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Two-Dimensional GaTe/Bi$_2$Se$_3$ Heterostructure: a Promising Direct Z-scheme Water Splitting Photocatalyst

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Among various photocatalytic materials, Z-scheme photocatalysts have drawn tremendous research interest due to high photocatalytic performance in solar water splitting. Here, we perform extensive hybrid density functional theory calculations to explore electronic structures, interfacial charge transfer, electrostatic potential profile, optical absorption properties, and photocatalytic properties of a proposed two-dimensional (2D) small-lattice-mismatched GaTe/Bi$_2$Se$_3$ heterostructure. Theoretical results clearly reveal that the examined heterostructure with a small direct band gap can effectively harvest the broad spectrum of the incoming sunlight. Due to the relative strong interfacial built-in electric field in the heterostructure and the small band gap between the valence band maximum of GaTe monolayer and the conduction band minimum of Bi$_2$Se$_3$ nanosheet with slight band edge bending, these photogenerated carriers transfer via Z-scheme pathway, which results in the photogenerated electrons and holes effectively separating into the GaTe monolayer and the Bi$_2$Se$_3$ nanosheet for the hydrogen and oxygen evolution reactions, respectively. Our results imply that the artificial 2D GaTe/Bi$_2$Se$_3$ is a promising Z-scheme photocatalyst for overall solar water splitting.

Key words: Z-scheme photocatalyst, Interfacial built-in electric field, Band edge alignment, Water splitting

I. INTRODUCTION

In recent years, due to the ever-increasing environmental problems and energy demand, the efficient use of natural energy such as solar energy has become the focus of attention [1, 2]. Since the pioneering work by Fujishima and Honda [3], photocatalytic H$_2$ production, directly converting solar energy to H$_2$ fuel via water splitting, has been regarded as one of the most promising strategies. Photocatalytic water splitting is a typical artificial photosynthesis process [4, 5], which refers to the use of solar energy to produce photogenerated carriers, and then photogenerated electrons and holes can participate in hydrogen evolution reaction (HER, 2H$^+$ + 2e$^-$ $\rightarrow$ H$_2$) and oxygen evolution reaction (OER, 2H$_2$O + 4h$^+$ $\rightarrow$ O$_2$ + 4H$^+$), respectively.

Compared with their bulk counterparts, 2D materials display different electronic, thermal and optoelectronic properties [6–12]. Till now, many 2D materials have been successfully synthesized in experiments via various methods including chemical vapor deposition, solvothermal self-assembly method, and molecular beam epitaxy [13–17], and show high photocatalytic efficiency because 2D structures can provide larger surface area, more active site, shorter carrier migration distance, rich and tunable electronic and optical properties [18–20]. In general, it is difficult for single 2D semiconducting material to meet the requirements of water oxidation and reduction reactions at the same time, which greatly limits the selectable range of 2D materials for solar water splitting. Among various 2D materials, the layered III–VI compounds (MX, M=Ga and In; X=S, Se, and Te) have attracted great research attention due to their high carrier mobility, high charge density, and high photoresponsivity and so on [21, 22]. As one member of the 2D-MX family, the theoretical predicted GaTe monolayer has an indirect band gap, which will prevent more applications in high-performance photocatalysts for water splitting, although Zhuang et al. have demonstrated that the band edges of all single-layer group-III monochalcogenide photocatalysts (namely, all MX) locate at energetically favorable positions compared with the water redox potentials [23]. Peng et al. has shown that the sunlight energy conversion efficiency of GaTe monolayer is up to 3.22% [24].

Fortunately, previous experimental and theoretical
investigations have shown that the coupling of two semiconducting nanosheets to form a regular type-II or a Z-scheme heterostructure provides an effective strategy to solve this problem [25–32]. For example, our previous investigations have shown that the g-C₃N₄/SnS₂ heterostructure and the 2D van der Waals heterostructure based on black- and blue-phosphorene are promising water splitting photocatalysts with regular type-II band edge alignment feature [25, 26]. In a common Z-scheme heterostructure, there is a photocathode (a photocatalyst for H₂ evolution) and a photoanode (a photocatalyst for O₂ evolution). Due to the direct recombination of the photogenerated holes in photocathode with the photogenerated electrons in the photoanode, then the OER and HER take place on the photoanode and photocathode, respectively. In fact, GaTe monolayer can act as a photocathode for HER since the conduction band edge is higher than the reduction potential, allowing photogenerated electrons to reduce water [23]. However, till now few reports have focused on the GaTe-based Z-scheme system for spontaneous water splitting photocatalysts with regular type-II heterostructure. According to the obtained electronic structures calculated at the PBE level, the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional [46] is employed to obtain accurate electronic structures in our calculations. Of course, the spin-orbit coupling is considered to well describe the topological insulator Bi₂Se₃, and dipole corrections are included to get correct band offsets of the examined GaTe/Bi₂Se₃ heterostructure.

In this work, converting the complex dielectric function to the optical absorption coefficient α(abs) according to the relation [47]:

$$\alpha_{\text{abs}} = \sqrt{2\omega \left[ \sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega) \right]}^{1/2}, \quad (1)$$

the optical absorption spectra of the GaTe monolayer and the Bi₂Se₃ nanosheet as well as the proposed 2D GaTe/Bi₂Se₃ heterostructure can be calculated. Here, the real and imaginary parts of frequency dependent complex dielectric function 𝜀(ω) are labelled with 𝜀₁(ω) and 𝜀₂(ω), respectively. Using the Kramer-Kronig relationship, 𝜀₁(ω) can be derived from 𝜀₂(ω), which is calculated by summing all possible transitions from the unoccupied to the occupied wave functions within the selection rules.

II. COMPUTATIONAL METHODS AND MODELS

All DFT calculations are carried out by using a projected-augmented plane wave method implemented in the Vienna ab initio simulation package (VASP) [40, 41]. The generalized gradient approximation of the Perdew-Burke-Ernzerhof (PBE) parametrization [42] is adopted for the exchange-correlation functional to optimize the geometric structures of isolated GaTe monolayer (see the left panel in FIG. 1(a)) and Bi₂Se₃ nanosheet (one quintuple layer with the Se-Bi-Se-Bi-Se sequence, see the left panel in FIG. 1(b)) as well as the 2D GaTe/Bi₂Se₃ heterostructure (see FIG. 2(a)). In order to accurately describe the weak interaction between GaTe monolayer and Bi₂Se₃ nanosheet in the heterostructure, we use the van der Waals correction of Grimme’s DFT-D3 model with Becke-Johnson damping with the PBE functional [43, 44]. The kinetic energy cutoff for plane-wave basis set is set to be 400 eV, and the Brillouin zone integration is carried out using the Γ-centered mesh of 8×8×1 k-points [45]. The vacuum region along the Z direction is set to be 20.0 Å to avoid the interaction between neighboring slabs. Geometric structures are optimized until the force on each atom is less than 0.02 eV/Å and the energy tolerance is 10⁻⁵ eV. Due to the less reliability of electronic structures of semiconductors calculated at the PBE level, the Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional [46] is employed to obtain accurate electronic structures in our calculations. Of course, the spin-orbit coupling is considered to well describe the topological insulator Bi₂Se₃, and dipole corrections are included to get correct band offsets of the examined GaTe/Bi₂Se₃ heterostructure.

III. RESULTS AND DISCUSSION

Firstly, we examine the geometric and electronic structures of the isolated GaTe monolayer and Bi₂Se₃ nanosheet to check the validity of the adopted computational methods and parameters in this work. The top and side views of a relaxed GaTe monolayer are plotted in left panel of FIG. 1(a). It is clear that GaTe monolayer displays bilayer Ga-Te buckling honeycomb hexagonal structure. The optimized lattice constant is 4.14 Å at the PBE level, and the Ga–Ga and Ga–Te distances are predicted to be about 2.47 and 2.71 Å, respectively. The conduction band minimum (CBM)
Two-Dimensional GaTe/Bi$_2$Se$_3$ heterostructure

FIG. 1 (a) The free GaTe monolayer, (b) The free Bi$_2$Se$_3$ nanosheet. Here, top and side views of are plotted in the left panel, while the band structure is illustrated in the right panel, in which the band positions are relative to the vacuum level (set to zero for clarity).

locates at the M point, while the valence band maximum (VBM) lies around the Γ point according to the calculated band structure of GaTe monolayer, as shown in the right panel of FIG. 1(a). This observation implies that GaTe monolayer is a semiconductor with an indirect bandgap of 1.97 eV. These optimized bond lengths and the predicted indirect band gap values are close to the previous reports [22]. The left panel of FIG. 1(b) illustrates the top and side views of the relaxed Bi$_2$Se$_3$ nanosheet. The optimized lattice constant, thickness of nanosheet, Bi-Se1 and Bi-Se2 distances are about 4.14, 7.07, 2.85, and 3.08 Å, respectively. As shown in the right panel of FIG. 1(b), the calculated band structure of the examined Bi$_2$Se$_3$ nanosheet shows also a semiconductor with an indirect bandgap of 0.92 eV, in which the CBM locates at the Γ point, while the VBM lies at the region between the points M and Γ points. These results agree well with the experimental and theoretical reports [33, 36]. Clearly, test calculations imply that these adopted computational parameters are suitable for exploring the following proposed 2D GaTe/Bi$_2$Se$_3$ heterostructure.

Here, it should be pointed out that the isolated GaTe monolayer and Bi$_2$Se$_3$ nanosheet are two indirect band gap semiconductors. Due to the misalignment with respect to momentum (K vector), namely, there is a momentum offset between the VBM and CBM, an electron must undergo a momentum change to produce an electron-hole pair in the GaTe monolayer or the Bi$_2$Se$_3$ nanosheet under light radiation, which leads to the low light harvesting ability. As a suitable photocatalyst, the band gap must exceed the free energy of water splitting of 1.23 eV. Clearly, the band gap of the isolated Bi$_2$Se$_3$ nanosheet is not large enough to complete the water oxidation and reduction. Moreover, the CBM of the Bi$_2$Se$_3$ nanosheet is lower than the reduction potential of H$^+/\text{H}_2$, implying that the HER can not occur on the isolated Bi$_2$Se$_3$ nanosheet. Note that the position of the VBM of the free GaTe monolayer is slightly higher than the oxidation potential of H$_2\text{O}/\text{O}_2$, indicating that the free GaTe monolayer can only act as a photocatalyst for producing H$_2$ in water splitting.

Many previous reports have shown that coupling two different 2D materials to form a heterostructure is an effective approach to enhance the photocatalytic performance [4, 27, 48, 49], even for spontaneous photocatalytic water splitting, due to the formation of built-in potentials at the interface region. The GaTe monolayer and the Bi$_2$Se$_3$ nanosheet are good candidates for constructing a heterostructure since the lattice mismatch between two 2D materials is very small (the lattice mismatch is less than 0.1%). In this work, we test three high symmetric stacking configurations, which are fully relaxed using the conjugate gradient algorithm. Their top and side views are plotted in FIG. 2. According to the calculated total energies, we find the stacking configuration shown in FIG. 2(a) is energetically most favorable. The vertical distance between the GaTe monolayer and Bi$_2$Se$_3$ nanosheet is about 3.07 Å, very close to the typical vdW equilibrium space (i.e. 3.1 Å). To check the thermodynamic stability of this GaTe$_x$/Bi$_2$Se$_3$ heterostructure, we calculate the formation energy, defined as

\[ E_f = E_{\text{GaTe}/\text{Bi}_2\text{Se}_3} - E_{\text{Bi}_2\text{Se}_3} - E_{\text{GaTe}} \]
here, $E_{GaTe/Bi_2Se_3}$, $E_{Bi_2Se_3}$, and $E_{GaTe}$ represent the total energies of the relaxed heterostructure, the free relaxed pristine Bi$_2$Se$_3$ nanosheet and GaTe monolayer, respectively. The calculated $E_f$ is about $-0.32$ eV per unit cell. This relative small formation energy indicates that the interlayer coupling between the Bi$_2$Se$_3$ nanosheet and GaTe monolayer is dominated by the vdW interaction. Of course, this negative formation energies imply that the examined stacking pattern is thermodynamically stable. To further confirm the stability of the examined GaTe/Bi$_2$Se$_3$ heterojunction, we perform the \textit{ab initio} molecular dynamics simulations at 300 K and the time step is 1 fs. We do not observe serious structure destruction, and the geometric structure is still robust within 8 ps, implying that the proposed heterostructure is also thermally stable. In the heterostructure, the Ga–Ga and Ga–Te distances are about 2.45 and 2.70 Å in the GaTe monolayer, and the Bi–Se1 and Bi–Se2 distances in the Bi$_2$Se$_3$ nanosheet are 2.87 and 3.08 Å, which are very close to these corresponding values in the free GaTe monolayer and Bi$_2$Se$_3$ nanosheet, due to the weak interlayer interaction.

The work functions, defined as energy difference between the electron energy in the vacuum and the Fermi level (equals to the VBM position, here), are predicted to be 5.61 and 6.31 eV for the isolated GaTe monolayer and the Bi$_2$Se$_3$ nanosheet, respectively. Once the GaTe monolayer connects to Bi$_2$Se$_3$ nanosheet, charge transfer spontaneously occurs due to the difference between two work functions of 0.70 eV. Based on the Bader charge analysis, we find that about 0.03 e per unit cell transfers from the GaTe monolayer to the Bi$_2$Se$_3$ nanosheet. To describe the charge transfer between the GaTe monolayer and Bi$_2$Se$_3$ nanosheet in the heterostructure more clearly, we calculate the charge density difference, defined as

$$\Delta \rho = \rho_{GaTe/Bi_2Se_3} - \rho_{GaTe} - \rho_{Bi_2Se_3}$$

here, $\rho_{GaTe/Bi_2Se_3}$, $\rho_{GaTe}$, and $\rho_{Bi_2Se_3}$ labels for the charge densities of the GaTe/Bi$_2$Se$_3$ heterojunction, the GaTe monolayer and Bi$_2$Se$_3$ nanosheet, respectively, and the obtained results are plotted in FIG. 3(a). Here, the red (blue) region stands for the charge depletion (accumulation). It is clear that the charge density redistributes mainly occurs at the interface, and the holes (electrons) accumulate close to the GaTe (Bi$_2$Se$_3$) region. FIG. 3(b) shows the planar averaged charge density difference along the Z direction, where the negative (positive) value implies electron depletion (accumulation). This verifies that the Bi$_2$Se$_3$ nanosheet gains electrons from the GaTe monolayer. The Z-direction planar-averaged charge density difference is plotted in FIG. 3(b), where the positive (negative) value stands for electron accumulation (depletion). Again, we observe that the charge transfer from the GaTe monolayer to the Bi$_2$Se$_3$ nanosheet mainly distributes around the interface region.

FIG. 4(a) shows the projected band structures of the GaTe/Bi$_2$Se$_3$ heterostructure at the HSE06 level, here, the energy bands contributed by the GaTe monolayer and Bi$_2$Se$_3$ nanosheet are labeled with the red and blue dots, respectively, and the Fermi level is set to zero for clarity. Similar to the free GaTe monolayer and Bi$_2$Se$_3$ nanosheet, this 2D heterostructure is also a semiconductor, but with a quasi-direct band gap of 0.26 eV, in which both CBM and VBM are located around the Γ point. This observation means that an indirect-direct transition for the band gap is realized by introducing

![FIG. 3](image1.png)

![FIG. 4](image2.png)
the interlayer interaction. The small direct band ensures that the GaTe/Bi$_2$Se$_3$ heterostructure can harvest broad spectrum of sunlight, and the efficiency to produce the photogenerated electron-hole pairs will be greatly enhanced, since the electron excitation from the VBM of the proposed 2D heterostructure to the CBM is easier than the isolated GaTe monolayer and Bi$_2$Se$_3$ nanosheet under solar light radiation. According to the spatial distribution of the VBM and CBM of the heterostructure, as shown in FIG. 4(b), clearly, the CBM of the GaTe/Bi$_2$Se$_3$ heterostructure is mainly contributed by the Bi$_2$Se$_3$ nanosheet, whereas the VBM mainly localizes at the GaTe monolayer. In the heterostructure, the VBM (CBM) of the GaTe monolayer locates at 0.00 (1.78) eV, leading to the band gap of 1.78 eV, while the Bi$_2$Se$_3$ nanosheet has a 1.08 eV band gap, spanning from −0.82 eV to 0.26 eV. These band gap values are close to the band gaps of the isolated GaTe monolayer (1.97 eV) and Bi$_2$Se$_3$ nanosheet (0.92 eV).

Actually, the charge transfer at the interface results in the built-in polarized electric field, which can be estimated following a previous study [27] using the relation:

$$E = \frac{P}{\varepsilon S d}$$  

(2)

here $P$ is the dipole moment, $\varepsilon$ is the dielectric constant, $S$ is the surface area of the heterostructure, and $d$ is the separation between the GaTe monolayer and Bi$_2$Se$_3$ nanosheet. As for the GaTe/Bi$_2$Se$_3$ heterojunction, $P = 0.022 \text{e}/\text{Å}, \varepsilon = 8.85 \times 10^{-12} \text{F/m}, S = 1.49 \times 10^{-19} \text{m}^2$, and $d = 3.07 \times 10^{-10} \text{m}$, then, originating from the interfacial charge transfer, the strength of the polarized electric field is predicted to be about $5.43 \times 10^8 \text{V/m}$. Due to this built-in polarized electric field originating from the work function difference of two semiconductors, the VB edge of the GaTe monolayer and the CB edge of the Bi$_2$Se$_3$ nanosheet in the heterostructure will slightly bend upward and downward, respectively.

Moreover, this built-in polarized interfacial electric field induces the electrostatic potential difference between the GaTe monolayer and Bi$_2$Se$_3$ nanosheet in the heterostructure, originating from the work function difference (0.7 eV) between the GaTe monolayer and the Bi$_2$Se$_3$ nanosheet, which is verified by the plotted results in FIG. 5, in which the water reduction and oxidation potentials locate at 4.44 and 5.67 eV below the vacuum level, respectively. The potential difference is about 0.27 eV, which is a key parameter for the band alignment of the heterostructure formed by two different 2D materials. Therefore, the water redox potentials on the Bi$_2$Se$_3$ nanosheet are 0.27 eV higher than that of the GaTe monolayer. From FIG. 5, it is clear seen that the proposed 2D heterostructure displays a typical type-II band alignment feature. Note that, in the proposed 2D heterostructure, the VBM of the GaTe monolayer is 0.41 eV higher than the water oxidation potential, while the CBM of the Bi$_2$Se$_3$ nanosheet is 0.82 eV lower than the water reduction potential, which imply that the H$_2$ and O$_2$ can not be produced on the Bi$_2$Se$_3$ nanosheet and the GaTe monolayer in the heterostructure, respectively. On the other hand, the VBM of the Bi$_2$Se$_3$ nanosheet is 0.68 eV lower than the water reduction potential, and the CBM of the GaTe monolayer is 0.96 eV higher than the water oxidation potential, indicating that the OER and HER can occur on the Bi$_2$Se$_3$ nanosheet and the GaTe monolayer in the heterostructure, respectively.

It is well established that one can design a typical Z-scheme photocatalyst based on a 2D heterostructure containing two semiconductors (i.e. C$_2$N and BCN nanosheets) with type-II band alignment [31]. According to the above obtained results, as shown in FIGs. 3–5, we illustrate the direct Z-scheme photocatalytic mechanism for solar water splitting in the proposed 2D GaTe/Bi$_2$Se$_3$ heterostructure in FIG. 6. Under solar light radiation, both GaTe monolayer and Bi$_2$Se$_3$ nanosheet in the heterostructure can effectively harvest light (i.e. absorb visible and near-infrared light), the electrons occupied on the VB are photoexcited to the CB, at the same time, the holes are generated in the VB, then the electron-hole pairs are generated on two semiconductors. Due to the slight band bending originating from the interfacial polarized electric field, in the proposed 2D heterostructure, the photogenerated electrons with a lower reduction ability in the Bi$_2$Se$_3$ nanosheet will combine with the holes with a lower oxidation ability in the VB of the GaTe monolayer. This is a fast process since the photogenerated electrons (holes) can freely flow out along the downward (upward) band bending [50]. As a result, the photogenerated holes and electrons with high oxidation and reduction abilities remain on the Bi$_2$Se$_3$ nanosheet and the GaTe monolayer in the heterostructure, respectively. One can see in FIG. 6 that the VB edge of the
FIG. 6 The proposed direct Z-scheme photocatalytic mechanism for solar water splitting in the proposed 2D GaTe/Bi$_2$Se$_3$ heterostructure.

Bi$_2$Se$_3$ nanosheet is 0.68 eV lower than the water oxidation potential and the CB edge of the GaTe monolayer is 0.96 eV higher than the water reduction potential, which imply that the photogenerated holes in the VB of the Bi$_2$Se$_3$ nanosheet have ample driving force for the oxygen evolution reaction, at the same time, water can also be reduced to H$_2$ by the electrons in the CB of the GaTe monolayer.

To effectively utilize solar energy, a photocatalyst with high photocatalytic efficiency is required to have a strong and wide optical absorption. The calculated optical absorption coefficients for the the parallel and vertical directions in the 2D GaTe/Bi$_2$Se$_3$ heterostructure as well as that of the free GaTe monolayer and the Bi$_2$Se$_3$ nanosheet as a function of photon energy are plotted in top and bottom panels of FIG. 7, respectively. Clearly, we observe two following features: (i) an obvious optical anisotropy appears in the proposed 2D heterostructure, and the optical absorption coefficients along the parallel direction are significantly larger than that along the vertical direction in a relative wide range (i.e. 0.2–3.0 eV); (ii) the heterostructure can capture a wide energy range of solar light, and the first absorption peak locating at about 0.30 eV, see the insert in FIG. 7, corresponds well with the predicted direct band gap of 0.26 eV. Compared with the free GaTe monolayer and the Bi$_2$Se$_3$ nanosheet, the optical absorption of the examined 2D heterostructure is significantly improved, which may enhance the photocatalytic efficiency for solar water splitting. Clearly, the optical properties of the proposed 2D GaTe/Bi$_2$Se$_3$ heterostructure are strongly related to the direction of injecting light as well as their electronic structures.

At last, we want to emphasize that, compared with photocatalyst based on one 2D semiconductor, either the GaTe monolayer or the Bi$_2$Se$_3$ nanosheet, the proposed Z-scheme photocatalytic heterostructure has three following required properties: (i) the light absorption is obviously improved due to the reduced direct band gap, (ii) due to the interlayer coupling via the interfacial charge transfer, the band alignment in the heterostructure is optimized for overall solar water splitting; (iii) the hydrogen and oxygen evolution reactions can be easily separated into the GaTe monolayer and the Bi$_2$Se$_3$ nanosheet, respectively.

IV. CONCLUSION

In summary, according to the calculated total energies, band structures, charge density difference, interfacial charge transfer, potential profile, and optical absorption, we find that the proposed 2D GaTe/Bi$_2$Se$_3$ heterostructure is thermodynamically and thermally stable. The heterostructure with a small direct band gap can effectively harvest solar light, and the photogenerated carriers transfer via Z-scheme pathway. Due to the relative strong interfacial built-in electric field in the heterostructure and the small band gap between the VBM of the GaTe monolayer and the CBM of the Bi$_2$Se$_3$ nanosheet with the slight band edge bending, the photogenerated holes in the VB of the GaTe monolayer will combine with the electrons in the Bi$_2$Se$_3$ nanosheet, and these uncombined electrons and holes are effectively separated into the GaTe monolayer and the Bi$_2$Se$_3$ nanosheet for the HER and OER, respectively. That is to say, we proposed a novel Z-scheme photocatalyst, namely, GaTe/Bi$_2$Se$_3$ heterostructure, for overall water splitting.

V. ACKNOWLEDGMENTS

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FIG. 7 Optical absorption coefficients for the parallel (top panel) and vertical (bottom panel) directions relative to the stacking direction in the 2D GaTe/Bi$_2$Se$_3$ heterostructure. Here, the optical absorption coefficients of the free GaTe monolayer and Bi$_2$Se$_3$ nanosheet are also plotted for comparison.
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