Flat bands in twisted bilayer WSe₂ with strong spin-orbit interaction

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Abstract

We study the influence of strong spin-orbit interaction on the formation of flat bands in relaxed twisted bilayer WSe$_2$. Flat bands, well separated in energy, emerge at the band edges for twist angles ($\theta$) close to 0° and 60°. For $\theta$ close to 0°, the interlayer hybridization together with a moiré potential determines the electronic structure. The bands near the valence band edge have non-trivial topology, with Chern numbers equal to +1 or −1. We propose that this can be probed experimentally for twist angles less than a critical angle of 3.5°. For $\theta$ near 60°, the flattening of the bands arising from the K point of the unit cell Brillouin zone is a result of atomic rearrangements in the individual layers. Our findings on the flat bands and the localization of their wavefunctions for both ranges of $\theta$ match well with recent experimental observations [2, 17].

Twisted bilayer transition metal dichalcogenides (TMD) have recently gained attention as potential platforms for hosting correlated phases and novel excitonic properties [2–20]. The absence of a ‘magic angle’ in twisted TMDs [1, 22–24] makes the experimental realisation of flat bands [2, 17] easier compared to twisted bilayer graphene. Large spin-orbit coupling can strongly influence the electronic structure of the moiré superlattice (MSL), and can cause the bands to have non-trivial topological character. Within the TMD family, WSe$_2$ is a prototypical example with large spin-orbit coupling, making twisted WSe$_2$ bilayers (tWSe$_2$) especially interesting.

The valence band maxima (VBM) in the band structure of high-symmetry-stacked bilayers of WSe$_2$ are at the K point of the unit cell Brillouin zone (UBZ), unlike other TMDs with small spin-orbit coupling where they are at the Γ point. As a consequence, the flat bands near the valence band (VB) edge in the MSL of tWSe$_2$ arise from the bands near the K points of UBZs of the two layers. The spin character of the flat bands is further determined by spin-valley locking in WSe$_2$. Recent spectroscopic imaging and transport measurements in tWSe$_2$ show evidence of such flat bands [2, 17,25]. Most theoretical studies, to date, on tWSe$_2$ [26–30] have been based on continuum models [18, 19]. In this letter, we study flat bands in relaxed MSL of tWSe$_2$ using density functional theory (DFT).

We focus our study on twist angles, $\theta$, near 0°, ranging from 7.3° to 1.89°, and near 60°, ranging from 52.7° to 57.72°. We find several well-separated flat bands near the band edges for both $\theta$ close to 0° and 60°. The spin-orbit splitting of the monolayer bands is preserved in tWSe$_2$. Flat bands near the VB edge for $\theta$ close to 0° are topologically non-trivial. We
**FIG. 1.** (a) Band structure of 2.28° tWSe$_2$ along the path $\Gamma_M - M_M - K_M - \Gamma_M$ with the VBM set to zero. (b) Bands near the VB edge along the path $K_M - M_M - K'M$. The spin orientations of the first two bands, each doubly degenerate, are indicated by red and blue arrows. The pink dashed lines represent the band structure of the two separate, twisted, relaxed monolayers of the MSL. For ease of viewing, the VBM of the monolayers has been set to -4 meV. (c) Variation of $E_{Ww}$ (brown line) and $E_{12}$ (purple line) with $\theta$. (d) Variation of $S_{ij}$ with energy. The red and blue lines represent spin-up and spin-down, respectively.

also find flat bands arising from the $\Gamma$ point of the UBZ lie inside the VB continuum for all $\theta$. The spatial localization of these flat bands is in excellent agreement with recent scanning tunneling measurements [17] (STM).

We performed electronic structure calculations using the atomic-orbital basis as implemented in the SIESTA package [6]. The commensurate tWSe$_2$ structures are generated using the Twister code [1] and relaxed using classical force fields as implemented in LAMMPS [2, 3, 5] (for other details, see Supplemental material (SM) [37]). The relaxation patterns agree well with previous studies on other TMDs [16, 22, 38, 40]. MSLs with $\theta$ close to 0° consist of regions with three high symmetry stackings (HSS): AA (also known as 3-R), AB (also known as BW-Se), BA (also known as BSe-W), as well as Bridge (Br) regions (which are the transition regions from one HSS to another) (see SM [37]). MSLs with $\theta$ close to 60° also consist of three HSSs: AA', A'B and AB' (also known as 2-H, BSe-Se, and BW-W respectively), as well as the bridge (Br) regions.

Fig. 1 presents our results for the band structures of tWSe$_2$ for $\theta$ close to 0°. For these $\theta$, bands near the $K_M$ point of the moiré Brillouin zone (MBZ) (subscript M denotes k-points in MBZ) arise from the monolayer bands near the K and K' points of the UBZ of the two layers. As the monolayer VBM at the K and K' points have anti-parallel spins, the VBM at
the K\textsubscript{M} point is doubly degenerate with anti-parallel spins. Fig. 1(a) shows the bands for the 2.28° tWSe\textsubscript{2}. Two-fold degenerate bands with opposite spins are evident near the VB edge (V1, V2, V3). These first few VBs are shown along the path K\textsubscript{M} − M\textsubscript{M} − K’\textsubscript{M} in Fig. 1(b). There is always a gap between V1 and V2, even at the M\textsubscript{M} point, due to the inter-layer hybridization (Fig. 1(b)); this is clear from the fact that the bands for the relaxed-MSL monolayer (i.e., without inter-layer interaction but the structural relaxation effects of the MSL included) along the same path (pink dashed line in Fig. 1(b)) show a band crossing at M\textsubscript{M}.

To study the topological aspects of the band-structure, we have calculated the Chern number (C\textsubscript{n}) for the first few bands near the VB edge. When \( \theta \) is <3.9°, C\textsubscript{n} is +1, −1, −1 respectively, for the V1, V2 and V3 same spin (say spin-down) bands. For larger \( \theta \) (3.9° to 7.3°), C\textsubscript{n} is +1 and −1 for V1 and V2 respectively. We only report C\textsubscript{n} for isolated bands. The bands with the opposite spin (spin-up) have C\textsubscript{n}’s with opposite sign. The variation of the bandwidth of V1 (E\textsubscript{W}) and the energy gap between V1 and V2 (E\textsubscript{12}) is shown in Fig. 1(c). While E\textsubscript{W} increases monotonically with \( \theta \), E\textsubscript{12} becomes negative at 3.5°. While non-zero C\textsubscript{n} is found for a large range of \( \theta \), the negative E\textsubscript{12} narrows the range of angles for observing quantum spin-hall insulating states in tWSe\textsubscript{2} [41, 42]. We compare our DFT results to continuum model [18]. While the model gives the Chern number of the first two bands correctly, it is unable to describe the DFT-calculated Chern number for the third band [37].

Fig. 1(a) also shows six split-off bands (C1) near the conduction band (CB) edge. These bands are degenerate at Γ\textsubscript{M} with three spin-up and other three spin-down. The Q point of the UBZ gives rise to the bands near conduction band minima (CBM) in the MBZ. The bands near the CBM at alternate Q points of the UBZ have anti-parallel spins. This determines the spin-character of C1 as well as of the next set of bands near the CBM in the MBZ, which are also 6-fold degenerate at Γ\textsubscript{M}.

In order to find the intrinsic spin-orbit split in MSL, we calculate the matrix element of the spin-raising/lowering operator: \( S_{ij} = \langle \psi_i^{K_M} | S^\pm | \psi_j^{K_M} \rangle \) where \( \psi_i^{K_M}, \psi_j^{K_M} \) are two wave functions at K\textsubscript{M} point of MBZ respectively and \( S^\pm (= S_x \pm iS_y) \) is spin raising/lowering operator. We calculate the \( S_{ij} \) for \( i = \text{VBM} \) at K\textsubscript{M} point and \( j \) are the states within the energy range 0–500 meV below \( i \)th state. We calculate \( S_{ij} \) for the two highest energy states with spin-up and down at K\textsubscript{M} point and find states 436 meV below the VBM for which \( S_{ij} \).
FIG. 2. (a), (b), and (c) ((d), (e), and (f)) The distribution of $|\psi_G M(r)|^2 (|\psi_K M(r)|^2)$ averaged along the out-of-plane ($z$) direction for V1, V2 and C1 bands for $\theta = 2.28^\circ$ tWSe$_2$. (g) Moiré potential (in eV) of the relaxed-MSL monolayer. (h) LDOS of the first flat band arising from the $\Gamma$ point of UBZ. (i) LDOS of the VB edge states arising from the K point of UBZ. The HSS regions are as marked in panel (a).

is large (Fig. 1(d)). This implies that the atomic spin-orbit remains unchanged in MSLs.

Next, we discuss the localization of the wavefunctions of the bands mentioned above. As the bands at the VB edge have a dispersion, even if small, their localization varies with the $k$-points in the MBZ. Fig. 2(a) and (b) depict the localization of the wavefunctions corresponding to V1 and V2 respectively at the $\Gamma_M$ point; and Fig. 2(d) and (e) show the same at $K_M$ for one of the spin (say spin-down). At $\Gamma_M$, the V1 wavefunction shows a hexagonal pattern avoiding AA stacking and is located in both layers, while the V2 wavefunction is localized on AA stacking. At $K_M$, the other spin (spin-up) of V1 localizes on AA and AB and the other spin of V2 localizes on BA. Figs. 2(c) and (f) depict the C1 wavefunctions at $\Gamma_M$ and $K_M$. C1 localizes on AB and BA stackings following the energy ordering of Q point in UBZ of HSSs.

A complimentary picture of the localization is provided by the coarse-grained “moiré potential” ($V_M$) of a relaxed MSL monolayer. The coarse-grained potential is obtained
by averaging the potential in a Voronoi cell centered at W atoms \((x_W, y_W)\) following Eqn. 1

\[
V_M(x_W, y_W) = \int_{\Omega_{or}(x_W, y_W)} V(x, y, z) \, d\mathbf{r} - \bar{V}
\]  

(1)

\(V(x, y, z)\) is the local potential obtained from the DFT calculation and \(\bar{V}\) is the mean. Fig. 2(g) shows the “moiré potential”. The variation of the potential is driven by the strain and relaxation patterns. The resulting \(V_M\) shows an alternate arrangement of maxima and minima in a hexagonal shape centred on the AA stackings. The other layer has a similar pattern with the positions of maxima and minima interchanged. The moiré potential along with the interlayer hybridization determines the electronic structure of the relaxed MSL of tWSe\(_2\) for \(\theta\) close to 0°.

STM on 3° tWSe\(_2\) show signatures of flat bands derived from the Γ point of UBZ and the local density of states (LDOS) corresponding to these bands [17]. We find flat bands arising from the Γ point of UBZ lie inside the VB continuum [37]. The LDOS associated with these Γ-derived states localizes strongly on AB, BA and Br regions, forming a hexagonal pattern (Fig. 2(h)). This is in excellent agreement with the STM image of the Γ-derived flat band [17]. The LDOS of V1, which arises due to the K point of UBZ, is shown in Fig. 2(i). The LDOS is delocalized in the moiré unit cell and is consistent with the experimental findings [17].

![FIG. 3. (a): Band structure of 57.72° tWSe\(_2\). The VBM is set to zero. Inset: Bands near the VB edge along the K\(_M\) – M\(_M\) – K’\(_M\) path. The spin-characteristic of the first two bands are shown in red and blue colours. (b) and (c) Bands near the valence and CB edges in (a) for relaxed-MSL bilayer (black) and relaxed-MSL monolayer (pink dashed). The VBMs and CBMs are set to zero. (d) \(E_W\) and \(E_{12}\) vs the twist angle \(\theta\). (e) \(S_{ij}\) vs energy for spin-up (red) and spin-down (blue) states.](image-url)
We next discuss our findings for the electronic structure, and the wavefunctions of the relaxed MSLs obtained for $\theta$ close to 60°. Fig. 3(a) depicts the band structure for the 57.72° MSL. Several well-separated flat bands emerge at the VB edge (Fig. 3(b)). These bands are four-fold degenerate at the $\Gamma_M$ point of the MBZ, and split into two sets of two-fold degenerate bands at the $K_M$ point, with each set having parallel spins (inset of Fig. 3(a)) but anti-parallel to the other set. This is because the first set of bands at $K_M$ point of MBZ arise from the VBM at the K point of the UBZ of the two layers, which have the same spin. The second set of bands with the opposite spin at the $K_M$ point arise from the VBs at ($K' +$ reciprocal lattice vector of MSL) point of the UBZ of the two layers. To further understand this spin-character of the bands, we plot the bands along the path $K_M - M_M - K'$ in the MBZ (Fig. 3(a) inset). As can be seen from the inset, the two sets of bands cross each other at the $M_M$ point of the MBZ and have opposite ordering at $K'_M$ point. The variation of the energy gap ($E_W$) at the $K_M$ point between these two sets of bands with $\theta$ is shown in Fig. 3(d) (brown line). $E_W$ decreases with increasing MSL size. It should be noted that $E_W$ is not a spin-orbit split but arises due to band folding. The variation of the energy gap between V1 and V2 ($E_{12}$) is also shown in Fig. 3(d) (purple line), and it becomes negative at $\theta > 54.9°$. Bands at the VB edge for $\theta$ close to 60° are topologically trivial. Furthermore, flat bands at CB edge are nearly 12-fold degenerate (Fig. 3(c)) (two sets of 6-fold degenerate bands with $\sim 4$ meV separation) and originate from the doubly-degenerate bands with anti-parallel spins at the Q point of UBZ. In order to look for the atomic spin-orbit partner of the V1 state at $K_M$ point, we calculate $S_{ij}$ matrix elements as discussed before. We find large $S_{ij}$ for states $\sim 440$ meV below the corresponding states at VB edge (Fig. 3(e)).

Figs 4(a)–(c) show the localization of the wavefunction for the flat bands labelled V1, V2, V3 in Fig. 3(b) at the $\Gamma_M$ point of the MBZ. The wavefunctions corresponding to the CBM (C1 of Fig. 3(c)) at the $\Gamma_M$ point are shown in Fig. 4(g). We find that V1 localizes on the AA' stacking regions, whereas V2 and V3 localize on the A'B and AA' stacking regions respectively. This is qualitatively different from what happens in other twisted homobilayer TMDs [1]. C1 has a very small dispersion ($< 1$ meV) and localizes strongly on the AB' stacking regions.

Some insight into the various features of the above band structure can be obtained by noting that the local stacking at any given point of the tWSe$_2$ MSL with $\theta$ close to 60° preserves the inversion symmetry as seen in the HSSs: AA', AB' and A'B (see [37]). This
inversion, together with time-reversal symmetry, makes the effective interlayer interaction zero at the K point of the UBZ \cite{18}. It is also responsible for the trivial topology of the bands in this system. As the flat bands near the VB edge arise from the K point of UBZ, we study the electronic structure of the relaxed-MSL monolayer. The results are shown as pink dashed lines in Fig. 3(b) (VB edge) and Fig. 3(c) (CB edge). Clearly, there is a remarkable similarity between flat bands near the VB edge originating from the bilayer MSL and the relaxed MSL monolayer. The dispersion of these monolayer bands, as well as the separation between them, agree very well with the results of the relaxed-MSL bilayer. This implies that the flat bands near the VB edge originate primarily from the in-plane strains and not from the interlayer hybridization. The first three wavefunctions at the VB edge of the relaxed MSL monolayer are depicted in Fig. 4(d)–(f) and also look the same as those of the MSL bilayer. On the other hand, the flat bands at the CB edge are derived from the Q point of the UBZ. Although the interlayer hybridization is non-zero at the Q point, the bands near the CB edge of bilayer MSL and of the relaxed MSL monolayer agree very well. Furthermore, the CB edge wavefunction at the $\Gamma_M$ point of the relaxed monolayer localizes...
at the same stacking as that of the full MSL.

In order to further understand the wavefunction localization, we have computed the moiré potential ($V_M$) of the relaxed MSL monolayer (Fig. 4(h)). $V_M$ has maxima at the AA’ and A’B regions and minima at the AB’ regions, which is consistent with the holes localizing at AA’ and A’B and the electrons localizing at AB’. Hence, a relaxed MSL monolayer for $\theta$ close to 60° is sufficient to study the electronic properties of MSL if one is interested in the first few bands at the band edge.

The monolayer band states near the $\Gamma$ point of the UBZ also give rise to flat bands in the MBZ. The flat band at 129 meV below the VBM (marked as $V_\Gamma$ in Fig. 3(b)) has this origin. This band has a bandwidth $< 1$ meV, and its wavefunction localizes strongly on the AA’ regions, similar to the findings in twisted MoS$_2$ [1, 22]. The localization corresponds to the ordering of the VBs at the $\Gamma$ point in the UBZ of the different HSS bilayers [37]. This flat band originating from the $\Gamma$ point is two-fold degenerate and has charge density in the interlayer region, unlike the states arising from the K point of the UBZ. The LDOS corresponding to this state is shown in Fig. 4(i). STM studies on 57.5° tWSe$_2$ find $\Gamma$ derived bands localized on AA’ stacking [17]. Our findings on the nature and localization of the relevant flat band are in excellent agreement with the STM results.

In conclusion, we have extensively studied the formation of flat bands in tWSe$_2$ for $\theta$ close to 0° as well as 60°, and have investigated the localization of the wavefunctions of the flat bands. Our study includes the strong spin-orbit coupling present in this system, as well as the atomic rearrangements arising from the relaxation of the rigidly rotated bilayer system. We find topologically non-trivial bands for tWSe$_2$ close to 0° where interlayer hybridization together with the moiré potential determines the electronic structure. For $\theta$ close to 60°, the moiré potential of relaxed MSL monolayer can account for the electronic structure and the localization characteristics of the first few flat bands at band edges. Furthermore, we have identified another set of flat bands arising from the $\Gamma$ point of the UBZ. Our findings are in excellent agreement with recent STM experiments. This study provides a detailed understanding of the origin of flat bands for twisted TMD bilayers with strong spin-orbit interaction. The K-derived flat bands at the VB edge should prove especially valuable for investigating the spin-valley physics in twisted homo-bilayer TMD systems.

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Supplementary materials for flat bands in twisted bilayer WSe$_2$ with strong spin-orbit interaction

COMPUTATIONAL DETAILS AND METHODOLOGY:

We use Twister code to generate the twisted WSe$_2$ (tWSe$_2$) [1]. As the twist angle approaches 0° or 60°, the number of atoms in the system becomes very large (Table 1). Relaxing the twisted structure is important to obtain the correct electronic structure and localization. Owing to the large number of atoms, relaxation of these large systems using standard density functional theory (DFT) calculations is challenging. Here, we employ a multiscale approach to relax our systems and calculate the electronic structure of the relaxed systems as discussed below.

The unit cell lattice parameter of WSe$_2$ is 3.25Å in all our calculations. We relax our twisted structure using classical force fields. The structures are relaxed using LAMMPS package [2]. The intralayer potential is described by Stillinger-Weber potential [3] and the interlayer interaction is described by Kolmogorov-Crespi forcefield [4, 5] which is fitted to van der Waals corrected DFT calculations. The forces are minimized using the conjugate gradient method till the force on each atom becomes less than $10^{-8}$ eV/Å.

With the relaxed moiré structure, we perform DFT calculation to obtain the electronic structure. Our DFT calculations are performed using the atomic-orbital based code; SIESTA [6]. We use polarized-double-zeta basis set to expand the wavefunctions. We use norm-

| Twist angle(θ) | No. of atoms | Length (Å) |
|---------------|--------------|------------|
| 7.3°, 52.7°   | 366          | 25.39      |
| 5.1°, 54.9°   | 762          | 36.63      |
| 3.5°, 56.5°   | 1626         | 53.51      |
| 2.88°, 57.12° | 2382         | 64.77      |
| 2.65°, 57.35° | 2814         | 74.80      |
| 2.28°, 57.72° | 3786         | 81.66      |
| 1.89°, 58.11° | 5514         | 98.55      |
conserving pseudopotentials and the exchange-correlation is approximated with the local density approximation (LDA) [7]. As vdW functional in DFT only affects the relaxation of structure, we do not use vdW correction further in our electronic structure calculations. 10Å vacuum is added to restrict interaction between periodic images along the out-of-plane direction. We use $12 \times 12 \times 1$ Monkhorst-Pack k-point sampling [8] to converge the ground state charge density for the unit cell. For moiré cell, we accordingly scale the k-grid, and the large moiré cells are only sampled at $\Gamma_M$ point at their moiré Brillouin zone (MBZ). All calculations include spin-orbit interaction.

GW calculation on the unit cell is performed using BerkeleyGW package [9] with a $12 \times 12 \times 1$ Monkhorst-Pack k-grid. The mean-field wavefunctions for GW calculations are calculated using LDA. To calculate the interlayer separation for the unit cells, we used the DF-C09 [10] van der waals functional. The dielectric matrix is expanded in plane-wave basis with energy up to 15 Ry and extended to finite frequencies using the generalized plasmon pole model [11]. The Coulomb interaction is truncated to compute the dielectric matrix, and self-energy [12]. We use 1000 bands (without spin-orbit coupling) to construct the epsilon matrix and 1000 spinors for calculating the self-energy. We use the static remainder technique [13] to accelerate the convergence of the self energy with respect to empty bands. While the number of bands is insufficient to obtain the absolute convergence of the band edges with respect to vaccuum, it is sufficient to calculate the relative position of the valence band maximum at $\Gamma$ point and K point in unit cell Brillouin zone. To check for convergence with respect to number of bands in epsilon, we have done calculations on AB stacking with 5000 bands (without spin-orbit) and 1000 spinors for the construction of the epsilon matrix. Our calculations show that 1000 bands in epsilon are sufficient to converge the relative energy difference. Table 2. shows our results on unit cells of different high symmetry stackings. In all stackings, the VBM at K point is higher in energy than the $\Gamma$ point.

Furthermore, we optimize AB stacking structure with generalized gradient approximation [14] and DF-C09 [10] van der waals functional. Even in this case, our GW calculations show that the VBM at K point is higher than the $\Gamma$ point by 191 meV.
TABLE II. The valence band energies at Γ and K point are reported. The first entry for each stacking is for the valence band, and the second one is for the next band. All energies are in eV. The structures are optimized with LDA, and the interlayer interaction is described by vdW-DFC09 (except the last row). The epsilon matrix for GW calculation is constructed with 1000 bands, and the quasiparticle energies are calculated using 1000 spinors for the first five rows. The sixth and seventh rows are calculated with 5000 bands and 1000 spinors in epsilon calculation. The epsilon matrix of the last row is again calculated with 1000 bands.

|        | DFT         | GW         |
|--------|-------------|------------|
|        | E_Γ | E_K | Δ(=E_K - E_Γ) | E_Γ | E_K | Δ(=E_K - E_Γ) |
| AA’ (2-H) | 1.96 | 2.06 | 0.10 | -0.12 | 0.0012 | 0.12 |
|         | 1.96 | 2.06 | 0.10 | -0.12 | -0.0005 | 0.12 |
| AB’ (BW-W) | 1.89 | 2.07 | 0.18 | -0.21 | 0.02 | 0.23 |
|         | 1.89 | 2.07 | 0.18 | -0.21 | 0.02 | 0.23 |
| A’B (BSe-Se) | 1.72 | 2.07 | 0.35 | -0.42 | 0.0052 | 0.42 |
|         | 1.72 | 2.07 | 0.35 | -0.42 | 0.0042 | 0.42 |
| AA (3-R) | 1.71 | 2.10 | 0.39 | -0.15 | 0.28 | 0.43 |
|         | 1.71 | 2.03 | 0.32 | -0.15 | 0.23 | 0.38 |
| AB (BW-Se) | 1.96 | 2.10 | 0.14 | -0.13 | 0.06 | 0.19 |
|         | 1.96 | 2.03 | 0.07 | -0.13 | -0.0058 | 0.13 |
| 5000 bands for constructing epsilon |
| AB (BW-Se) | 1.96 | 2.10 | 0.14 | -0.20 | -0.0027 | 0.20 |
|         | 1.96 | 2.03 | 0.07 | -0.20 | -0.07 | 0.13 |
| 1000 spinors for constructing epsilon |
| AB (BW-Se) | 1.96 | 2.10 | 0.14 | 0.21 | 0.41 | 0.20 |
|         | 1.96 | 2.03 | 0.07 | 0.21 | 0.34 | 0.13 |
| The structure is optimized with GGA and vdW-DFC09. 1000 bands are used to construct epsilon. |
| AB (BW-Se) | 0.96 | 1.08 | 0.12 | 0.0006 | 0.19 | 0.19 |
|         | 0.96 | 1.02 | 0.06 | 0.0006 | 0.12 | 0.12 |
Moiré superlattices (MSLs) in TMDC have different sets of high symmetry stackings (HSS) depending on whether $\theta$ is close to $0^\circ$ or $60^\circ$. For $\theta$ close to $0^\circ$, the MSL has three HSSs: AA (W on top of W and Se on top of Se), AB (Se on top of W and W on top of hollow at the centre of the hexagon) and BA (W on top of Se and Se on top of the hollow at the centre of the hexagon) (Fig. 5(a–b)). Staggered stacking AB and BA are of lower energy than the eclipsed stacking AA. In AA stacking, the Se atoms from both layers face each other, and due to steric hindrance, the interlayer separation (ILS) is maximum at 7.1 Å. In the moiré supercells, the ILS is minimum (6.5 Å) for AB and BA stackings. The ILS of any given stacking in WSe$_2$ is larger than that of MoS$_2$ because of the denser electron cloud in Se compared to S. In Fig. 6 (a–c), we show band structures of these high-symmetry structures. Additionally, we show the band structure of WSe$_2$ monolayer in Fig. 6(b) (red dashed line). The valence band maxima (VBM) and conduction band minima (CBM) of all these bilayer structures are located at K and Q points, respectively. The VBM at the K point and the next band have parallel spins (Fig. 6(a)), and there is a splitting of 30–50 meV between them depending on the stacking. The split due to spin-orbit coupling is 445 meV which is also present in monolayer (Fig. 6(b)). Spin-orbit splitting is also present at CBM at Q point. Additionally, there is interlayer splitting due to hybridization in the bilayers, which is absent in the monolayer [15]. In this regard, it is to be noted that the interlayer split at K point is very small as the bands at K point have very localized wavefunctions. On the other hand, the CBM wavefunctions at Q point and VBM wavefunctions at Γ point are more delocalized, leading to large interlayer splitting at these points.

The other set of MSL with $\theta$ close to $60^\circ$ contains AA’ (W on top of Se and Se on top of W), AB’ (W on top of W and Se on top of the centre of hexagon) and A’B (Se on top of Se and W on top of the centre of hexagon) HSS (Fig. 5 (c–d)). AA’ (also known as 2H stacking) is the most stable structure of bilayer WSe$_2$ and has an ILS of 6.5 Å. In A’B, Se atoms from both layers face each other leading to increased ILS of 7.1 Å due to electron-electron repulsion. A’B stacking has the highest energy among these three HSS. Fig. 6 (d–f) show band structures of AA’, AB’ and A’B, respectively. Due to the presence of inversion symmetry in these HSS, the VBM are two-fold degenerate at the K point and have anti-parallel spin (Fig. 6(d)). The CBMs at Q point are doubly degenerate.
FIG. 5. Relaxed MSL of tWSe₂ with θ (a) 2.28° and (c) 57.72°. The rectangular boxes show different high symmetry stackings present in these structures. (b) and (d) are side views of (a) and (c) respectively. W and Se atoms are shown in red and green colours respectively.

**STRUCTURAL ASPECTS**

We study the relaxed MSLs. As the eclipsed stacking (AA) region has higher energy compared to the staggered stacking regions (AB and BA, which are degenerate), upon relaxation, the AB, BA regions expand equally while the AA region shrinks, giving rise to a hexagonal pattern in MSL with twist angle (θ) close to 0°. The relaxation effect becomes more evident as θ approaches 0°. The relaxation pattern is depicted by the variation of ILS. We plot the ILS distribution in Fig. 7(a). The ILS varies between 6.5–7.1 Å. AB and BA have the minimum ILS. The relaxation process also induces local strain and corrugation in the MSL. As a result, the structure of MSL is determined by the competition between strain-energy cost and stacking-energy gain. Fig. 7(b) and (c) show the strain distribution in layer 1 (L1) and layer 2 (L2), respectively. We plot the strain for every W atom along the direction of its six nearest W neighbours. In both layers, the strains are zero at HSS but are localized in the domain walls. The strain distribution in each layer is conjugate to the other i.e. at a given point in MSL along a certain direction, if the strain is compressive in L1, it becomes tensile in L2.

The MSL with θ close to 60° has AA’, AB’ and A’B. The fact that AA’ has lower energy than AB’ manifests in reduced symmetry in relaxed MSL and gives rise to Reuleaux triangles in the moiré patterns. The area of higher energy stacking A’B reduces, and the area of AB’
FIG. 6. Band structure of (a) AA, (b) AB, (c) BA, (d) AA', (e) AB' and (f) A'B HSS. The inset in (a) and (d) show the spin configuration of top two bands at valence band edge at K point. The red dashed lines in (b) represents the band structure of monolayer.

is smaller than the area of AA’ region. The ILS varies between 6.5–7.1 Å. The relaxation pattern can be visualized by plotting the variation of ILS in MSL (Fig. 8(a)). We also plot the distribution of strain induced by relaxing the MSL in Fig. 8(b) and (c). We again find that the strains are localized on the domain walls and are zero at the HSS. It is to be noted that lattice reconstruction, where the lattice constant of the MSL changes, is not observed in the angle range of our interest [16].

COMPARISON WITH EXPERIMENTS

Scanning tunnelling measurements show flat bands coming from Γ point of the unit cell Brillouin zone (UBZ) for both kinds of MSL [17]. We show the local density of states (LDOS) plots corresponding to those states in the main text. To further compare with experimental
findings, we calculate the projected density of states (PDOS). We first consider a $3^\circ$ tWSe$_2$. We plot the PDOS of $3^\circ$ tWSe$_2$ in Fig. 9(a). Fig. 9(b) shows the zoomed view of PDOS near valence band (VB) edge. The first few states (up to 178 meV below the VBM of MSL) arise from K point of UBZ. It is evident from Fig. 9(b) that the first peak has a non-zero contribution from AA, AB, BA and Br (domain walls between AB and BA). Hence, the LDOS calculated in the energy range of the first band at the VB edge is delocalized in the whole MSL. The violet dashed line in Fig. 9(b) marks the first peak due to the band arising from Γ point of the UBZ. This band is primarily localized in AB, BA and Br region. The wavefunction at Γ point of UBZ consists of $d_{z^2}$ orbital of W atom and $p_z$ orbitals of Se atoms. We call these orbitals as Orb$_{z^2}$. The component along the out-of-plane direction of these orbitals makes the interlayer interaction stronger, and hence larger interlayer split is found at Γ point. On the other hand, $d_{x^2-y^2}$ and $d_{xy}$ of W atom and $p_x$, $p_y$ orbitals of Se
FIG. 9. Fig. (a) The PDOS contribution of AA, AB, Br and BA. (b) Enlarged view of PDOS near valence band edge. The violet dashed line marks the first peak due to $\Gamma$. (c)-(f) The contribution of $\text{Orb}_x$ (green line) and $\text{Orb}_{xy}$ (red line) to the PDOS of AB, AA, Br and BA respectively. $\text{Orb}_x$ consists of $d_{z^2}$ of W and $p_z$ orbital of Se while $\text{Orb}_{xy}$ represents $d_{x^2-y^2}$ and $d_{xy}$ of W atom and $p_x$, $p_y$ of Se atom.

atoms ($\text{Orb}_{xy}$) contribute to K point wavefunction of UBZ. We plot the contributions of $\text{Orb}_x$ (green line) and $\text{Orb}_{xy}$ (red line) to PDOS of AB and BA (Fig. 9(c) and (f)). The peak marked by violet dashed line has the main contribution from $\text{Orb}_x$ confirming the fact that this peak arises from $\Gamma$ point of UBZ. We also show the contribution of $\text{Orb}_x$ and $\text{Orb}_{xy}$ to PDOS of AA and Br region in Fig. 9(d) and (e), respectively.

We consider the 57.72° $t\text{WSe}_2$ to compare with the STM on 57.5° $t\text{WSe}_2$. We plot the PDOS in Fig. 10(a). Fig. 10(b) shows the enlarged view of PDOS near the VB edge. The peak marked by the violet dotted line in Fig. 10(b) arises from $\Gamma$ point of UBZ and has contribution from AA' stacked region, which implies that the $\Gamma$ derived flat band localizes on AA'. We plot the contributions of $\text{Orb}_x$ (green line) and $\text{Orb}_{xy}$ (red line) to PDOS of AA’, AB’, Br (bridge region between AA’ and AB’) and A’B in Fig. 10(c)–(f). The large contribution of $\text{Orb}_x$ to the peak marked by violet dashed line (Fig. 10(c)) shows the onset of $\Gamma$ derived state. Furthermore, this peak has a large value for AA’ stacking and negligible
FIG. 10. (a)(b) The PDOS (PDOS near VB edge) due to AA’, A’B, Br and AB’. The violet dashed line in (b) corresponds to the peak arising due to Γ point. (c) The contribution of Orb_{z} and Orb_{xy} to PDOS of AA’ to identify the Γ and K derived peaks. The green and red lines correspond to Γ, and K derived states, respectively. (d), (e) and (f) show the orbital resolved PDOS for A’B, Br and AB’.

contribution from other stackings.

MOIRÉ HAMILTONIAN

The electronic structure of the relaxed MSL can be fit to a continuum model [18] which can be used to go beyond one-particle physics in these systems. The moiré Hamiltonian at K valley for a particular spin state:

\[ H = \begin{pmatrix} \frac{-\hbar^2(k-\kappa_\pm)^2}{2m^*} + \Delta_+(\mathbf{r}) & \Delta_T(\mathbf{r}) \\ \Delta_T^\dagger(\mathbf{r}) & \frac{-\hbar^2(k-\kappa_\pm)^2}{2m^*} + \Delta_-(\mathbf{r}) \end{pmatrix} \]  

(2)

\( \kappa_\pm \) are located at MBZ corners and correspond to K_{M} and K’_{M} points. For \( \theta \) close to 0°, the layer dependent moiré potential (\( \Delta_\pm \)) is given by:

\[ \Delta_\pm(\mathbf{r}) = \sum_{j=1,3,5}^{2} 2V\cos(G_j . \mathbf{r} \pm \psi) \]  

(3)
FIG. 11. (a) and (b): Band structures of 3.5° and 2.28° tWSe₂ with no interlayer interaction (i.e. of relaxed MSL monolayer). The blue solid and black dashed lines show the model band structure and DFT result respectively. (c) and (d): Band structures of 5.1° and 2.28° MSLs. (e) and (f) ((g) and (h)): Localization of wavefunctions of V₁ and V₂ (marked in Fig. (d)) at Γₘ (Kₘ) point.

V represents the potential amplitude and ψ describes the spatial pattern. Gⱼ is the moiré reciprocal lattice vectors in the first shell and obtained by anti-clockwise rotation of the first vector G₁ by (j − 1)π/3. The interlayer tunneling (∆ₜ) is given by:

\[
\Delta_T(r) = w(1 + e^{-iG₂}.r + e^{-iG₃}.r)
\]

where \( w \) is the interlayer tunneling strength.

First, we fit the model with no interlayer interaction to the DFT results of the relaxed MSL monolayer. Fig. 11(a) and (b) (blue lines) show the band structures obtained by solving the model with \( w = 0 \) for 3.5° and 2.28°. Setting \( V = 21 \) meV and \( ψ = 94° \), the model band structures are in good agreement with DFT results. Fitting the model band structures including the interlayer interaction, we find \( w = 29 \) meV. The band structures with \((V, ψ, w) = (21 \) meV, 94°, 29 meV) for 5.1° and 2.28° are shown in Fig. 11(c) and (d). The Chern number for the first two bands are consistent with the DFT results. We plot the wavefunctions of the first two bands of 2.28° MSL (V₁ and V₂ in Fig. 11(d)) at Γₘ and Kₘ (Fig. 11(e)–(h)) and they are in good agreement with the DFT wavefunctions (Fig. 2 in the main manuscript). Hence, the model is able to describe the first two bands. A limitation of the model is that neither the Chern number nor the localization of the third band is correctly
FIG. 12. (a): Band structures of $57.72^\circ$ tWSe$_2$. Blue solid line shows the model band structure. (b)–(d): Localization of V1, V2 and V3 at $\Gamma_M$.

represented by it. It is to be noted that F. Wu et al. [18] gives a different set of parameters obtained from the unit cell. Although the parameters are very different, they also represent the first two bands correctly. The wide range of parameters can describe the same band structure because of the fact that the bands are mostly determined by kinetic energy. The intralayer and interlayer potential act as a perturbation to split and modulate the bands. The parameters given by H. Tang et al. [19] describes the MSL with $\theta > 2$ degree, but it is unable to predict the DFT-calculated Chern number for the first two bands for smaller $\theta$.

For $\theta$ close to $60^\circ$, the intralayer potential becomes:

$$\Delta(r) = \sum_{j=1,3,5} 2V \cos(G_j \cdot r + \psi)$$  \hspace{1cm} (5)

and the effective interlayer interaction is zero. Hence, fitting the model with DFT results for $57.72^\circ$ tWSe$_2$ (Fig. 12(a)), we find the parameters to be $(V, \psi, w) = (26 \text{ meV}, 0, 46^\circ)$. Furthermore, we plot the wavefunctions (Fig. 12(b)–(d)) and they are in excellent agreement with the DFT results.

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