Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures

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Abstract

Compared with their bulk counterparts, 2D materials can sustain much higher elastic strain at which optical quantities such as bandgaps and absorption spectra governing optoelectronic device performance can be modified with relative ease. Using first-principles density functional theory and quasiparticle GW calculations, we demonstrate how uniaxial tensile strain can be utilized to optimize the electronic and optical properties of transition metal dichalcogenide lateral (in-plane) heterostructures such as MoX2/WX2 (X = S, Se, Te). We find that these lateral-type heterostructures may facilitate efficient electron–hole separation for light detection/harvesting and preserve their type II characteristic up to 12% of uniaxial strain. Based on the strain-dependent bandgap and band offset, we show that uniaxial tensile strain can significantly increase the power conversion efficiency of these lateral heterostructures. Our results suggest that these strain-engineered lateral heterostructures are promising for optimizing optoelectronic device performance by selectively tuning the energetics of the bandgap.

Two-dimensional (2D) transition-metal dichalcogenides (TMDs) have recently received considerable attention owing to their intriguing properties [1–5]. For example, most of the TMD semiconductors, such as MoS2, MoSe2, WS2, and WSe2, have a direct and finite bandgap in a monolayer [6–9]; thus they have been regarded as promising candidates for optoelectronic devices [7, 9]. Furthermore, unlike most bulk-scale TMD materials that can rarely survive beyond 1% strain, their 2D counterparts can sustain much higher strain [10] (e.g. monolayer MoS2 can sustain up to 11% strain [11]), making their material properties amenable to strain engineering. The concept of strain engineering has been demonstrated in TMDs as a powerful technique for tuning physical quantities and generating novel properties. It has been reported [12, 13] that strain is a remarkable modifier of optical quantities, such as bandgaps and absorption spectra, which govern optoelectronic device performance and carrier mobility, and can even induce magnetic instability. However, to-date most strain engineering studies have focused on single layers of TMDs [8, 14–17] or their vertically stacked heterostructures [4, 18–23], where precise control of stacking orientation, with its significant impact on overall materials properties, is still a challenge. On the other hand, the relatively new class of TMD lateral (in-plane) heterostructures [24] which have been successfully synthesized experimentally [25–28], do not suffer from the stacking orientation issue of vertically stacked heterostructures, and can equally offer enormous advantages in realizing novel properties through strain engineering.

In this work, we investigate the influence of uniaxial tensile strains on the electronic and optical properties of TMD-based lateral heterostructures (TLHs) such as MoX2/WX2 (X = S, Se, Te) by performing first-principles density functional and quasiparticle GW calculations. These TLHs consist of different transition metals (either Mo or W) but the same chalcogenides. We only focus on the TLHs consisting of 2H-phase semiconductors and exclude 1T (or 1T′)–phase metals [29]. We note that experimentally observed WTe2, unlike other TMDs, adopts 1T′ as a stable phase [30]. However, our modeling is still based on the semiconductor 2H
phase in order to examine systematically the trend for the series of lateral MoX$_2$/WX$_2$ heterostructures. Such TLHs feature a type II bandgap alignment, where both the conduction band edge and the valence band edge of the MoX$_2$ segment are lower than the corresponding band edges of the WX$_2$ segment [12, 26, 31–33]. Thus the MoX$_2$ and WX$_2$ segments serve as the electron acceptor and donor of the TLHs, respectively. We find that these TLHs may facilitate efficient electron–hole separation for light detection/harvesting and they preserve a type II characteristic up to 12% of uniaxial strain. Based on the strain–dependent bandgap and the band offset, we show that uniaxial tensile strains can significantly increase the power conversion efficiency (PCE) of these lateral heterostructures. For example, relative to the unstrained structures, a 4% uniaxial tensile strain increases the PCE of the lateral MoSe$_2$/WSe$_2$ heterostructure by ~15%, and the same strain increases the PCE of the lateral MoS$_2$/WS$_2$ heterostructure by ~35%. Therefore, our study suggests that these strained TLHs can be utilized as novel architectures for efficient optoelectronic device development by selective control of the bandgap in energetic distributions.

First-principles calculations were performed with the Vienna Ab initio Simulation Package (VASP, version 5.3.5) [34, 35]. Density functional theory (DFT) calculations were performed for both WX$_2$ (X = S, Se, Te) monolayers and MoX$_n$/WX$_2$ (X = S, Se, Te) TLHs mainly by employing the local-density approximation (LDA) for the exchange–correlation functional as parameterized by Perdew and Zunger [36]. The projector–augmented wave method was used to mimic the ionic cores. The kinetic energy cutoff for the plane wave basis set was set to 500 eV, and the ‘accurate’ precision setting was adopted to avoid wrap around errors. K-point samplings of 4 × 8 × 1 and 2 × 10 × 1 were used for the WX$_2$ (X = S, Se, Te) monolayers and the MoX$_n$/WX$_2$ (X = S, Se, Te) TLHs, respectively. The lattice parameter perpendicular to the 2D plane was fixed at ~20 Å to ensure a large separation between lateral heterostructures in neighboring supercells and was carefully checked to avoid any spurious interactions. Atomic positions as well as the in-plane lattice parameters were fully optimized with a conjugate gradient algorithm. Convergence criteria of $1 \times 10^{-2}$ eV Å$^{-1}$ per ion and $10^{-3}$ eV per electronic step were applied to ionic and electronic relaxations, respectively. Following structural optimizations, band structures were calculated for the WX$_2$ (X = S, Se, Te) monolayers and the MoX$_n$/WX$_2$ heterostructures, while optoelectronic quantities including the bandgaps of WX$_2$, conduction band offsets between MoX$_2$ and WX$_2$, and the PCEs were calculated for the MoX$_n$/WX$_2$ heterostructures. The band structures of WX$_2$ (X = S, Se, Te) monolayers calculated at the LDA level were compared with Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional [37] calculations. For comparison of optoelectronic characteristics, quasiparticle GW calculations [38] were also performed for the WS$_2$ monolayer and the MoS$_2$/WS$_2$ heterostructure under selected uniaxial strains based on their respective LDA geometries. Specifically, single-shot $G_0W_0$ calculations were performed on the basis of the wavefunctions and eigenvalues from the HSE06 functional, using the same kinetic energy cutoff for the plane wave basis set of 500 eV and an energy cutoff for the response function of 150 eV. A total of 192 bands and 64 frequency points for the WS$_2$ monolayer and a total of 252 bands and 84 frequency points for the MoS$_2$/WS$_2$ heterostructure were included in the $G_0W_0$ calculations. The $k$-mesh was increased to $4 \times 12 \times 1$ and $2 \times 12 \times 1$ for the WS$_2$ monolayer and the MoS$_2$/WS$_2$ heterostructure, respectively. The 12 points along the $Y$ direction guarantee that both the conduction band minimum (CBM) and valence band maximum (VBM) will be correctly sampled.

Monolayers of constituent MoX$_2$ and WX$_2$ are each composed of two hexagonal planes of chalcogen (X = S, Se, Te) atoms and a hexagonal plane of transition metal (M = Mo, W) atoms sandwiched in between. The M atoms are coordinated through ionic–covalent interactions with the X atoms in a trigonal prismatic arrangement ($2H$-crystal symmetry). The mismatch of the lattice constants between the MoX$_2$ and WX$_2$ components is less than 0.01%, which results in the formation of favorable lateral MoX$_2$/WX$_2$ heterostructures. Here we considered the interfacial atomic configurations of MoX$_2$/WX$_2$ with zigzag types that are found as the most stable interfaces in experiments [28]. The lateral MoX$_2$/WX$_2$ heterostructures contain units of MoX$_2$ and WX$_2$ in a supercell (see figure 1(a)). As the anionic species change from S, Se, to Te, the electron affinity of the elements gradually decreases; that is, the electron affinity is highest with S and lowest with Te. Consequently, the net charges gradually decrease; the net charges of individual species in WTe$_2$/MoTe$_2$ are only about half those of the Se counterpart (see table S1 (stacks.iop.org/TDM/4/021016/mmedia)). The decreased ionicity at the interfaces ultimately results in the MoTe$_2$/WTe$_2$ heterostructures exhibiting the lowest formation energy among the considered configurations. This observation is consistent with the cohesive energy of MX$_2$ monolayers (see table S1). Hereafter, we will only focus on the energetically most stable heterostructures.

First we explored the electronic band structures of zigzag-interfaced MoX$_2$/WX$_2$ heterostructures, as illustrated using (MoX$_2$)$_n$(WX$_2$)$_m$(MoX$_2$)$_n$ (X = S, Se, Te) containing a total of twenty MoX$_2$ and WX$_2$ units per supercell (figure 1(a)), in order to lay the groundwork for subsequent discussions of the influence of uniaxial strain on the band alignment and optoelectronic properties. The W 5$d$ orbitals are located at higher energies than the Mo 4$d$ orbitals, such that both the CBM and VBM of WX$_2$ are higher than those of MoX$_2$, resulting in type II band alignment at zero strain (figure 1(b)). The isosurfaces of band decomposed electron densities confirm the type II band alignment (figure 1(c)); CBM charge densities are confined in the MoS$_2$ region while VBM charge densities are confined in the WS$_2$ region.
It is worth noting that both the VBM and CBM of the heterostructure are located at 2/3 along the $\Gamma$–$Y$ line, which corresponds to the K point in the reciprocal space for a conventional hexagonal unit cell. This direct K–K bandgap (table S2, supporting information) is advantageous for efficient optical transitions without involving phonons. Therefore, at the MoX$_2$/WX$_2$ junction, interfacial excitons could be created directly upon the adsorption of light in the solar spectrum, where electrons are accumulated at the CBM of MoX$_2$ while holes are accumulated at the VBM of WX$_2$. However, this one-step process could be limited due to the small area at the junction compared to the large areas of the donor WS$_2$ and the acceptor MoS$_2$. Alternatively, interfacial excitons may be created indirectly through a two-step process where excitons are first created on the donor WS$_2$ or acceptor MoS$_2$ side, which then diffuse to the interface and are separated by the band offsets due to the type II band alignment [39]. More specifically, if the exciton is formed on the acceptor first, the valence band offset may serve as the driving force to shift the hole to the donor; if the exciton is formed instead on the donor first, the conduction band offset may drive the electron toward the acceptor. The second process also involves direct K–K bandgaps for the donor or acceptor (table S2, supporting information), which are beneficial in utilizing the heterostructures to convert solar energy into electricity.

Our focus concerns how to utilize tensile strains to optimize the electronic and optical properties of TLHs. The effect of strain can be readily illustrated using single-component TMDs, e.g. WS$_2$, for which a centered rectangular supercell containing two WS$_2$ units per supercell was adopted in replacement of the conventional hexagonal unit cell. Uniaxial strains were applied to the direction normal to the zigzag edge direction, while biaxial strains were applied to both normal and parallel directions to the zigzag edge direction. Based on electronic structure calculations at both LDA and HSE06 levels, strains significantly affect the size of the bandgaps of WS$_2$, which decreases monotonically as uniaxial strain increases (see figures S1 and S2, supporting information). One of the most promising features of monolayer TMDs is the direct bandgap characteristics, which can be intact up to a few percent strain. For instance, monolayer WS$_2$ preserves the direct bandgap characteristics up to ~4% biaxial strain, and is even more immune to uniaxial strain (see figures S1 and S2 for LDA and HSE results, respectively). Similar to the (MoX$_2$)$_6$(WX$_2$)$_7$(MoX$_2$)$_7$ TLH (figure 1(a)), the direct bandgap of monolayer WS$_2$ is also located at the K-point in the reciprocal space as defined for a conventional hexagonal unit cell (figure S3, supporting information).

Next we turn to the electronic and optical properties of two-component TLHs, which are also affected by tensile strain. Specifically, we find that uniaxial strain can be useful to enhance their optoelectronic properties, and make the TMD heterostructures more promising as an optoelectronic device. Uniaxial strain $\varepsilon$ was imposed...
to the lateral MoX2/WX2 heterostructures by elongating the lateral heterostructures along the armchair direction (x direction of figure 1(a)) that is perpendicular to the zigzag interfaces, while the perpendicular cell dimension (y direction of figure 1(a)) is fully relaxed. The open circuit voltage is determined by the direct K–K bandgap between CBM and VBM, which is related to the bandgap ($E_g$) of WX2 and conduction band offset ($\Delta E_c$). Thus, these two quantities are critical for quantifying the optoelectronic properties of lateral MoX2/WX2 heterostructures. (Our analysis is presented on the basis of the donor’s $E_g$ and conduction band offset $\Delta E_c$ but using the acceptor’s $E_g$ and valence band offset $\Delta E_v$ should lead to the same trend.) The bottom panel of figure 2 shows the change of $E_g$ for WX2 and $\Delta E_c$ between MoX2 and WX2 as a function of uniaxial strain in lateral MoX2/WX2 heterostructures. The WX2 bandgaps monotonically decrease under the uniaxial strain, while the conduction band offsets remain almost constant in the range between $\sim 0.1$ eV and $\sim 0.2$ eV. Characteristics of the CBMs are mainly from the $d_{xy}$ orbitals of weakly interacting cations in $xy$-plane [12], where tensile strain cannot enhance their overlap, thus resulting in a robust conduction band offset under the tensile strain. On the other hand, VBM, contributed by both $d_{xy}$ and $d_{x^2−y^2}$ orbitals [12], are sensitively changed under strain and thus dominate the strong dependence of the bandgaps on tensile strains. In addition, the valence band offset also remains constant, which is due to the fact that the VBM of both MoX2 and WX2 are concurrently raised by the strain in comparable amount. Consequently, uniaxial strain monotonically decreases the bandgaps of MoX2 and WX2, while maintaining type II band alignment. The overall changes of $E_g$ and $\Delta E_c$ with uniaxial strains display similar trends across different MoX2/WX2 heterostructures, as supported by all the materials under our consideration. Here, the bandgaps can be tuned up to $\sim 1$ eV by applying uniaxial strain up to 12%. Note that the maximum uniaxial strain of 12% is based on recent experimental report [11], demonstrating that monolayer TMDs can sustain up to $\sim 11$% strain.

Based on the type II band alignment of lateral heterostructures, the upper limit of the PCE can be estimated in the limit of 100% external quantum efficiency as follows [9, 40]:

$$\eta = \frac{J_{sc}V_{oc}FF}{P_{solar}} = \frac{0.65(E_g - \Delta E_c - 0.3) \int_{E_g}^{\infty} \rho(h\omega) d(h\omega)}{\int_{0}^{\infty} \rho(h\omega) \omega d(h\omega)},$$

where the band-fill factor is assumed to be 0.65, $P(h\omega)$ is taken to be the air mass AM1.5 solar energy flux (in the unit W m$^{-2}$ eV$^{-1}$) at the photon energy $h\omega$ [41], $E_g$ is the bandgap of the WX2 segment, and the $(E_g - \Delta E_c - 0.3)$ term is an estimation of maximum open circuit voltage $V_{oc}$. Here, AM refers to the relative path length of the solar beam through the atmosphere and depends on the angle of the Sun from the vertical. AM is important because with longer path lengths (higher AM values), there is a greater opportunity for scattering and absorption of solar radiation by atmospheric constituents, such as clouds. AM is 1.5 when the Sun is 48.2° from the vertical. For efficient charge separation, an additional adjustment of 0.3 eV, an empirical value, is used [40, 42]. The integral in the numerator corresponds to the short circuit current, $J_{sc}$, in the limit of 100% external quantum efficiency, and that in the denominator corresponds to an AM1.5 solar flux. The top panel of figure 2 presents a 2D contour plot of PCE as a function of $E_g$ and $\Delta E_c$. Computed PCEs of lateral MoX2/WX2 heterostructures based on the LDA results in the bottom panel of figure 2 are overlaid on the contour as data points of solid triangles. We find that both lateral heterostructures of MoS2/WS2 and MoSe2/WSe2 reach a maximum PCE value of 23% at 4% uniaxial strain. At the maximum PCE points, they preserve a direct bandgap characteristic (table S2, supporting information), which makes these strained lateral MoX2/WX2 (X = S, Se) heterostructures promising as future solar energy conversion materials. In comparison, the PCE of the pristine lateral MoTe2/WTe2 heterostructure is about 21% at 0% strain, which decreases gradually with increasing strains.

To complement the results from the LDA functional, which is known to underestimate bandgaps for many semiconductors [43, 44], we employed Green’s function-based many-body perturbation theory by performing non-self-consistent quasiparticle G0W0 calculations on top of the wavefunctions and eigenvalues obtained with the HSE06 hybrid functional (G0W0@HSE06). Because of high computational cost, G0W0@HSE06 calculations were performed only for a narrower lateral (MoS2)$_7$(WS2)$_7$ heterostructure containing only 42 atoms per supercell under selected strains (0%, 6%, and 12%). The smaller heterostructure is manageable for GW calculations, while it is still large enough to result in comparable electronic structures as the larger (MoS2)$_7$(WS2)$_7$(MoS2)$_7$ heterostructure (figure S4, supporting information). The overall changes of $E_g$ and $\Delta E_c$ with uniaxial strains at the GW level display essentially the same trend as that observed at the LDA level for the lateral MoS2/WS2 heterostructure. However, the bandgaps of WS2 calculated by G0W0@HSE06 are noticeably larger ($\sim 1.1–1.2$ eV) than those calculated using the LDA functional (see the comparison in the bottom panel of figure 2). In this regard, it should be noted that the bandgap in PCE formula (equation (1)) corresponds to an optical bandgap (i.e. onset transition), whereas the GW approximation yields fundamental bandgaps associated with the photoemission and inverse photoemission processes [45]. The difference between the optical and fundamental bandgaps boils down to the exciton binding energies. Excitons, or electron–hole pair interactions, play a fundamental role in determining the optical spectrum of semiconductors. In order
to include the excitonic effects accurately, one should solve the Bethe–Salpeter equation (BSE) on top of GW approximation. The GW + BSE method has already been applied to monolayer TMDs, giving an exciton binding energy of 1.0–1.1 eV for MoS2 following strict convergence studies [46, 47]. On the other hand, the exciton binding energy of WS2 is expected to be similar to or even slightly larger than that of MoS2 [17, 48], and therefore the large exciton binding energy of WS2 may bring the GW fundamental bandgaps for WS2 down to optical bandgap values close to the LDA results (see the bottom panel of figure 2). (Note that compared to the large theoretical binding energy, the experimental values for WS2 are often found to be reduced to a range of 0.3–0.7 eV depending on the substrates used [49–51], which can be ascribed to the strong dielectric screening of the electron–hole pair interactions by the substrates [46].) In other words, due to an error cancellation associated with the underestimation of bandgaps and lack of excitonic effects, LDA turns out to be a good approximation for our purpose in that it gives a fortuitous agreement of optical bandgaps between theory and experiments [17]. This is indeed observed for MoS2 with an LDA bandgap of 1.87 eV [52] that is in good agreement with experimental 1.83–1.88 eV [53, 54]. For the donor WS2 under 0% strain, the LDA bandgap of 1.98 eV [52] (figure 2 and table S2) also agrees with the experimental 1.94–1.99 eV obtained from both differential reflectance and photoluminescence spectroscopy [55, 56], which provides a direct support for using the LDA bandgaps for PCE calculations. Based on these results, hereafter we will continue our discussions of PCEs based on the LDA values.

As shown in figures 3(a) and (b), both lateral MoS2/WS2 and MoSe2/WSe2 heterostructures can achieve a PCE as high as ~23% under the 4% uniaxial strain. This value is higher than the literature values for comparable 2D systems, including PCBM (Phenyl-C61-butyric acid methyl ester)/CBN (monolayers of hexagonal BN and graphene) (10–20%) [9], inhomogeneously strained monolayer MoS2 (16%) [10], AA-/AB-stacked bilayer phosphorene (18%) [20], and the recently predicted γ-SiC2-based systems (12–20%) [57]. On the other hand, strain is not beneficial for the PCE of the lateral MoTe2/WTe2 heterostructure that already has a bandgap close to the desirable values at zero strain, where it continuously decreases under the uniaxial strains (figure 3(c)). It is worth pointing out that the PCEs are estimated in the limit of 100% external quantum efficiency, so the actual PCE values might be lower. However, the relative change of PCEs with respect to

Figure 2. Optoelectronic quantities and PCE under uniaxial strain. Computed PCE contours as a function of the bandgap ($E_g$) of $WX_2$ and conduction band offset ($\Delta E_c$) between $MoX_2$ and $WX_2$ are shown in the top panels, where the computed $E_g$ and $\Delta E_c$ at each strain are overlaid on the contours. Bottom panel displays changes of $WX_2$ ($X = S, Se, Te$) bandgap ($E_g$) and conduction band offset ($\Delta E_c$) between MoX2 and WX2 as a function of uniaxial strain in lateral MoX2/WX2 heterostructures. For the MoS2/WS2 heterostructure, the $E_g$ of WS2 and the $\Delta E_c$ between MoS2 and WS2 are also calculated using the $G_0W_0@HSE06$ approach and compared with the LDA values. The bandgap difference between the GW and LDA results is denoted as the exciton binding energy (B.E.) which is discussed in the main text.

2D Mater. 4 (2017) 021016
that of unstrained heterostructure shown in figure 3(d) clearly demonstrates the strain-improved PCE values. For example, a 4% uniaxial tensile strain increases the PCE of the lateral MoS$_2$/WS$_2$ heterostructure by about 35% while the same strain applied to MoSe$_2$/WSe$_2$ increases PCE by 15%. Overall, our study demonstrates that a few percentage (≤ 4%) of uniaxial tensile strain can remarkably improve the solar energy conversion processes of lateral MoX$_2$/WX$_2$ (X = S, Se) heterostructures.

In summary, we have shown that lateral MoX$_2$/WX$_2$ (X = S, Se, Te) heterostructures formed by fusing various TMDs may establish a promising class of materials for solar energy harvesting. These lateral-type heterostructures may facilitate efficient electron–hole separation for light detection/harvesting and preserve their type II characteristic up to 12% of uniaxial strain. Uniaxial tensile strains can be utilized to optimize the electronic and optical properties of MoX$_2$/WX$_2$ (X = S, Se, Te), and thereby can maximize solar energy harvesting. A 4% uniaxial tensile strain could increase the PCE of the lateral MoS$_2$/WS$_2$ heterostructure by about 35% compared with that of the pristine system. In comparison, a 4% strain would increase the power efficiency of a lateral MoSe$_2$/WSe$_2$ heterostructure by 15%. Consequently, we expect these strained TLHs to be novel architectures for future development of efficient optoelectronic devices, due to the selective control of their bandgap in terms of energetic distribution.

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