequency) for characterization:

\[ \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \]  

where \( \varepsilon_1(\omega) \) and \( \varepsilon_2(\omega) \) represent the real and imaginary parts, respectively. Based on the Kramers–Kronig transformation (Kuzmenko, 2005), the real part \( [\varepsilon_1(\omega)] \) can be expressed as follows:

\[ \varepsilon_1(\omega) = 1 + \frac{2}{\pi} \int_0^\infty \frac{dw}{(w^2 + \omega^2)\omega^2} \varepsilon_2(\omega) \]  

where \( \omega \) is the frequency. In addition, the imaginary part \( \varepsilon_2(\omega) \) can be described as (Saha et al., 2000):

\[ \varepsilon_2(\omega) = 4\pi e^2 m_p^2 \omega^2 \sum_{i,j} \int \frac{d^2k}{(2\pi)^2} \langle ik|P|jk \rangle^2 \epsilon_i^2(\omega) (1 - \epsilon_j^2) \delta(E_j - E_i - \omega) \]  

where \( \omega, E, F, P, \epsilon \rangle \) and \( \langle k|j \rangle \) represent the incident photon frequency, the incident photon energy, the Fermi function, the transition matrix, the CB state and VB state, respectively. Finally, the absorption coefficient \( [a(\omega)] \) can be calculated by (Cheng et al., 2022a):

\[ a(\omega) = \frac{\sqrt{2\omega}}{c} \left( \varepsilon_1(\omega) + \varepsilon_2(\omega) - \varepsilon_1(\omega) \right)^{\frac{1}{2}} \]

where \( c \) denotes the speed of light in vacuum.

The carrier mobility is calculated by the following formula (Qiao et al., 2014):

\[ \mu = \frac{eB^2}{k_B T m^* m_0 E_{\text{edge}}} \]

where \( C_{2D} \) is the elastic modulus, which can be expressed by \( C_{2D} = \frac{1}{2} \int B^2 \sigma \), here \( B \) is the total energy of monolayer after deformation, \( S_B \) is the lattice area of monolayer under equilibrium and \( \delta \) is the uniaxial strain. Besides, \( k_B \) is the Boltzmann constant, \( T \) is the temperature. \( m^* \) is the effective mass along the transport direction and \( m_0 \) is the average effective mass determined by \( m_0 = \frac{m_p m_d}{m_p^2 + m_d^2} \). \( E_d \) represents the deformation potential constant, which is expressed by \( E_d = \frac{1}{3} \frac{E_{\text{edge}}}{\frac{1}{6}} \), here \( E_{\text{edge}} \) represents the shift of the band edge position with respect to the uniaxial strain \( \delta \).

**Results and discussions**

Crystal structures, stability, and electronic properties

Figure 1A shows the top and side views of 4 × 2 supercell of MoWS₄ monolayer, which has a space group of Pnm2₁. The light green area is the unit cell of MoWS₄ monolayer, which contains four atoms. The pink, blue, and yellow balls represent Mo, W, and S atoms, respectively. MoWS₄ monolayer is a honeycomb structure from the top view, while sandwich structure from the side view, which is very similar to the structure of MoS₂ monolayer (Kan et al., 2014). After fully geometric optimization, the lattice constants are \( a = 3.188 \) Å and \( b = 5.526 \) Å with a layer thickness of 3.119 Å.

To confirm the stability of MoWS₄ monolayer, the formation energy \( (E_{\text{form}}) \), defined as:

\[ E_{\text{form}} = |E_{\text{MoWS}} - E_{\text{Mo}} - E_{\text{WS}} - 4E_{\text{S}}|/b, \]

where \( E_{\text{MoWS}} \) presents the total energy of the unit cell of MoWS₄ monolayer, and \( E_{\text{Mo}}, E_{\text{WS}}, E_{\text{S}} \) present the energies of each Mo, W, and S atom in itself bulk phase, respectively. The calculated formation energy of MoWS₄ monolayer is \(-1.1\) eV/atom (<0),
implying the procedure of synthesizing MoWS₄ monolayer is exothermic and favorable. Besides, the dynamic and thermal stabilities of MoWS₄ monolayer are further investigated. As shown in Figure 1B, the calculated phonon spectra exhibit no imaginary frequency, indicating high dynamic stability of MoWS₄ monolayer. The thermal stability is further studied via AIMD calculations. As illustrated in Figure 1C, the total energy of the MoWS₄ monolayer remains essentially stable and no deformation occurs in its final structure. These results suggest that MoWS₄ monolayer exhibits good dynamic and thermal stability, which deduces the possibility of experimental synthesis of MoWS₄ monolayer.

Figure 2 shows the top and side views of MoWS₄ bilayer. Three stacking patterns (AA, AB, and AC) are considered in the bilayer structures of MoWS₄. The results of the calculated total energy are $-94.2727 \text{ eV}$, $-94.4175 \text{ eV}$, and $-94.2726 \text{ eV}$ for AA, AB, and AC stacking patterns, respectively. AA and AC stacking structures have the same layer spacing of 6.76 Å, and AB stacking has a spacing of 6.13 Å. Obviously, the AB stacking structure is most stable energetically.

Figures 3A,B shows the electronic band structures of MoWS₄ monolayer and bilayer obtained by using the PBE functional (blue) and the HSE06 functional (red). The Fermi level and the high symmetry path are set as 0 eV and $\Gamma$-X-M-Y-$\Gamma$, respectively. The MoWS₄ monolayer and bilayer are indirect band gap semiconductors and their band gaps calculated by HSE06/PBE functional are 2.01/1.67 eV and 1.48/1.14 eV, respectively. The band gaps obtained by the HSE06 functional are larger than that obtained by the PBE functional since the PBE functional tends to underestimate the band gap. Figures 3C,D shows the maps of charge density for MoWS₄ monolayer at the conduction band minimum (CBM) and the valence band maximum (VBM), and it
can be concluded that the CBM is mainly contributed by the Mo atoms, whereas the VBM comes from a combination of Mo, W, and S atoms.

Photocatalytic water splitting and optical properties

Considering the excellent semiconductor properties of MoWS4 monolayer and bilayer, we systematically study their feasibility as photocatalysts for water splitting. It is well known that a photocatalytic candidate should meet the following conditions: Firstly, its band gap should exceed the free energy of water splitting (1.23 eV). Obviously, the band gaps of MoWS4 monolayer and bilayer both exceed 1.23 eV; Secondly, its band edges must cross the redox potentials of water. The CBM energy should be higher than the reduction potential of H⁺/H₂ (−4.44 eV), and the VBM energy should be lower than the oxidation potential of O₂/H₂O (−5.67 eV) (Abe, 2010; Sun et al., 2019; Cheng et al., 2022b). For 2D materials, the band edges with respect to the vacuum level (∊_{VBM/CBM}^{DFT}) can be obtained by: ∊_{VBM/CBM}^{DFT} = ∊_{VBM/CBM}^{DFT} − V_{vacuum}, where ∊_{VBM/CBM}^{DFT} represents the value of CBM/VBM obtain by DFT and V_{vacuum} represents the electrostatic potential in the vacuum region. We plot the map of band edges relative to the vacuum level of MoWS₄ monolayer and bilayer in Figure 4A, and find that the band edge positions of MoWS₄ monolayer and bilayer can perfectly satisfy the redox potential for the water splitting reaction at pH = 0. Specifically, the band edges of CBM/VBM for MoWS₄ monolayer and bilayer are −4.202/−5.713 eV and −4.230/−5.712 eV, respectively. Thus, the results suggest that the MoWS₄ monolayer and bilayer can be promising candidates for water splitting photocatalysts.

Besides, efficient light absorption is also an important feature for water splitting photocatalysts. Figures 4B,C shows the light absorption spectra of the MoWS₄ monolayer and bilayer within the visible-ultraviolet light range. The result can be summarized as follows: 1) Their light absorption coefficients in the ultraviolet light range are higher than visible light region (up to ~10⁶ cm⁻¹); 2) Their light absorption coefficients of MoWS₄ bilayer overall are higher than that of MoWS₄ monolayer; 3) Their light absorption coefficients are significantly anisotropic: that is higher in the z direction, but have a wider range of light absorption spectra in the x and y directions. It is known that the high light absorption coefficients can guarantee the effective use of solar energy, which is very favorable for water splitting photocatalysts (Zhao et al., 2018; Fan et al., 2021). Therefore, both MoWS₄ monolayer and bilayer can be promising potential candidates as photocatalysts.

Strain engineering and high carrier mobility

We further investigate the effect of strain engineering on the photocatalytic performance of MoWS₄ monolayer. Figure 5 shows the band structures of MoWS₄ monolayer under the in-plane biaxial strain from −2 to 2%. Its band gap increases when compressive strain increases or tensile strain decreases, and its band gap varies in the range of 1.508–2.378 eV. In addition, when it is subjected to compressive strain, the indirect bandgap changes to be a direct bandgap; while when it is subjected to tensile strain, it remains an indirect bandgap semiconductor. As illustrated in Figure 6, we study the changes of its band edge positions under the applied in-plane biaxial strain. All of VBM positions are lower than the oxidation potential of O₂/H₂O under the −2−2% in-plane biaxial strain, which indicates that MoWS₄ monolayer always serves as a potential photocatalyst to generate
oxygen. Besides, when the applied tensile strain reaches 2%, its CBM positions become lower than the reduction potential of H⁺/H₂. Thus, excessive tensile strain will lead to its inability to produce hydrogen. In general, compressive strain does not cause MoWS₄ monolayer to deviate from the basic requirements for water splitting photocatalyst, but tensile strain can easily affect its hydrogen production performance.

As we know, the fast carrier migration capability is necessary for high performance photocatalysts. Thus, the PBE functional is used to calculate the carrier mobility of MoWS₄ monolayer according to Eq. 5. Subsequently, we calculate its carrier effective masses ($m'$), in-plane stiffness ($C_{2D}$) and deformation potential constants ($E_d$). Therein, to obtain $E_d$ of MoWS₄ monolayer, the linear fitting maps of band edge positions are plotted as the function of the applied uniaxial strain $\delta$ along the $x$ and $y$ directions (Bardeen and Shockley, 1950; Zhang et al., 2021a), as illustrated in Figure 7 and the result is summarized in Table 1. It is notable that the values of $E_d$ have a small difference along the $x$ and $y$ directions, which shows that the scattering ability of its carriers in different directions is also similar. In addition, the carrier effective masses of MoWS₄ monolayer have a small difference along the $x$ and $y$ directions. The electron effective masses of MoWS₄ monolayer are much lower than its hole effective masses ($m_e = 0.377m_0$ and $0.374m_0$ along the $x$ and $y$ directions), which are smaller than that of many 2D photocatalytic materials, such as Penta-PdSSe ($m_e = 2.16m_0$).
Penta-PdSe$_2$ ($m_e$ = 1.88$m_0$), δ-SnS ($m_e$ = 1.01$m_0$), SnP$_3$ ($m_e$ = 0.9$m_0$) (Long et al., 2018; Sun et al., 2018; Zhang et al., 2021b; Xiao et al., 2021). The smaller carrier effective masses benefit the transfer rate of photogenerated carriers in the photocatalytic process. What’s more, the calculated electron mobility along $x$ and $y$ directions are 529 cm$^2$V$^{-1}$s$^{-1}$ and 557 cm$^2$V$^{-1}$s$^{-1}$, respectively, whereas the calculated hole mobility along $x$ and $y$ directions are both 38 cm$^2$V$^{-1}$s$^{-1}$. The reason for this difference is that the hole effective mass is much larger than the electron effective mass. More importantly, as shown in Figure 8, the electron mobility of MoWS$_4$ monolayer can significantly exceed that of many other 2D photocatalytic materials such as MoS$_2$ ($\mu_e$ = 72.16 cm$^2$V$^{-1}$s$^{-1}$, $\mu_h$ = 200.52 cm$^2$V$^{-1}$s$^{-1}$), Penta-PdS$_2$ ($\mu_e$ = 40.97 cm$^2$V$^{-1}$s$^{-1}$, $\mu_h$ = 339.25 cm$^2$V$^{-1}$s$^{-1}$), Penta-PdSe$_2$ ($\mu_e$ = 29.40 cm$^2$V$^{-1}$s$^{-1}$, $\mu_h$ = 534.55 cm$^2$V$^{-1}$s$^{-1}$), SnP$_2$S$_6$ monolayer ($\mu_e$ = 148.48 cm$^2$V$^{-1}$s$^{-1}$, $\mu_h$ = 143.12 cm$^2$V$^{-1}$s$^{-1}$), As$_2$S$_3$ monolayer ($\mu_e$ = 253.11 cm$^2$V$^{-1}$s$^{-1}$, $\mu_h$ = 10.85 cm$^2$V$^{-1}$s$^{-1}$) (Cai et al., 2014; Wang et al., 2015; Long et al., 2018; Jing et al., 2019; Liu et al., 2021). It is well known that materials with high carrier mobility can effectively reduce their photogenerated electron and hole recombination rates and increase the participation rate in redox reactions, which are beneficial for
photocatalytic processes. Thus, our results suggest that MoWS$_4$ monolayer is a promising 2D photocatalyst candidate for water splitting.

**Conclusion**

Based on the first-principles calculations, we systematically investigate photocatalytic properties of two-dimensional MoWS$_4$. It is found that both the MoWS$_4$ monolayer and bilayer are semiconductors with indirect band gaps and show high and anisotropic light absorption coefficients in the visible-ultraviolet range. The band edge positions of the materials can satisfy the redox potentials perfectly and the electron mobility of MoWS$_4$ monolayer is up to 557 cm$^2$ V$^{-1}$ s$^{-1}$, which outperforms many other 2D photocatalytic materials, such as MoS$_2$ monolayer, Penta-PdS$_2$, Penta-PdSe$_2$, and SnP$_2$S$_6$ monolayer. These results indicate that MoWS$_4$ can be a promising photocatalyst for water splitting with outstanding performances.

**Data availability statement**

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding authors.

**Author contributions**

FW: Methodology, Investigation, Writing—original draft. ZC: Conceptualization, Investigation, Methodology, Writing—original draft. XZ: Investigation, Writing—original draft. CX: Validation, Resources. FL: Data curation, Validation. CC: Conceptualization, Writing—original draft, Supervision, Funding acquisition. GL: Validation, Data curation, Supervision.

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**Conflict of interest**

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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