Stacking-tailoring quasiparticle energies and interlayer excitons in bilayer Janus MoSSe

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Keywords: exciton, radiative lifetime, MoSSe

Abstract
Stacking sequence of bilayer van der Waals transition metal dichalcogenides determines their electronic and related optical excitations. When the Janus monolayer structure has been taken to construct bilayer TMDs, it would introduce another degree of freedom, the out-of-plane intrinsic dipole moment, to tune the electronic and optical properties. Here we reveal that the electronic band structures and interlayer excitons can be dramatically tuned via the stacking sequence of the bilayer MoSSe with the different intrinsic dipole orientations. Moreover, the lowest energy interlayer excitons exhibit diverse spatial extensions, and the corresponding radiative lifetimes can be tailored within the range of $\sim 10^{-8}$ to $\sim 10^{-2}$ seconds at room temperature, by means of optimizing the dipole orientation and stacking sequence, and when the dipole moment keeps the same orientation for the constituent layer, it will slower the radiative recombination. Our findings shed a light on the applications of the interlayer excitons in Janus MoSSe on optoelectronics.

1. Introduction

Atomically thin transition metal dichalcogenides (TMDs) are essential members of the two-dimensional (2D) materials family, with potential applications in optoelectronic [1–4], photonic [2, 5–7] and valleytronic devices [8–11]. These applications are the performance of light-mater interactions in TMDs. In particular, due to the reduced dielectric screening, excitonic effects are significantly enhanced in monolayer 2D TMDs, with the exciton binding energies as high as several hundred meV [12–20]. The 2D TMDs with tightly bound excitons extend our studies to intriguing physics, such as exciton-polariton interactions [21, 22], linearly polarized photoluminescence [23], excitonic laser [24] and even exciton Hall effect [25, 26].

Whereas the light-mater interactions induced phenomena in monolayer 2D TMDs are quite appealing, the van der Waals (vdW) structures, stacking monolayer TMDs vertically into multilayer system, provide a unique platform to explore the exciton related properties [27–34]. Compared to the monolayer 2D TMDs, vdW structures are capable of realizing type-II band alignment via choosing monolayer constituent and stacking sequence [35–37]. With the type-II band alignment, vdW structures can form interlayer excitons (IX) where electrons and holes residing in distinct layers, accompanying with long radiative lifetime than intralayer excitons [29, 32, 38]. Long lifetime excitons can be potentially used to realize Bose–Einstein condensation [39] and excitonic superfluidity [40].

Recently, a Janus monolayer of TMDs, MoSSe, has been successfully synthesized which breaking the out-of-plane symmetry [41, 42]. Owing to the different electronegativity between S and Se atom, there exists a net out-of-plane electric dipole moment which is absent in symmetric MoS2 and MoSe2. MoSSe with intrinsic out-of-plane dipole moment has been shown large piezoelectricity [43], excellent water-splitting photocatalyst [44, 45] and extremely long carrier lifetime [46, 47]. Moreover, stacking the monolayer MoSSe into bilayer vdW structure, one should take into account the stacking sequence and the
dipole moment orientation simultaneously, and thus introduce an extra degree of freedom for constructing the Janus bilayer vdW structure.

In this work, we investigate the intrinsic dipole moment orientation- and stacking- dependent interlayer excitations in bilayer Janus MoSSe, which are not fully understood currently in symmetric homo- and hetero- bilayers of TMDs due to the missing of out-of-plane dipole moment. Different from homo- and hetero- bilayers of TMDs, bilayer Janus MoSSe can be stacked into eighteen configurations taking into account the dipole orientation and stacking sequence. We perform density functional theory (DFT) combining with GW and Bethe–Salpeter equation (BSE) to explore the interlayer excitons of nine stacking configurations, including spin–orbit coupling (SOC) in the various configurations with the binding energies, spatial distribution and radiative lifetime. Our findings reveal that the radiative lifetimes of interlayer excitons in bilayer Janus MoSSe can be tuned from tens of nanoseconds to tens of milliseconds at room temperature, which is crucial for precise control of the radiative lifetime of excitons for future MoSSe based optoelectronic devices. Furthermore, the stacking types here with out-of-plane dipole moment orientation shed a new light on tuning the interlayer excitons for bilayer Janus structures.

2. Methods

The ground state calculations are performed using the Quantum-ESPRESSO package [48, 49] with the Perdew–Burke–Ernzerhof (PBE) approximation, and we use fully relativistic norm-conserving pseudopotentials [50] including semicore electrons $s$ and $p$ of Mo to describe the SOC. The plane-wave energy cutoff is taken as 80 Ry. The vacuum thickness is set to 16 Å to mimic the isolated system. The vdW corrections are taken into account via PBE + D2 scheme [51]. Quasiparticle energies are computed by many-body perturbation theory through the one-shot GW0 approximation within plasmon-pole model [52]. 60 Ry and 15 Ry are used to calculate exchange and response function. 250 empty bands with an extrapolation correction method [53] are used to represent the converged quasiparticle energies. Then, the optical absorption spectra within direct transition are obtained through solving the BSE. 4 valence and 4 conduction bands are considered here since we are only interested in the low-energy excitons. Brillouin zone is sampled with $32 \times 32 \times 1$ $k$-point both in GW and BSE calculations by Yambo code [54, 55].

The radiative lifetime of exciton $S$ in 2D system at 0 K is computed by the Fermi’s golden rule written as

$$\tau_S(0) = \gamma_S(0)^{-1} = \frac{\hbar^2 c A}{8 \pi e^2 E_S(0) \mu_S},$$

where $\gamma$ is the recombination rate, $c$ is the speed of light, $A$ is the area of the unit cell, $E_S(0)$ is the excitation energy of exciton $S$, and $\mu_S$ is the exciton transition dipole from the BSE [23, 29, 56]. At finite temperature, the lifetime is [23, 29, 56]:

$$\langle \tau_S(T) \rangle = \gamma_S(0)^{-1} \times \frac{3}{4} \frac{2 M_S c^2 k_B T}{E_S(0)^2},$$

where $M_S$ is the exciton mass, and approximated as the sum of the electron and hole effective masses which deriving from the quasiparticle band structures in our calculations.

3. Results and discussion

3.1. Stacking configurations and band structures of bilayer Janus MoSSe

The stacking configurations of bilayer Janus MoSSe are shown in figure 1. Nine stacking configurations are considered here when taking into account the dipole orientation in Janus MoSSe, while they reduce to only three configurations when the mirror symmetry is kept in symmetric monolayers. The vertical stacking configurations represent the different out-of-plane dipole moment orientations of the monolayer constituent. Herein we classify the stacking into three types with type-1 keeping the same orientation of the dipole moment for both of the monolayer, and type-2 is the opposite orientation while type-3 is the back-facing orientation. We define the formation energy $\Delta E$ of the bilayer MoSSe as $\Delta E = E_{\text{bilayer}} - 2E_{\text{monolayer}}$, where $E_{\text{bilayer}}$ is the total energy of the bilayer configuration and $E_{\text{monolayer}}$ is the energy of the monolayer MoSSe. Obviously, the negative $\Delta E$ means the system are stable, agreeing well to the previous results with various vdW functionals [57]. The calculated $\Delta E$ of the nine configurations are listed in table 1. As can be seen, all the nine configurations are stable, and type-2 and type-3 are favorable stacking compared to type-1. We also calculate the interlayer distance and the formation energy of the nine configurations with vdW-DF2, showing the same results as PBE-D2 in which type-1 holds the higher formation energy than the other two stacking though all of them are stable. Generally, in each stacking type, the AA’ undergoes a 180° relative rotation of the constituent layers compared with the AA configuration.
Figure 1. Top and side views of nine stacking configurations of Janus bilayer MoSSe. 1, 2 and 3 represent the dipole moment orientation is same, opposite and back-facing, respectively. S/Se atoms are represented by yellow/green balls.

Table 1. The distance $d$ between the Mo atomic plane of bilayer MoSSe, formation energy $\Delta E$, potential drop $\Delta V$, band gap of PBE, $G_0W_0$, and the band gap at $K$ point.

| Stacking configurations | $d$ (Å) | $\Delta E$ (eV) | $\Delta V$ (eV) | $E^{\text{PBE}}_{\pm x}$ (eV) | $E^{\text{G0W0}}_{\pm x}$ (eV) | $E^{\text{G0W0}}_{\pm K}$ (eV) |
|-------------------------|---------|----------------|----------------|-------------------------------|-------------------------------|-------------------------------|
| 1-AA                    | 6.97    | −0.118         | 1.47           | 0.93                          | 1.82                          | 1.82                          |
| 1-AA'                   | 6.37    | −0.189         | 1.43           | 0.79                          | 1.61                          | 1.73                          |
| 1-AB                    | 6.37    | −0.183         | 1.48           | 0.75                          | 1.58                          | 1.65                          |
| 2-AA                    | 6.75    | −0.099         | 0              | 1.19                          | 2.14                          | 2.32                          |
| 2-AA'                   | 6.14    | −0.157         | 0              | 0.94                          | 1.83                          | 2.52                          |
| 2-AB                    | 6.10    | −0.160         | 0.065          | 0.87                          | 1.83                          | 2.12                          |
| 3-AA                    | 7.21    | −0.130         | 0              | 1.41                          | 2.19                          | 2.32                          |
| 3-AA'                   | 6.62    | −0.213         | 0              | 1.23                          | 2.02                          | 2.27                          |
| 3-AB                    | 6.63    | −0.207         | 0.042          | 1.25                          | 2.04                          | 2.11                          |

The total energy of the nine configurations are comparable with the largest energy difference about 0.016 eV between them. The distance $d$ of adjacent Mo atomic plane of the bilayers is listed in table 1, ranging from 6.10 to 7.21 Å. The distance $d$ is determined by the size and the electronegativity of atom S and Se in the adjacent layers, resulting in the largest and shortest $d$ in type-3 and type-1 stacking, respectively. For all the configurations, AA stacking holds the largest $d$ because of the S/Se atoms of the adjacent layers are over against each other.

On account of the different stacking sequences and the intrinsic out-of-plane dipole moments, the electrostatic potential drops $\Delta V$ in the nine configurations must be different. We calculate the electrostatic potentials of the nine configurations as shown in figure S1 (https://stacks.iop.org/NJP/23/013003/mmedia), and the results are listed in table 1. With the same dipole orientation in both layers of type-1 stacking, $\Delta V$ is as large as $\sim$1.5 eV. The large potential drop, introducing a strong net electric field along the $+z$ direction (from lower layer to upper layer here), would affect the electron-hole separation or combination processes [46, 47]. For AA and AA' configurations in type-2 and type-3, due to $D_{3h}$ and $D_{3d}$ symmetry with mirror and inversion symmetry respectively, the observed $\Delta V$ is zero and thus no net interface electric field. While the $\Delta V$ in 2-AB and 3-AB is as small as 0.065 eV and 0.042 eV respectively compared with 1-AB.

The spin-projected quasiparticle band structures including SOC of the nine stacking configurations are presented in figure 2 around $K$ point, and the whole band structures can be found in figure S2. The $G_0W_0$
band gap of all systems are various from 1.58 to 2.19 eV, while it is from 1.65 to 2.32 eV at K point. Overall, the type-1 configurations, i.e. the dipole moment along the same directions in the bilayer MoS\textsubscript{2}, possess the relative small band gaps among the three types, while the back-facing configurations type-3 hold the largest band gaps, as listed in table 1. The insets of figure 2 indicate the charge distributions of the top 4 valence (VB, VB-1, VB-2, VB-3) and bottom 4 (CB, CB + 1, CB + 2, CB + 3) conduction bands at K point. The zero energy is set to the top of the valence band. The spin-up (down) is denoted as the upward (downward) arrow. For 2-AA’ and 3-AA’, the energy bands of the two single monolayer MoS\textsubscript{2} are degenerate each other.

**Figure 2.** Spin-projected quasiparticle band structures of the nine bilayer MoS\textsubscript{2} around K point. The inset is the charge distributions of the top 4 valence (VB, VB-1, VB-2, VB-3) and bottom 4 (CB, CB + 1, CB + 2, CB + 3) conduction bands at K point. The zero energy is set to the top of the valence band. The spin-up (down) is denoted as the upward (downward) arrow. For 2-AA’ and 3-AA’, the energy bands of the two single monolayer MoS\textsubscript{2} are degenerate each other.

3.2. Type-1 stacking

Based on the quasiparticle energy band structures, here we firstly discuss the optical absorption properties including excitonic effects of the type-1 stacking configurations as shown in figure 3. The lowest-energy interlayer exciton is denoted as $I X_{0}$, which are all below the first strong absorption peak corresponding to
Figure 3. Optical absorption spectra of three type-1 configurations. $I_{X_0}$ is the lowest-energy interlayer exciton. The vertical red lines are the oscillator strength, and the dashed lines represent the energy gap at $K$ point.

Table 2. The positions, binding energy $E_b$ and lifetime $\tau$ (at 300 K) of the excitons. The calculated lifetime of a exciton in monolayer MoS$_2$ is 0.67 ps at 0 K, agrees well with the data in reference [29].

| Stacking configurations | $I_{X_0}$ (eV) | $E_b$ ($I_{X_0}$ (eV)) | $\tau$ ($I_{X_0}$ (s)) |
|-------------------------|----------------|------------------------|------------------------|
| 1-AA                    | 1.31           | 0.51                   | $1.1 \times 10^{-5}$   |
| 1-AA'                   | 1.29           | 0.44                   | $1.5 \times 10^{-2}$   |
| 1-AB                    | 1.21           | 0.44                   | $3.5 \times 10^{-5}$   |
| 2-AA                    | 1.84           | 0.62                   | $1.4 \times 10^{-7}$   |
| 2-AB                    | 1.83           | 0.69                   | $1.9 \times 10^{-7}$   |
| 2-AB'                   | 1.74           | 0.38                   | $1.2 \times 10^{-5}$   |
| 3-AA                    | 1.84           | 0.54                   | $4.8 \times 10^{-4}$   |
| 3-AA'                   | 1.77           | 0.50                   | $3.7 \times 10^{-4}$   |
| 3-AB                    | 1.87           | 0.24                   | $3.9 \times 10^{-4}$   |

The first bright intralayer exciton. For 1-AA stacking, $I_{X_0}$ is at 1.31 eV with the binding energy $E_b$ of 0.51 eV, originating from the transition between the VBM and the CBM at $K$ point. In case of 1-AA', $I_{X_0}$ locates at 1.29 eV with the lifetime as long as $1.5 \times 10^{-2}$ s. In case of 1-AB, $I_{X_0}$ is at 1.21 eV with a lifetime of $3.5 \times 10^{-6}$ s, which is shortest in all the type-1 stacking configurations here, as listed in table 2. We also find $I_{X_0}$ are doubly degenerate, originating from the spin–orbit splitting, mixed transitions between VBs and CBs, and energy degeneracy at $K$ and $-K$ points due to the time-reversal symmetry. For instance, all the $I_{X_0}$ of type-1 stacking attribute to the VBM to CBM transitions at $K$ and $-K$ points. These electronic transitions are also known as excitonic weights, as shown in figure S3, where the transitions at $K$ and $-K$ points dominate the components.

The radiative lifetime of exciton is strongly dependent on the distribution of exciton wave functions. Figure 4 shows the real-space wave function of the first interlayer exciton in type-1 stacking, where the hole/electron is fixed around the Mo atom. For 1-AA, electron wave function of the interlayer exciton $I_{X_0}$ is confined within the lower layer with the fixed hole in upper layer, as shown in lower panel of figure 4(a). When the electron is fixed in the lower layer, the hole wave function just extends over the upper layer. Consequently, the overlap of electron and hole wave functions is negligible, and the reduced overlap gives rise to the lifetime of $I_{X_0}$ in 1-AA as long as $1.1 \times 10^{-5}$ s at 300 K. In addition, 1-AA' and 1-AB exhibit the same interlayer charge distributions as 1-AA where the electron and hole is separately confined in distinct layers. However, the lifetime of $I_{X_0}$ in 1-AA' is as high as 15 ms, which is far longer than that in 1-AA and 1-AB. We find that the states participating in the transitions of $I_{X_0}$ in 1-AA' originate from a spin-flip transition $|V, U, \downarrow\rangle$ to $|C, L, \uparrow\rangle$, while in 1-AA and 1-AB, the formation of $I_{X_0}$ is a spin-conserving transition, and thus the radiative lifetime of $I_{X_0}$ in 1-AA' is longest in type-1. The finite lifetime of $I_{X_0}$ with spin-flip transition in 1-AA' probably arising from the strong SOC of MoSSe, which can mix a small amount of spin-allowed character into the spin-forbidden process.

3.3. Type-2 stacking
Absorption spectra of type-2 stacking configurations are shown in figure 5, where all $I_{X_0}s$ locate above the first strong absorption peak. The $I_{X_0}$ in 2-AA is at 1.84 eV and mixed the transitions of VB-1 to CB and VB to CB + 1 at K point. While in 2-AA' and 2-AB, transitions between VB and CB at K dominate the contributions to $I_{X_0}$. $I_{X_0}$ is four-fold degenerate in 2-AA, and for other two configurations, it is doubly degenerate. The excitonic weights can be found in figure S3 for $I_{X_0}$, in which the transitions at K and $-K$
Figure 4. Top and side views of exciton wave functions in type-1 stacking for lowest-energy interlayer exciton. The fixed hole and electron around Mo atom denoted as black dot and red square. In side views, the electron and the hole wave functions are shown for each configuration.

Figure 5. Optical absorption spectra of three type-2 configurations. $\text{IX}_0$ is the lowest-energy interlayer exciton. The vertical red lines are the oscillator strength, and the dashed lines represent the energy gap at $k$ point.

point dominate the components of $\text{IX}_0$. The binding energy of $\text{IX}_0$ for 2-AA $'$ is larger than that of others, which is the consequence of the strong overlap of electron and hole wave functions as shown in figure 6. The radiative lifetimes of type-2 are listed in table 2, where we can find the 2-AA configuration holds the shortest lifetime for $\text{IX}_0$. The exciton wave functions of $\text{IX}_0$ for type-2 configurations are depicted in figure 6. For 2-AA, the electron wave function spreads mainly over lower layer with the percentage of 97.6% for the hole fixed in upper layer, and around the hole there exists almost no electron distributions within the radius of 5 Å. For 2-AB, the hole and electron is perfectly localized in distinct layers. This causes a relative longer radiative lifetime of $\text{IX}_0$ in 2-AB than 2-AA. A striking exciton wave functions emerge in 2-AA $'$ as shown in figure 6(b), where the electron and hole wave functions exhibit strong overlap due to the inversion symmetry, yielding a mixed intra- and interlayer exciton. The mixed feature produces a large binding energy of $\text{IX}_0$ in 2-AA $'$. However, the spin character of the participated bands determines the
Figure 6. Top and side views of exciton wave functions in type-2 stacking for lowest-energy interlayer exciton. The fixed hole and electron around Mo atom denoted as black dot and red square. In side views, the electron and the hole wave functions are shown for each configuration.

Figure 7. Optical absorption spectra of three type-3 configurations. IX$_0$ is the lowest-energy interlayer exciton. The vertical red lines are the oscillator strength, and the dashed lines represent the energy gap at K point.

lifetime of the exciton. The same as in 1-AA', it is a transition of $|V, U, \downarrow\rangle$ to $|C, L, \uparrow\rangle$ for IX$_0$ in 2-AA', resulting in a dark exciton state. For 2-AB, electron and hole wave functions are completely confined in distinct layers, and thus the exciton lifetime is longer than in 2-AA.

3.4. Type-3 stacking

Finally we explore the optical properties of type-3 stacking configurations, as shown in figure 7, and all IX$_0$s are above the first intralayer exciton related absorption peak as in type-2. The IX$_0$ in 3-AA locating at 1.84 eV stems mainly from the mixed transitions of VB-1 to CB and VB to CB $+ 2$ at K point, both are spin-allowed as depicted in figure 2. In case of 3-AA' and 3-AB, the transitions between VB and CB at K point dominate the contribution to the IX$_0$. The excitonic weights of IX$_0$ are shown in figure S5. The binding energy of 3-AB are about half of the 3-AA and 3-AA', which is from the separate distribution of
exciton wave function as revealed in figure 8, and accompanying with the enhanced screening due to the reduced interlayer distance of 3-AB.

The exciton wave functions of \( \text{IX}_0 \) for 3-AA are shown in figure 8(a). When the hole is fixed in the lower layer, 92% of the electron wave functions are localized in the upper layer, giving rise to a mixed \( \text{IX}_0 \). The mixed character shortens the radiative lifetime of \( \text{IX}_0 \) to \( 4.8 \times 10^{-8} \) s for 3-AA. For \( \text{IX}_0 \) in 3-AA', it is a transition of \( \mid V, U, \downarrow > \) to \( \mid C, L, \uparrow > \) as in 2-AA', which is still a spin-forbidden process with a long exciton lifetime. The electron and hole wave functions of \( \text{IX}_0 \) are well separated in distinct layers in 3-AB, which supports the long lifetime of exciton. However, \( \text{IX}_0 \) in 3-AB is comparable with 3-AA and shorter than in 1-AB and 2-AB. We suppose the net electric field in these structures and wave functions distributions determine the exciton lifetime together. The net electric fields in type-1 stacking are much stronger than type-2 and type-3, and thus reduce the overlap of electron and hole wave functions effectively, causing the shorter exciton lifetimes overall.

4. Conclusions

In summary, we performed \textit{ab initio} many-body perturbation calculations to investigate the quasiparticle energies and the interlayer excitons of bilayer Janus MoSSe with BSE. Our results show that the electronic structures of bilayer MoSSe are strongly dependent on the stacking configurations. According to the intrinsic dipole orientation, we classify the bilayer structures into 3 types where the type-1 possess type-II band alignment. The quasiparticle band gaps can be tuned from 1.58 to 2.19 eV for the 9 configurations considered here, and the corresponding lowest energy interlayer excitons hold the diverse spatial extensions, and thus the exciton radiative lifetimes can be modulated from \( \sim 10^{-8} \) to \( \sim 10^{-2} \) s at room temperature. Our findings reveal that the intrinsic dipoles together with stacking sequence play an central role to tune the interlayer exciton lifetimes, making bilayer Janus MoSSe potential candidate for the optoelectronics.
Acknowledgments

The authors acknowledge funding from the National Natural Science Foundation of China (Grant Nos. 12064032, 11804173, 11547004, 11764031), and the Young Science and Technology Talents Training Program (NJYT-19-B02). The authors also thank the computational resources at the IMU.

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