Electrically tunable charge transfer and charge orders in twisted transition metal dichalcogenide bilayers

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Moiré superlattices of transition metal dichalcogenide (TMD) bilayers have been shown to host correlated electronic states, which arises from the interplay of emergent moiré potential and long-range Coulomb interactions. Here we theoretically investigate structural relaxation and single-particle electronic properties in moiré superlattices of transition metal dichalcogenide homobilayer and study the ground state charge orders in the effective honeycomb lattice of MX and XM region. From the large-scale density functional theory calculation and continuum model with layer degrees of freedom, we find that the out of plane gating field creates a tunable charge transfer gap and introduces a mass term in the Dirac spectrum. At the flat band limit, we observe a series of charge-ordered insulating states at various filling $n = 1/4, 1/3, 1/2, 2/3, 1$ with Monte Carlo simulations, and predict that gating field induces a phase transition between different electron crystals at fixed filling $n = 1/2, 2/3$. Our work demonstrates that transition metal dichalcogenide homobilayer provides a powerful platform for the investigation of tunable charge transfer insulator and charge orders.

In TMD bilayers, moiré bands are formed from parabolic bands of individual layers. In twisted TMD homobilayers, the moiré bandwidth can be made arbitrarily small by reducing the twist angle, which gives rise to strong correlation without fine tuning. Electrons or holes in these moiré bands are tightly localized in high-symmetry stacking regions, which can be well described by a simple effective tight binding model. This description offers a convenient starting point for investigating interaction-induced states at finite density. Despite the conceptual simplicity, a quantitative modeling of moiré interaction-induced states at finite density offers a convenient starting point for investigating symmetry stacking regions, which can be well described by continuum model approach and Monte Carlo simulations.

In this work, using the large scale density functional theory, continuum model approach and Monte Carlo simulation, we study the effect of structural relaxation and electric field on the moiré band structure in twisted TMD homobilayers and predict novel charge orders at fractional fillings in the strong-coupling regime. We focus on the moiré valence bands originating from the Γ pocket. Due to interlayer tunneling and lattice relaxation, these moiré bands are derived from localized orbitals in MX and XM stacking regions that form a honeycomb lattice. We find a pair of massless Dirac fermions at $K, K'$ points of the mini Brillouin zone (BZ), which is protected by the $D_3$ point group symmetry of the moiré superlattice. Applying an out-of-plane electric field breaks the sublattice symmetry of the honeycomb lattice and opens a tunable gap $\Delta$ at the Dirac point. We introduce a new continuum model for twisted TMD homobilayers, which captures the layer degrees of freedom and the electrically tunable gap.

We further use an extended Hubbard model on the honeycomb lattice and perform Monte Carlo simulations to study the insulating electron crystals in the flat band limit. We find a distinctive set of charge orders at filling $n = 1/4, 1/3, 1/2, 2/3, 1$ on the honeycomb lattice. Interestingly, the electron crystals at $n = 1/2$ and $2/3$ both break the rotational symmetry and differ from the proposed states in WSe$_2$/WS$_2$ heterobilayer. These symmetry breaking charge orders can be directly probed by the optical anisotropy experiments. Moreover, we predict that phase transitions between distinct charge-ordered states at the same filling can be induced by the electric field, which tunes the charge-transfer gap $\Delta$. Our work shows that twisted homobilayer MoS$_2$ provides an ideal platform for investigating electrically tunable charge transfer gap and charge orders.

In particular, $d_0 = 0, -(a_1 + a_2)/3, (a_1 + a_2)/3$, where $a_1, a_2$ is the primitive lattice vector for untwisted bilayers, correspond to three high-symmetry stacking configurations of untwisted TMD bilayers, which we refer to as MM, XM, MX. In MM (MX) stacking, the M atom on the top layer is locally aligned with the M (X) atom on the bottom layer, see Fig. 1. Likewise for XM. The
bilayer structure in these stacking configurations is invariant under three-fold rotation around the z axis.

In homobilayer TMD, the spin degenerate Γ pockets in the valence band arise from electron tunneling between the two layers. The $k \cdot p$ Hamiltonian takes the form:

$$\mathcal{H}(d_0) = \begin{pmatrix} \frac{\hbar^2 k^2}{2 m^*} + \epsilon_b(d_0) & \Delta_T(d_0) \\ \Delta_T^*(d_0) & -\frac{\hbar^2 k^2}{2 m^*} + \epsilon_t(d_0) \end{pmatrix}. \quad (1)$$

Here $m^* = 1.07 m_e$ is the effective mass for the valence band. $\Delta_T(d_0)$ is the interlayer tunneling amplitude which depends on the in-plane displacement between the two layers. In contrast to the complex tunneling amplitude for the $K$ pockets [13], here the time reversal symmetry at Γ pocket enforces $\Delta_T(d_0)$ to be real. The potential term $\epsilon_{t,b}(d_0)$ denotes the energy of the valence band maximum in the absence of tunneling, which arises from the unequal layer weight of the wavefunction at MX and XM stacking configuration.

We expand $\Delta_T(d_0)$ in Fourier components up to the second harmonic:

$$\Delta_T(d_0) = w_0 + 2w_1 \sum_{j=1}^{3} \cos(G_j \cdot d_0) + 2w_2 \sum_{j=1}^{3} \cos(2G_j \cdot d_0), \quad (2)$$

where $G_i (i = 1, 2, 3)$ is the three reciprocal lattice vector in monolayer TMD. Due to three-fold rotation symmetry, $\Delta_T$ is a local extreme for MM, MX and XM stackings, with $\Delta_T = w_0 + 6w_1 + 6w_2$ for $d_0 = 0$ (MM) and $w_0 - 3w_1 - 3w_2$ for $d_0 = (a_1 + a_2)/3$ (MX or XM). The zero momentum transfer tunneling term $w_0$ is responsible for the large bonding and antibonding energy splitting for all $d_0$, while $w_1, w_2$ capture the variation of the tunneling amplitude at different lateral displacements.

The interlayer tunneling strength depends significantly on the layer spacing $d$. From the DFT calculation, we find the equilibrium layer spacing of untwisted TMD bilayers in MM, MX and XM stacking: $d_{MM} = 6.63 \text{Å}$ and $d_{MX} = d_{XM} = 5.99 \text{Å}$. The 10% variation of layer spacing is comparable with that in bilayer graphene [14] and strongly impacts the energy splitting of Γ pockets.

By calculating the work function, we plot in Fig. [1] the band structure of MM and MX-stacked bilayers, with reference energy $E = 0$ chosen to be the absolute vacuum level. Using the relaxed layer spacings, we find the energy splitting in MX (or XM) stacking to be stronger than in $MM$, as a result of its smaller layer distance. From the different energy splitting at Fig. [2], we obtain the tunnelling parameter as $w_0 = 338 \text{meV}$, $w_1 + w_2 = -18 \text{meV}$. If the same layer spacing were used for both MX and MM bilayers, the opposite (and incorrect) conclusion about the energy splitting would be found, see Fig[1]. Thus lattice relaxation is crucial for obtaining the correct moiré band structure.

The structure of twisted TMD homobilayers can be described by a lateral shift $d_0$ that varies slowly in space: $d_0 = \theta \hat{x} \times \mathbf{r}$. We therefore construct the following continuum Hamiltonian for the moiré bands from Γ pocket two band $kp$ model:

$$\mathcal{H} = \begin{pmatrix} -\frac{\hbar^2 k^2}{2 m^*} + \epsilon_b(r) & \Delta_T(r) \\ \Delta_T^*(r) & -\frac{\hbar^2 k^2}{2 m^*} + \epsilon_t(r) \end{pmatrix}. \quad (3)$$

The position dependent tunneling term is obtained by replacing $d_0$ with $\theta \hat{x} \times \mathbf{r}$ in Eq.[2]:

$$\Delta_T(r) = w_0 + 2w_1 \sum_{j=1}^{3} \cos(G_j^m \cdot r) + 2w_2 \sum_{j=1}^{3} \cos(2G_j^m \cdot r) \quad (4)$$

Where $G_j^m = G_i \theta \times \hat{z} (i = 1, 2, 3)$ is the three reciprocal lattice vector in moiré superlattice. Likewise, the intralayer potential $\epsilon_{t,b}$ ($t,b$ stand for top and bottom layer, respectively) can be expressed as the first order Fourier expansion over moiré reciprocal lattice vector:

$$\epsilon_{t,b}(r) = 2V_0 \sum_{j=1,2,3} \cos(G_j^m \cdot r \pm \phi) \quad (5)$$

The sign of phase factor $\phi$ changes under layer exchange, enforced by $C_{2y}$ symmetry as shown in Fig. [2b]. The potential term is crucial for the later modelling with out of plane gating field.

We now compare the band structure from continuum model with the large scale density functional theory. The moiré superlattice is fully relaxed with van der Waals correction incorporated by the vdW-DF (optB86) function.
θ (XM) region, in Fig. 2b. At small twist angle, layer distance, \( d \) \[46\]. We plot the twist-angle dependent initioals \[45\] as implemented in the Vienna Ab initio Simulation Package\[46\]. We plot the twist-angle dependent layer distance, \( d_{far} \) at MM region, and \( d_{near} \) in MX (XM) region, in Fig. 2. At small twist angle \( \theta \approx 0 \), the two layers are corrugated, and the layer distance of MM, MX or XM stacking region approaches to that of the untwisted structure. The interlayer tunneling amplitude is maximum at MX and XM region, which are identical on-site potential.

We perform the large scale DFT simulation to calculate the band structures for various twist angles, shown in Fig. 3. We find that above a small moiré period \( L_m \sim 4.7 \) nm with twist angle \( \theta = 3.89^\circ \), the topmost moiré \( s \) bands are well separated from the remaining bands. Similar band structures are also found in large-scale DFT calculation with fully relaxed lattice structure for homobilayer MoS\(_2\)\[37, 38\] and WS\(_2\)\[39\]. Fitting the moiré band structure to continuum model, we obtain the parameters as \( w_0 = 338 \) meV, \( w_1 = -16 \) meV and \( w_2 = -2 \) meV, \( V_0 = 6 \) meV, \( \phi = 121^\circ \) at twist angle \( \theta = 2.876^\circ \). These values are consistent with the estimation from untwisted structures.

As shown in Fig. 3(a,c), the moiré bands exhibit Dirac points at \( K \) and \( K' \) points of the moiré Brillouin zone. These Dirac points are protected by the \( D_3 \) point group of twisted TMD homobilayer: the doublet at \( K \) or \( K' \) form a two-dimensional \( E \) representation. The bandwidth of Dirac bands changes monotonously from 250 meV to 10 meV when twist angle \( \theta \) ranges from \( 0^\circ \) to \( 2^\circ \) as shown in Fig. 3(a). This provides an ideal platform to study the tunable correlation physics of Dirac electrons at the filling of \( n = 2 \) holes per moiré unit cell.

In the case of twisted bilayer graphene \[47\], the low energy Dirac fermion is protected by the \( C_{2z} \) symmetry, which can not be broken by out of plane field. However, in MX and XM region of the twisted homobilayer MoS\(_2\), the wavefunctions have unequal layer weight as indicated from the untwisted calculation. Thus the out of plane gating field breaks the \( C_{2y} \) symmetry and gaps out the Dirac fermion. A simplified continuum model targeting at antibonding orbitals well captures the topmost moiré bands, but can not describe the band structure and charge distribution involving layer degrees of freedom.

We further calculate the band structure of the fully relaxed moiré superlattice of homobilayer MoS\(_2\) with the applied gating field. As shown in Fig. 3(b), an out of plane gating field 0.5 \( V/nm \) creates a 2.4 meV gap at \( K \) point, while the bandwidth of the first energy-separable moiré band is 12 meV. At \( K \) point of the band edge, the wavefunction of the first band is localized at MX region, while the second band at XM region. For small twist angle \( \theta = 2^\circ \) with wavelength \( L_m = 9.1 \) nm, the gating field \( E_d = 1V/nm \) induces a charge transfer gap \( \Delta \) up to 5 meV, even larger than the bandwidth for the topmost moiré band (see supplementary material). A larger field-induced \( \Delta \) can be achieved in twisted TMD homobilayers with reduced interlayer tunneling (which competes with the layer potential asymmetry). This can be realized by inserting an hBN layer in between the top and bottom TMD layers \[24\].

In the TMD superlattice, the local minimums of the periodic moiré potential can be viewed as the effective moiré atoms to host charge. Under the harmonic approximation, the size of Wannier orbital for the topmost moiré
band is given by $\xi = \sqrt{\frac{n}{m^* \omega}} = 2(\pi)^{-\frac{1}{2}} \sqrt{L_m(n^2 \epsilon_{L_m})^\frac{1}{2}}$ ($\epsilon_{L_m}$ is the moiré potential integrated to antibonding orbitals). In homobilayer system without lattice mismatch, the kinetic energy over nearest neighbor interaction strength is plotted in Fig. S2 up to $\Delta = \epsilon_{L_m} \approx 3.8$ meV can be reached by realistic gating field. We note the critical $\Delta_c$ can be further lowered by increasing moiré wavelength.

At filling factor $n = 2/3$, the charges form a zigzag stripe order with $6 \times 6$ periodicity breaking the $C_3$ rotation symmetry. This zigzag type charge configuration is energetically favored compared to a linear stripe at screening distances from $d = 1/2 L_m$ to $d = 10 L_m$. As $\Delta$ increases, the zigzag charge stripe transitions to the $\sqrt{3} \times \sqrt{3}$ crystal that occupies one sublattice sites only, as shown in Fig. 4. We find the critical charge transfer gap $\Delta_c = \Delta_c = \sqrt{V_2 - V_3 - \frac{3}{4} V_4 + \frac{1}{4} V_5 - \frac{1}{3} V_6} = 0.04 \epsilon_{L_m} \sim 1.3$ meV at $d = L_m = 9.1$ nm.

The transition between distinct electron crystals at the same filling is first order. This should lead to a kink in the sublattice/layer charge imbalance as a function of the gating field. This prediction, which is a main result of our work, can be tested in MoSe$_2$/hBN/MoSe$_2$ heterostructure [24], where the gating field induced charge transfer between the top and bottom layers has already been observed at relatively high temperature.

For $n = 1$, we find that even at $\Delta = 0$, the ground state is fully sublattice polarized, which spontaneously breaks the honeycomb lattice symmetry. For filling $n > 1$, charge-2e trimer can be the lowest energy excitations when tuning the charge transfer gap $\Delta$, providing a platform to design unconventional superconductivity [33].

For homobilayer WSe$_2$, the valence band maximum is located at $K$ with weak interlayer tunneling amplitude and intralayer potential both on the order of 10 meV. The complex tunneling term between two layers brings further complications for the theoretical and experimental investigation of the insulating states [26, 28, 43]. In the case of heterobilayer TMD such as WSe$_2$/WS$_2$, the existence of secondary moiré potential minima is proposed [35]. However, due to the large band offset between WSe$_2$ and WS$_2$, charges are localized at the WS$_2$ layer, which limits the tunability of potential difference between two moiré regions.

In conclusion, we present a combined study of lattice relaxation, single-particle electronic structure, and ground state charge orders on the twisted homobilayer MoS$_2$. Unlike the previous moiré charge transfer insulator in WSe$_2$/WS$_2$ heterobilayer, here out of plane gating field breaks $C_2$ symmetry and induces a controllable charge transfer gap. With Monte Carlo simulation, we predict additional stripe type charge orders at filling factor $n = 1/2$, we find an emerging rectangular lattice with $\sqrt{3} \times 2$ periodicity. This state breaks the three-fold rotation symmetry and can be viewed as the combination of the stripe states on both sublattices, each at 1/4 filling. This rectangular electron crystal is energetically favorable compared to the $2 \times 2$ crystal at all gate screening distance. In contrast, at large $\Delta$, the ground state becomes a simple stripe state on the triangular sublattice with lower on-site potential, as shown in Fig. 3.
filling $n = 1/2, 2/3$ in the emergent honeycomb lattice with $\Delta = 0$. When increasing $\Delta$, these electron crystals transit to fully sublattice polarized states. Our work demonstrates that the interplay between two moiré regions leads to the charge transfer insulator \cite{35, 49} and serves as a platform for creating novel correlated states, such as unconventional density wave, charge stripes \cite{34}, spin superfluid\cite{50} and superconductivity \cite{48}.

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