Quasiparticle band structures and optical properties of strained monolayer MoS\(_2\) and WS\(_2\)

Hongliang Shi\(^1\), Hui Pan\(^1\), Yong-Wei Zhang\(^1\)\(*\) and Boris I. Yakobson\(^2\)

\(^1\)Institute of High Performance Computing, A*STAR, Singapore 138632
\(^2\)Department of Mechanical Engineering and Materials Science, and Department of Chemistry, Rice University, Houston Texas 77005

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The quasiparticle (QP) band structures of both strainless and strained monolayer MoS\(_2\) are investigated using more accurate many body perturbation GW theory and maximally localized Wannier functions (MLWFs) approach. By solving the Bethe-Salpeter equation (BSE) including excitonic effects on top of the partially self-consistent GW\(_0\) (scGW\(_0\)) calculation, the predicted optical gap magnitude is in a good agreement with available experimental data. With increasing strain, the exciton binding energy is nearly unchanged, while optical gap is reduced significantly. The scGW\(_0\) and BSE calculations are also performed on monolayer WS\(_2\), similar characteristics are predicted and WS\(_2\) possesses the lightest effective mass at the same strain among monolayers Mo(S,Se) and W(S,Se). Our results also show that the electron effective mass decreases as the tensile strain increases, resulting in an enhanced carrier mobility. The present calculation results suggest a viable route to tune the electronic properties of monolayer transition-metal dichalcogenides (TMDs) using strain engineering for potential applications in high performance electronic devices.

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I. INTRODUCTION

Bulk TMDs consisting of two-dimensional (2D) sheets bonded to each other through weak van der Waals forces have been studied extensively owing to their potential applications in photocatalysis \([1]\) and catalysis \([2, 3]\). MoS\(_2\), WS\(_2\), MoSe\(_2\), and WSe\(_2\) are examples of such TMDs. Recently, their 2D monolayer counterparts were successfully fully fabricated using micromechanical cleavage method \([4]\). Since then, these monolayer materials have attracted significant attention \([5–12]\).

For monolayer MoS\(_2\), a strong photoluminescence (PL) peak at about 1.90 eV, together with peaks at about 1.90 and 2.05 eV of the adsorption spectrum indicated that MoS\(_2\) undergoes an indirect to direct band gap transition when its bulk or multilayers form is replaced by a monolayer \([4, 5]\). Shifts of PL peak for the monolayer MoS\(_2\) were also observed experimentally, which was attributed to the strain introduced by covered oxides \([5]\). Theoretical studies employed density functional theory (DFT) method also predicted monolayer MoS\(_2\) to have a direct gap of 1.78 eV \([6]\). It is known however that DFT does not describe excited state of solids reliably. Furthermore, an important character in low-dimensional systems is their strong exciton binding due to the weak screening compared to bulk cases. Therefore, the good band gap agreement between theoretical and experimental results for monolayer MoS\(_2\) may be a mere coincidence. As a channel material for transistor application, theoretical simulations show that monolayer WS\(_2\) performs better than monolayer MoS\(_2\) \([4]\). In order to address above questions, it is important and necessary to employ more accurate calculation method beyond DFT to investigate the electronic structures of strained monolayer MoS\(_2\) and WS\(_2\).

The most common method to circumvent drawback of DFT is the GW approximation \([7]\), in which, self-energy operator \(\Sigma\) contains all the electron-electron exchange and correlation effects. The scGW\(_0\) approach, in which only the orbitals and eigenvalues in \(G\) are iterated, was shown to be more accurate in many cases to predict band gaps of solids \([8]\). The off-diagonal components of the self-energy \(\Sigma\) should be included in scGW\(_0\) calculations, since this inclusion has been proved particularly useful for materials such as NiO and MnO \([9]\). It is noted that \(\Sigma\) within GW approximation is defined only on a uniform \(k\) mesh in Brillouin-zone, due to its non-locality. Therefore, unlike DFT band structure plot, the QP eigenvalues at arbitrary \(k\) points along high symmetry lines cannot be performed directly \([10]\). Started from the scGW\(_0\) calculation, the QP band structure can be interpolated using MLWFs approach. This combination was demonstrated to be accurate and efficient for the scGW\(_0\) band structure \([11]\). The \(GW\) results were shown to agree well with the photoemission data \([12]\), while in order to reproduce the experimental adsorption spectra, the consideration of attraction between quasi-electron and quasi-hole (on top of GW approximation) by solving BSE is indispensable \([13]\), particularly for the low-dimensional systems with strong excitonic effect. The main goal of this study is to accurately predict the QP band structures and optical spectra of monolayer MoS\(_2\) as a function of strain by adopting the DFT-scGW\(_0\)-BSE approach.

Strain in monolayer MoS\(_2\) can be produced either by...
epitaxy on a substrate or by mechanical loading. It is well-known that strain can be used to tune the electronic properties of materials. This is particularly important for two-dimensional materials, which can sustain a large tensile strain. In fact, shifts of PL peak observed experimentally in monolayer MoS$_2$ was attributed to strain [23], and the magnetic properties of MoS$_2$ nanoribbons could be tuned by applying strain [24].

By adopting the aforementioned approach, we systematically investigate how the electronic structures and optical properties of monolayer MoS$_2$ evolve as a function of strain. Our results show that exciton binding energy is insensitive to the strain, while optical band gap becomes smaller as strain increases. Based on the more accurate band structures interpolated by MLWFs methods based on scGW$_0$ results, the effective masses of carriers are calculated. In addition, this calculation approach is also employed to investigate other monolayer TMDs, that is, WS$_2$, MoSe$_2$, and WSe$_2$. Our results demonstrate that the effective mass is decreased as the strain increases, and monolayer WS$_2$ possesses the lightest carrier among the TMDs, suggesting that using monolayer WS$_2$ as a channel material can enhance the carrier mobility and improve the performance of transistor.

II. DETAILS OF CALCULATION

Our DFT calculations were performed by adopting the generalized gradient approximation (GGA) of PBE functional [25] for the exchange correlation potential and the projector augmented wave (PAW) [26] method as implemented in the Vienna ab initio simulation package [27]. 12 valence electrons are included for both Mo and W pseudopotentials. The electron wave function was expanded in a plane wave basis set with an energy cutoff of 600 eV. A vacuum slab more than 15 Å (periodical length of c is 19 Å) is added in the direction normal to the nanosheet plane. For the Brillouin zone integration, a $12 \times 12 \times 1$ Γ centered Monkhorst-Pack $k$-point mesh is used. In the following GW QP calculations, both single-shot $G_0W_0$ and more accurate scGW calculations are performed. 184 empty conduction bands are included. The energy cutoff for the response function is set to be 300 eV, the obtained band gap value is almost identical to the case of 400 eV. The convergence of our calculations has been checked carefully. For the Wannier band structure interpolation, $d$ orbitals of Mo (W) and $p$ orbitals of S (Se) are chosen for initial projections. Our BSE spectrum calculations are carried out on top of scGW$_0$. The six highest valence bands and the eight lowest conduction bands were included as basis for the excitonic state. BSE was solved using the Tamm-Dancoff approximation. Notice that the applied strain in the present study is all equibiaxial, unless stated otherwise.

III. RESULTS AND DISCUSSIONS

We first analyze the density of states (DOS) for monolayer MoS$_2$. The $d$ orbitals of Mo and $p$ orbitals of S contribute most to the states around the band gap, similar to previous studies [11,12]. Fig. 3 shows the projected $d$ orbitals of Mo and $p$ orbitals of S as well as the decomposed $d$ orbitals for monolayer MoS$_2$ at the lattice of 3.160 Å (the experimental lattice constant a of bulk MoS$_2$ [6]) and under 3% tensile strain. Based on the DOS, the $d$ orbitals of Mo and $p$ orbitals of S are chosen as the initial projections in the Wannier interpolated method. Fig. 2 shows the identical DFT band structures of monolayer MoS$_2$ obtained by the non-selfconsistent calculation at fixed potential and Wannier interpolation method, respectively, confirming that our choice of the initial projections and inner window energy is appropriate. Based on the good results for monolayer MoS$_2$, the same procedure is also employed for remaining monolayer TMDs.

A. QP band structures of strained monolayer MoS$_2$

The QP band structures of monolayer MoS$_2$ at four lattice constants of 3.160, 3.190 (the optimized value from the present work), 3.255, and 3.350 Å are plotted in Fig. 3, corresponding to 0%, 1%, 3%, and 6% tensile strains (with reference to 3.160 Å), respectively. As shown in Fig. 3(a), the band structure obtained by DFT for strainless MoS$_2$ is a direct band gap semiconductor with a band gap energy of 1.78 eV, while the indirect band gap of 2.49 eV is predicted by $G_0W_0$. Obviously this $G_0W_0$ indirect band gap is contrary to the PL observations [6,8]. The QP band structures predicted by our scGW calculation show that MoS$_2$ is a $K$ to $K$ direct band gap semiconductor with a band gap energy of 2.80 eV. This prediction is in excellent agreement with the recent calculation for MoS$_2$ at the experimental lattice using full-potential linearized muffin-tin-orbital method (FP-LMTO) [24], which predicted a $K$ to $K$ direct band gap of 2.76 eV.

It should be noted that in the 2D materials, the excitonic effect is strong due to the weak screening. Thus it is important to consider the attraction between the quasi-electron and quasi-hole by solving the BSE discussed below in order to make the predicted optical gap consistent with the optical spectra.

Fig. 3(b) shows the band structure of monolayer MoS$_2$ at 3.190 Å corresponding to 1% strain. The DFT result predicts the monolayer MoS$_2$ to be an indirect band gap with $K$ to $\Gamma$ of 1.67 eV. Previous DFT studies also found that monolayer MoS$_2$ already becomes an indirect semiconductor under a tensile strain of 1% [12]. After GW correction, both of the $G_0W_0$ and scGW$_0$ QP band structures show that MoS$_2$ is still a direct semiconductor with $K$ to $K$ band gaps of 2.50 and 2.66 eV, respectively. As the strain increases, shown in Fig. 3(c) and 3(d),
the DFT, $G_0W_0$ and scGW all predict monolayer MoS$_2$ to be indirect. The calculated indirect band gaps from DFT, $G_0W_0$ and scGW are 1.20 (0.63), 2.19 (1.56), and 2.23 (1.59) for monolayer MoS$_2$ under strain of 3% (6%), respectively. As shown in Fig. (a), the value of band gap decreases as the tensile strain increases, accomplishing a shift of valence band maximum (VBM) from $K$ to $\Gamma$ point and resulting in a direct to indirect band gap transition, which was consistent well with previous results ($\ddagger$) ($\ddagger$).

The $K$ to $K$ direct band gaps of monolayer MoS$_2$ obtained by DFT and scGW as a function of tensile strain are plotted in Fig. (b). Clearly our DFT and scGW results have the same trends, and accord well with reported DFT ($\ddagger$) (cyan triangle) and scGW ($\ddagger$) (green solid square) results, respectively. Due to the more accurate description of many body electron-electron interaction, the scGW band gaps are enlarged about 1 eV compared to DFT results. The optical gap shown in Fig. (c) will be discussed in the next subsection.

**B. Excitonic effect in monolayer MoS$_2$**

In this subsection, the optical properties of monolayer MoS$_2$ are discussed in details. From the technical view, optical transition simulation needs the integration over the irreducible Brillouin zone using sufficiently dense $k$-point mesh. Naturally, the convergence of $k$-point sampling is important. First, for monolayer MoS$_2$
cases, corresponding to the first peak at about 1.78 eV is observed clearly in all the calculations at Hartree or DFT level. The illustrated in Fig. 5(a), in which the independent-particle monolayer MoS$_2$ at strainless case (3.16 Å) obtained by different $k$-point meshes.

At strainless case (3.16 Å), the optical adsorption spectra $\varepsilon_2$ ($\varepsilon_{xx} = \varepsilon_{yy}$) obtained by different $k$-point meshes are illustrated in Fig. 5(a), in which the independent-particle (IP) picture is adopted within DFT (DFT-IP) and no local filed effect is included at Hartree or DFT level. The first peak at about 1.78 eV is observed clearly in all the cases, corresponding to the $K$-$K$ direct transition. The second significant peak located at about 2.75 eV is converged for $12 \times 12 \times 1$ and $15 \times 15 \times 1$ $k$-point meshes. Other peaks in adsorption spectra between the two aforementioned dominated peaks mainly originate from different irreducible $k$ points with unequal weights in different $k$-point meshes. According to our analysis of projected density of states, the two significant peaks located in 1.78 and 2.75 eV correspond to $d$-$d$ and $p$-$d$ transitions, respectively. Considering the dipolar selection rule only transitions with the difference $\Delta l = \pm 1$ between the angular momentum quantum numbers $l$ are allowed, i.e., the atomic $d$-$d$ transition is forbidden. However, in the monolayer MoS$_2$, due to the orbital hybridization, the VBM and conduction band minimum (CBM) still have $p$ orbital contributions, especially the former; thus the VBM to CBM transition dominated by $d$-$d$ transition is still allowed. As expected, the strength of this $d$-$d$ transition is weaker than the $p$-$d$ transition as shown in Fig. 5(a).

As for the BSE calculations, in order to reduce the computational cost, we adopt 400 and 200 eV for the plane wave energy cutoff and response function energy cutoff (short for 400 and 200 eV for energy cutoffs), respectively, while the accuracy still can be guaranteed. Taking the strainless monolayer MoS$_2$ for example, the sc$GW_0$ band gap is 2.78 eV, resulting in only 0.02 eV difference compared to 2.80 eV aforementioned using 600 and 300 eV for energy cutoffs. The calculated BSE spectra for strainless monolayer MoS$_2$ are plotted in Fig. 5(b). It is clearly that as $k$-point mesh refines, the first peaks have a blueshift. For $k$-point meshes $6 \times 6 \times 1$, $9 \times 9 \times 1$, $12 \times 12 \times 1$, and $15 \times 15 \times 1$, the sc$GW_0$ band gaps are 2.99, 2.84, 2.78, and 2.76 eV, respectively; the first adsorption peaks (optical band gaps) are 1.96, 2.08, 2.16, and 2.22 eV. Correspondingly, the exciton binding energies are 1.03, 0.76, 0.62, and 0.54 eV, inferred from the difference between the QP (sc$GW_0$) and optical (sc$GW_0$-BSE) gaps. These calculated QP band gaps, optical gaps and exciton binding energies are also listed in Table I. The convergence trend is obvious, particularly for the electronic band gap. However, due to the limitation of computation resource, sc$GW_0$ calculations with more dense $k$-point mesh are not performed here. Note that previous theoretical results showed a large value of exciton binding energy for monolayer MoS$_2$. For example, a value of 0.9 eV for monolayer MoS$_2$ (3.16 Å) was obtained using empirical Mott-Wannier theory [24]; and a value of 1.03 eV was obtained by $G_0W_0$-BSE calculations for monolayer MoS$_2$ (3.18 Å) using $6 \times 6 \times 1$ $k$-point mesh and including spin-orbital coupling [25], which is the same as our above results using the same $k$-point mesh without spin-orbital coupling.

Experimentally, two close peaks observed in adsorption spectrum of monolayer MoS$_2$ around 1.9 eV are due to the valence band splitting caused by spin-orbital coupling. In our calculations, the spin-orbital coupling is omitted unless otherwise stated and this will not alter our main conclusions presented in the current study. In or-
can be tuned by depositing monolayer MoS$_2$. Importantly, our results demonstrate that the optical gap of MoS$_2$ is very sensitive to tensile strain, which can be tuned by depositing monolayer MoS$_2$ on different substrates [13], whereas the exciton binding energy is insensitive to it according to our current results. This insensitivity is mainly because the hole and electron are derived from the topmost valence and lowest conduction edge states close to VBM and CBM that are significantly localized on Mo sites (contributed by Mo $d$ orbitals) irrespective of the magnitude of strain according to our DOS analysis.

We also notice that layer-layer distance or the length of vacuum zone implemented in the periodical supercell methods has important influence on the magnitude of the $G_0W_0$ band gap and the exciton binding energy [26, 27]. That is because the long-range van der Waals forces originating from the nonlocal electron-electron correlation is important in the layer TMDs. In order to obtain an accurate exciton binding energy, the convergence of k-point mesh, the truncation of Coulomb interaction [27], and the resulting accurate QP band structure ($G_0W_0$ or sc$GW$) are necessary. Compared to exciton binding energy of 1.1 eV obtained by interpolation of $G_0W_0$ band gap [25], our exciton binding energy obtained using denser k-point mesh is underestimated [28], due to the finite thickness of vacuum layer adopted in our periodical supercell calculations. However, the magnitude of the optical gap is not affected by the vacuum layer height according to our test (not shown here). An interesting observation is that the optical gap of monolayer MoS$_2$ is sensitive to the strain while the exciton binding energy is not. Our results also show that the spin-orbital coupling does not change the magnitude of exciton binding energy, while the optical gap reduces towards experimental results due to the band splitting at $K$ points and better consistency is achieved.

### Table I: QP band gap, optical band gap and exciton binding energy for monolayer MoS$_2$ and WS$_2$ are obtained by QP sc$GW_0$ and BSE with and without spin-orbital coupling (SOC) adopting different energy cutoffs and $k$-point mesh. All energies are in the unit of eV.

| Energy cutoffs | $k$-point mesh | E$_g$ | E$_g$(optical) | Binding energy |
|---------------|----------------|------|----------------|----------------|
| Monolayer MoS$_2$ (3.160 Å) | 400 and 200 | 6×6×1 (SOC) | 2.89 | 1.87 | 1.01 |
| | 6×6×1 | 2.99 | 1.96 | 1.03 |
| | 9×9×1 | 2.84 | 2.08 | 0.76 |
| | 12×12×1 | 2.78 | 2.16 | 0.62 |
| | 15×15×1 | 2.76 | 2.22 | 0.54 |
| | 600 and 300 | 12×12×1 | 2.80 | 2.17 | 0.63 |
| Monolayer MoS$_2$ (3.190 Å) | 600 and 300 | 12×12×1 | 2.66 | 2.04 | 0.62 |
| Monolayer WS$_2$ (3.155 Å) | 400 and 200 | 6×6×1 (SOC) | 3.02 | 1.97 | 1.05 |
| | 6×6×1 | 3.28 | 2.21 | 1.07 |
| | 9×9×1 | 3.12 | 2.34 | 0.78 |
| | 12×12×1 | 3.06 | 2.43 | 0.63 |
| | 15×15×1 | 3.05 | 2.51 | 0.54 |
| | 600 and 300 | 12×12×1 | 3.11 | 2.46 | 0.65 |
| Monolayer WS$_2$ (3.190 Å) | 600 and 300 | 12×12×1 | 2.92 | 2.28 | 0.64 |

For the evolution of exciton binding energy as a function of strain, our results demonstrate that it is almost unchanged, i.e., 0.63 eV (strainless), 0.62 eV (1% strain), 0.62 eV (3% strain), and 0.59 eV (6% strain) (using 600 and 300 eV for energy cutoffs and 12×12×1 $k$-point mesh). The direct optical gaps are 2.17, 2.04, 1.81, 1.52 eV for the four cases shown in Fig. 8, respectively, and also shown in Fig. using the orange left triangles. The experimental optical gap for monolayer MoS$_2$ was shown to be about 1.90 eV [13]. Since there was no mention of specific lattice parameter, here it is assumed to be the strainless case as shown in Fig. 8. Notice that the consistency is good between our theoretical and experimental results. If spin-orbital coupling is taken into account, the consistency will be improved further, since the first peak in the adsorption spectrum moves towards lower energy due to the top valence band splitting. Most importantly, our results demonstrate that the optical gap of monolayer MoS$_2$ is very sensitive to tensile strain, which can be tuned by depositing monolayer MoS$_2$ on different pseudopotentials [25]. Notice that the exciton binding energy obtained with and without spin-orbital coupling for monolayer MoS$_2$ as shown in Table I is nearly the same, while the optical gap in the former case shifts about 0.1 eV towards lower energy due to the top valence band splitting of 0.17 eV according to our sc$GW_0$ calculation.

**Note:** The table contains the QP band gap ($E_g$), optical band gap ($E_g$(optical)), and exciton binding energy for monolayer MoS$_2$ and WS$_2$ using different energy cutoffs and $k$-point meshes. The data is derived from GW and BSE calculations with spin-orbital coupling (SOC) using 600 and 300 eV for energy cutoffs and 12×9×1, 15×9×1, 600 and 300 12×12×1 6×6×1, 9×9×1, and 12×12×1 $k$-point meshes. The results demonstrate that the optical gap is sensitive to strain, while the exciton binding energy is insensitive. The theoretical and experimental results are compared, showing good consistency.

**Further Details:**
- The QP band gap ($E_g$) is the energy difference between the top of the valence band and the bottom of the conduction band.
- The optical band gap ($E_g$(optical)) is the energy difference between the top of the valence band and the first conduction band.
- The exciton binding energy is the energy required to remove an electron-hole pair.

**Implications:**
- The results highlight the importance of strain in modulating the electronic properties of monolayer TMDs.
- The insensitivity of the exciton binding energy to strain indicates that it may not be a suitable probe for strain sensing.
- The consistency between theoretical and experimental results suggests a promising approach for the study of TMDs.

**References:**
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The CBM at shows the topmost valence bands. Isosurface plots of from constructed in two groups. The first group was generated of solids [29]. The MLWFs shown in Fig. 6 were constructed in two groups. The first group was generated from d orbitals. The second group that MLWFs for the low-lying conduction bands were also generated from Mo d orbitals. Isosurface plots of the Mo d-orbitals in Fig. 6(a) show d-orbitals form covalent bonding with p(x) orbitals. The chemical bonding characters demonstrated by MLWFs are consistent well with our DOS analysis shown in Fig. 1.

C. Chemical bonding properties of monolayer MoS2

In order to gain further insight into the electronic structures under the tensile strain, we revisit the DOS shown in Fig. 1. For the strainless case, the VBM states at K mainly originate from Mo (dxy + dxz−yz) and S (px + py) orbitals not shown in Fig. 1. The CBM at K is mainly contributed by Mo dz2 and S (px + py). The Mo d and S p orbitals hybridize significantly, therefore Mo and S form covalent bond. MLWFs can also illustrate the chemical bonding properties of solids [30]. The MLWFs shown in Fig. 1 were constructed in two groups. The first group was generated from d guiding functions on Mo. The energy window contains the topmost valence bands. Isosurface plots of the Mo d-orbital MLWFs shown in Fig. 6(a) show dz2−yz orbitals form covalent bonding with px(py) orbitals. The chemical bonding characters demonstrated by MLWFs are consistent well with our DOS analysis shown in Fig. 1.

D. QP band structures and optical properties of strained monolayer WS2

The QP band structures of monolayer WS2 under tensile strain are also investigated, motivated by its better performance than monolayer MoS2 used as a channel in transistor devices [8]. The calculation results are illustrated in Fig. 7. Similar to monolayer MoS2, the scGW0 QP band structures of monolayer WS2 also undergo a direct to indirect band gap transition as tensile strain increases. The direct band gaps for the strainless (at the experimental lattice of 3.155 Å) and under 1% tensile strain cases are 3.11 and 2.92 eV, respectively, and the latter corresponds to the optimized lattice constant for monolayer WS2 from this work. The corresponding indirect band gaps under 3% and 6% tensile strains are 2.49 and 1.78 eV, respectively. Note that for the strainless case, our DFT result predicts monolayer WS2 to be an indirect band gap semiconductor with CBM only about 16 meV lower than the lowest conduction band at K points, which is contrary to recent full potential methods [7]. The difference may be originated from the technical aspect of these calculations, such as the employed pseudopotential method [9]. However, after the GW correction, a correct direct band gap is achieved.

For optical properties of monolayer WS2, our calculated QP band gaps, optical gaps and exciton binding energies are also listed in Table I. It is obvious that the monolayer WS2 presents many similar properties compared to monolayer MoS2, for example, the gaps and exciton binding energy also demonstrate a convergence trend as k-point mesh increases; the spin-orbital coupling has little influence on the magnitude of the exciton binding energy. Notice that our scGW0 calculation predicts the top valence band splitting of monolayer WS2 to be 0.44 eV, larger than that of monolayer MoS2 of 0.17 eV, because W is much heavier than Mo. The resulting first peak in BSE adsorption spectrum shifts 0.24 eV towards lower energy, also larger that that of monolayer MoS2 of 0.17 eV correspondingly. As for the strain effect, the BSE optical gap at our optimized lattice constant of 3.190 Å is 2.28 eV, while at 3.16 Å it is 2.46 eV, as shown in Table I. The former corresponding to 1% tensile strain, results in 0.18 eV reduction of band gaps. This demonstrates that the band gaps and optical gaps are also very sensitive to tensile strain, whereas the exciton binding energy is not. Based on above analysis, we predict the exciton binding energy of monolayer WS2 is similar to that of MoS2. Experimentally, the PL maximum of monolayer
WS$_2$ locates between 1.94 and 1.99 eV \cite{31}. Considering the large shift of the peak in the BSE adsorption spectrum caused by spin-orbital coupling, our results at optimized lattice of 3.190 Å are consistent well with above experimental result \cite{31}.

According to our above sc$GW_0$ and BSE calculations for monolayer MoS$_2$ and WS$_2$, it is clear that the self energy within the sc$GW_0$ calculations enlarges the band gap by accounting for the many body electron-electron interactions more accurately, while the strong excitonic effect results in a significant reduction of the band gap. Combining the two opposite effects on band gaps, the final resulting optical gap is consistent well with DFT band gaps. Therefore, the good band gap agreement between DFT and experiment is only a coincidence due to the fact that QP band gap correction is almost offset by exciton binding energy. This phenomenon was also observed in monolayer of hybridized graphene and hexagonal boron nitride, which also have strong excitonic effect \cite{23}.

We also perform the sc$GW_0$ QP band structures for monolayer MoS$_2$ and WS$_2$ under 1\% compressive strains. Our results show that the compressed MoS$_2$ has a direct band gap of 2.97 eV, while the compressed WS$_2$ has an indirect band gap of 3.13 eV and $K$ to $K$ direct gap of 3.30 eV.

Our sc$GW_0$ results show that both MoSe$_2$ and WSe$_2$ are also a direct semiconductor at the strainless state. The experimental lattice constants \cite{9} for MoSe$_2$ and WSe$_2$ are 3.299 and 3.286 Å and the optimized lattice constants are 3.327 and 3.326 Å, respectively; their direct $K$-$K$ band gaps are 2.40 and 2.68 eV at experimental lattices and 2.30 and 2.50 eV at the optimized lattices. Compared to the experimental lattice, the optimized lattice corresponds to 0.86\% (1.22\%) tensile strain for MoSe$_2$ (WSe$_2$), and the band gap also decreases with increasing tensile strain.

### E. Effective mass

Based on the more accurate sc$GW_0$ QP band structures, the effective mass of carriers for TMDs are calculated by fitting the bands to a parabola according to $E = \frac{k^2}{2m_m}$, where $m_e$ is the electron static mass. A $k$-point spacing smaller than 0.03 Å$^{-1}$ is used to keep parabolic effects. Electron and hole effective masses ($m^\ast$) at different strains are collected in Table \ref{table:effective_mass}. For MoS$_2$ under different strains, the CBM always locates in $K$ point, and the electron effective mass $m_e^\ast$ increases with increasing compressive strain while decreases with increasing tensile strain. As for hole, initially the effective mass also decreases as the tensile strain increases. After the direct to indirect gap transition, VBM shifts to $\Gamma$ with heavier hole, which also decreases as the tensile strain increases. Compared to the effective masses of 0.64 and 0.48 for hole and electron at $K$ point based on DFT calculation performed at the experimental lattice \cite{1} for MoS$_2$, the effective masses are reduced due to the $GW$ correction in our study.

It is noted that the carrier effective masses obtained by our sc$GW_0$ calculations do not include the spin-orbital coupling effect. Compared with those including spin-orbital effect for monolayer MoS$_2$ \cite{24}, it is found that the electron effective masses are in good agreement while the present hole effective mass is slightly smaller. This is mainly because the spin-orbital coupling alters the curvature of the topmost valence band close to VBM while the lowest conduction band close to CBM is not affected. The large difference between sc$GW$ (sc$GW_0$) and $G_0W_0$ result \cite{25} may be due to the poor $k$-points sampling and non-self-consistent (one-shot) GW calculations of the latter.

For WS$_2$, MoSe$_2$, and WSe$_2$, their masses also show similar behaviors. It is noted that at the same strain level, the electron effective mass of WS$_2$ is the lightest; and electron effective mass decreases as strain increases, making WS$_2$ more attractive for high performance electronic device applications since a lighter electron effective mass can lead to a higher mobility. Theoretical device simulations also demonstrated that as a channel material, the performance of WS$_2$ is superior to that of other TMDs \cite{4}.

### IV. SUMMARY

In summary, the QP band structures of monolayer MoS$_2$ and WS$_2$ at both strainless and strained states have been studied systematically. The sc$GW_0$ calculations are found to be reliable for such calculations. Using this approach, we find they share many similar behaviors. For the optical properties of monolayer MoS$_2$, exciton binding energy is found to be insensitive to the strain. Our calculated optical band gap is also consistent with experimental results. In addition, we find that the electron effective masses of monolayer MoS$_2$, WS$_2$, MoSe$_2$, and WSe$_2$ decrease as the tensile strain increases, and WS$_2$ possesses the lightest mass among the four monolayer materials at the same strain. Importantly, the present work highlights a possible avenue to tune the electronic properties of monolayer TMDs using strain engineering for potential applications in high performance electronic devices.

### V. ACKNOWLEDGMENTS

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TABLE II: Electron and hole effective masses ($m^*$) derived from partially scGW$_0$ QP band structures for monolayer MoS$_2$, WS$_2$, MoSe$_2$, and WSe$_2$ at different strains. The effective masses at $K$ and $\Gamma$ points are along $\Gamma K$ and $\Gamma M$ directions, respectively.

|        | Compressive (1%) | Experimental lattices | Optimized lattices | Tensile (3%) | Tensile (6%) |
|--------|------------------|-----------------------|--------------------|--------------|--------------|
| MoS$_2$ | $K_e$ 0.40        | 0.36 (0.35,0.60$^b$)  | 0.32               | 0.29         | 0.27         |
|        | $K_h$ 0.40        | 0.39 (0.44,0.54$^b$)  | 0.37               |              |              |
| WS$_2$ | $K_e$ 0.27        |                       | 0.24               | 0.22         | 0.20         |
|        | $K_h$ 0.32        |                       | 0.31               |              |              |
| MoSe$_2$ | $K_e$ 0.38       |                       | 0.36               |              |              |
|        | $K_h$ 0.44        |                       | 0.42               |              |              |
| WSe$_2$ | $K_e$ 0.29        |                       | 0.26               |              |              |
|        | $K_h$ 0.34        |                       | 0.33               |              |              |

$^a$Effective masses listed here are averages of the longitudinal and transverse values in Ref. [24].

$^b$Effective masses listed here are averages of the curvatures along the $\Gamma K$ and $\Gamma M$ directions in Ref. [27].

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