Massive Dirac fermions in moiré superlattices: a route toward correlated Chern insulators

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We demonstrate a generic mechanism to realize topological moiré minibands by considering a massive Dirac fermion moving in a moiré potential, which can be achieved in a heterobilayer of transition metal dichalcogenides. We take the MoTe2/WSe2 heterobilayer as an example and show that the topological phase can be driven by a vertical electric field due to the lattice corrugation. Thus a correlated Chern insulator can be stabilized by the Coulomb interaction that breaks the time-reversal symmetry spontaneously. Our work explains the recent experiment on the observation of Chern insulating state in the AB-stacked MoTe2/WSe2 and unveils a general strategy to design topological moiré materials.

Introduction.— Moiré superlattices (MSL) of van der Waals materials have evoked great interest due to their flat minibands and hence strong electronic correlation that enables novel quantum states, such as superconductivity and correlated insulator states [1–25], Mott insulator and generalized Wigner crystal states [26–34]. Furthermore, these minibands can be topologically nontrivial. Indeed, the topological moiré minibands have been identified in the twisted multilayer graphene [35–53], ABC-stacked-trilayer graphene/hBN heterostructure [54–56], and transition metal dichalcogenide (TMD) homobilayer [57]. The interplay between electronic correlation and nontrivial topology in MSL can stabilize exotic quantum states including unconventional superconductivity [58–76] and fractional Chern insulator [77–81].

TMD heterobilayers are one important class of MSL and are being considered platforms to simulate the Hubbard model. Their single-particle physics is modeled by holes with parabolic dispersion subject to a periodic moiré potential that yields topologically trivial moiré minibands [82, 83]. This theoretical framework can describe the experimentally observed Mott insulator and Wigner crystal in the WSe2/WS2 heterobilayer [26–30].

Strikingly, a recent experimental work reports the observation of correlated Chern insulator at half filling (ν = 1 hole per moiré unit cell) and quantum valley-spin Hall insulator at full filling (ν = 2 holes per moiré unit cell) in an AB-stacked MoTe2/WSe2 heterobilayer under a vertical electric field [84]. The topological phases are absent in its AA-stacked counterpart [85]. The experimental observations suggest valley-contrasting Chern bands in the AB-stacked heterobilayer that cannot be explained by the existing model [82, 83]. Several proposals have been put forward to account for the experiments by including interlayer tunneling [86] and pseudomagnetic field [87] in the AB-stacked MoTe2/WSe2 heterobilayer.

In this work, we reexamine the low-energy continuum model describing the TMD heterobilayer MSL by emphasizing the Dirac structure of low-energy bands in constituent layers. The low-energy physics in the TMD monolayer is described by massive Dirac fermions with opposite chirality at two distinct valleys [88]. In TMD heterobilayers, such as WSe2/WS2 and MoTe2/WSe2, the Dirac bands of two different layers are weakly coupled due to the large energy offset and lattice mismatch. When focusing on the conduction or valence band edge from one layer, the other layer provides a periodic modulation, and the whole system can be described by a massive Dirac fermion moving in a moiré potential. In previous studies, the massive Dirac structure is often neglected via dropping the conduction (remote) band, which is far away from the Fermi energy (of the order of 1eV) [82, 83]. Although this approximation provides an accurate description of the band dispersion, our study indicates that the Dirac nature plays a crucial role in the topology of the moiré minibands. In particular, we find that in the presence of a vertical electric field, the Berry curvature induced by Dirac remote bands opens up a topological phase, which is absent if remote bands are ignored. Moreover, the Coulomb interaction can stabilize a correlated Chern insulator by spontaneously breaking the time-reversal symmetry (TRS). Our work provides a natural explanation for the quantum anomalous Hall effect observed in a TMD heterobilayer under a vertical electric field [84].

Continuum model reexamined.—The standard continuum model describing the valence minibands in a TMD heterobilayer reads [82, 83]

$$H_0 = -\frac{k^2}{2m} + V(r), \quad V(r) = 2V_0 \sum_{j=1}^{3} \cos(g_j \cdot r + \phi),$$

(1)

where $k = -i\nabla$ is the momentum operator, $g_j = 4\pi/\sqrt{3a_M} \cos(2\pi j/3) $ denotes the moiré wave vector, and $\phi$ is the phase of the moiré potential. The MSL constant is $a_M = a/\sqrt{\delta + \theta^2}$ where $\delta = (a - d)/d'$ is the mismatch of lattice constants and $\theta$ is the twist angle. The continuum model has an emergent intravalley TRS, i.e., $\mathcal{K}H_0\mathcal{K}^{-1} = H_0$ that enforces antisymmetric Berry curvature $\Omega(k) = -\Omega(-k)$ and hence no Chern band. The corresponding time-reversal operator is defined as $\mathcal{T} = \mathcal{K}$ where $\mathcal{K}$ is the complex conjugate operator. The moiré potential couples Bloch states at the momenta differed by $\pm g_j$ that folds the energy bands into the mini Brillouin zone (MBZ) and leads to the moiré minibands.

To emphasize the Dirac structure of low-energy bands of the constituent layers, we propose a revised continuum model...
in which the massive Dirac fermion couples to the moiré potential
\[ H_t = h_{k,\tau} + V(r), \quad h_{k,\tau} = at ( \tau k_x \sigma_x + k_y \sigma_y) + \frac{\Delta}{2} \sigma_z, \]  
(2)
where \( t \) is the intralayer hopping energy, \( \Delta \) is the band gap, and \( \tau = \pm 1 \) is the index of the locked valley and spin degrees of freedom in TMD. \( \sigma_{x,y,z} \) are the Pauli matrices acting on the two basis orbitals \( \{|d,z\rangle, \frac{1}{\sqrt{2}}(|d,z\rangle + i\tau|d,-z\rangle)\) of the conduction and valence band, respectively [88]. \( H_t \) is invariant under the threefold rotation since \( \mathcal{E}_3 h_{k,\tau} \mathcal{E}_3^{-1} = h_{R\mathbf{R},k,\tau} \) and \( V(R\mathbf{R},r) = V(r) \) where \( \mathcal{E}_3 = \text{diag}(e^{-\frac{2\pi i}{3}}, 1) \) [89] and \( R_3 \) are the threefold rotation operator and matrix. Eq. (1) can be derived from Eq. (2) through the second order perturbation theory for \( \Delta \gg atk \) and \( V_0 \), and the effective mass \( m = \Delta/2a^2t^2 \). In contrast to Eq. (1), the intravalley TRS is broken in the revised continuum model as \( \mathcal{H} h_{k,\tau} \mathcal{F}^{-1} = h_{-k,-\tau} \) where the time-reversal operator reverses the valley index and momentum. As will be shown below, the Dirac nature of low-energy states in TMD makes it possible to achieve the valley-contrasting Chern bands, even though the Dirac band gap \( \Delta \sim 1 \) eV is much larger than the energy scale of the moiré miniband.

Topological phases.—Due to the \( \mathcal{C}_3 \) symmetry, the valley Chern number \( C_\tau \) of the top valence band can be determined by its \( \mathcal{C}_3 \) eigenvalues \( \eta_\tau(k) \) at the \( \mathcal{C}_3 \)-invariant points [90], i.e.,
\[ e^{\pm \frac{2\pi i}{3} C_\tau} = \eta_\tau(\gamma) \eta_\tau(\kappa) \eta_\tau(-\kappa), \]
(3)
where \( \gamma \) represents the MBZ center and \( \pm \kappa \) are the MBZ corners. It is easy to show \( \eta_\tau(\gamma) = 1 \), while \( \eta_\tau(\pm \kappa) \) can be evaluated to the leading order by the degenerate perturbation theory in which the coupling among three degenerate Bloch states at \( \pm \kappa \) are considered, as shown in Fig. 1(a). In the basis of the Bloch states of the valence band without a moiré potential, i.e., \( \{|u_{\pm \kappa},\tau\rangle, |u_{\pm \kappa},\tau\rangle, |u_{\pm \kappa},\tau\rangle\} \) with \( h_{k,\tau} |u_{\pm \kappa},\tau\rangle = -\sqrt{\Delta^2/4 + \pi^2k^2} |u_{\pm \kappa},\tau\rangle \), the matrix representation of the moiré potential operator is
\[ V_{\pm \kappa,\tau} = V^*_{\pm \kappa,\tau} = \begin{pmatrix} 0 & w(\pm \phi) & w(\pm \phi)^* \\ w(\pm \phi)^* & 0 & w(\pm \phi) \\ w(\pm \phi) & w(\pm \phi)^* & 0 \end{pmatrix}, \]
(4)
whose element
\[ w(\pm \phi) = (u_{\pm \kappa,\tau} | V | u_{\pm \kappa,\tau}^*) = V_0 e^{i(\pm \phi - \pi/3)} \left( \frac{1}{2} + \frac{i\sqrt{3}}{2\sqrt{1+s}} \right), \]
(5)
depends on the dimensionless \( s = 64\pi^2/\tau^2(\delta^2 + \theta^2)/9\Delta^2 \).

The eigenvalues of Eq. (4) are \( E_0 = 2Re(w) \) and \( E_{\pm 1} = -Re(w) \pm \sqrt{3}Im(w) \), and the corresponding eigenstates have the \( \mathcal{C}_3 \) eigenvalues \( \mathcal{C}_3 | E_j \rangle = e^{i\frac{2\pi j}{3}} | E_j \rangle \). In Fig. 1(b), the three eigenvalues are shown as a function of arg\( w \) and the top valence band at \( \pm \kappa \) changes among \( E_0 \) and \( E_{\pm 1} \) through the band crossing at arg\( w \) = \( \pm \pi/3 \) and \( \pi \) where the topological transition can occur. In this way, we can identify \( \eta_\tau(\pm \kappa) \) and hence the valley Chern number \( C_\tau \) according to Eq. (3). Moreover, the TRS guarantees \( \eta_\tau(\pm \kappa) = \eta_\tau(\mp \kappa)^* \) and \( C_+ = -C_- \). A global phase diagram in terms of \( \phi \) and \( s \) is constructed in Fig. 1(c). Three topological phases with \( C_+ = -1 \) and \( C_- = 1 \) emerge at \( \phi = \pm \pi/3 \) and \( \pi \), and then expand in a wider range of \( \phi \) as \( s \) increases from zero. The topological phase boundaries can be obtained analytically by demanding arg\( |w(\pm \phi)\rangle = \pm \pi/3 \) and \( \pi \) that yields the critical \( s \) as
\[ s_c = 3\cot^2(\phi - \alpha) - 1, \]
(6)
with \( \phi \in [-\pi/3 + \alpha, \pi/3 + \alpha] \) where \( \alpha = 0, \pm 2\pi/3 \).

Interestingly, \( s \) is proportional to the intrinsic Berry curvature \( \Omega_\tau(k) \approx 2a^2t^2/\Delta^2 \) (which is valid for \( \Delta \gg atk \) in the MBZ) of the Dirac model in Eq. (2) times the MBZ area \( A_\text{MBZ} = 8\pi^2(\delta^2 + \theta^2)/\sqrt{3}a^2 \). Namely, \( s \) measures the intrinsic Berry phase of the top valence band and the topological phase appears only when \( s > 0 \), as shown in Fig. 1(c). This also explains why the topological phase is absent when the Dirac nature of low-energy states in TMD is neglected, as described by Eq. (1).

To verify the topological phase, we take the MoTe\(_2\)/WSe\(_2\) heterobilayer as an example. MoTe\(_2\) and WSe\(_2\) have a valence band offset of about 200–300 meV and lattice mismatch \( \delta \sim 7\% \) [84, 85]. The top valence band is from MoTe\(_2\)
whose model parameters are $\Delta = 1.017$ eV, $a = 3.565$ Å, and $t = 0.709$ eV [91, 92]. By employing the plane wave expansion of the continuum model to the fifth shell, we obtain the topological phase diagram in terms of $\phi$ and $\theta$ in Fig. 1(d). Here the red dashed lines are the topological phase boundary predicted by Eq. (6) and are consistent with the numerical results. In Fig. 1(d), only the topological phase around $\phi = \pi/3$ is shown, and another two topological phases can be obtained by shifting $\phi$ by $\pm 2\pi/3$. For $\theta = 1^\circ$, $\phi = 59^\circ$, and $V_0 = 8$ meV, the top valence band displayed in Fig. 2(a) is topological with $C_+ = -1$. The red and blue lines are bands from the continuum models in Eqs. (1) and (2), respectively, and show good agreement with each other. Here we only show the valence bands from the +K valley, and those from the −K valley can be obtained by TRS. The corresponding Berry curvatures of the top valence band from the two different models are displayed in Figs. 2(b) and 2(c). The Berry curvature in Fig. 2(b) is antisymmetric due to the emergent intravalley TRS in Eq. (1), while that in Fig. 2(c) yields a Chern band with $C_+ = -1$. Deep inside the topological trivial phase, the Berry curvature derived from Eq. (1) could be a good approximation to that from Eq. (2) [93].

The moiré potential is inversion symmetric when $\phi = n\pi/3$ ($n$ is an integer). Especially for an odd $n$, the minima of the moiré potential for holes form a honeycomb lattice where the top two valence bands with opposite Chern numbers can be mapped to the Haldane model [93, 94]. By further including the time-reversal counterparts from the other valley and the Coulomb interaction, the system can simulate the Kane-Mele-Hubbard model [95]. The deviation of $\phi$ from $n\pi/3$ for an odd $n$ translates into a staggered potential in the Haldane model that can drive the topological transition, as shown in Fig. 1(c).

**Electric-field-driven topological transition.**—According to the first-principle calculation, the phase of the moiré potential in AA- and AB-stacked TMD heterobilayer is unlikely close to $\phi = \pm \pi/3$ or $\pi$ [82, 83, 86]. Here we show that $\phi$ actually can be tuned by a vertical electric field. We notice that the two stacking configurations have different lattice corrugations that have been identified in both the STM measurement [96, 97] and the first-principal calculation [86, 98]. The electric field couples to the lattice corrugation and modifies the moiré potential as

$$
H'_e = \hbar k_z + V(r) + e E_\perp z(r) = \hbar k_z + 2V_0' \sum_{j=1}^3 \cos \left( G_j \cdot r + \phi + \phi' + \beta \right),
$$

where $E_\perp$ is the vertical electric field and the topography of the corrugated layer is approximated by the lowest harmonics $z(r) \approx z_0 \sum_{j=1}^3 (G_j \cdot r + \phi')$. The role of electric field can be described by a modified moiré potential with $V_0' = \sqrt{V_0^2 + e^2 E_\perp^2 z_0^2/4 + V_0 e E_\perp z_0 \cos(\phi - \phi')}$, and $\tan \beta = 2V_0 - e E_\perp z_0 / 2V_0 + e E_\perp z_0$. As $E_\perp$ ramps up, the phase of the moiré potential in Eq. (7) changes continuously from $\phi$ to $\phi'$ when $eE_\perp z_0 \gg V_0$, which points to an electric-field-driven topological phase transition.

In AA-stacked TMD heterobilayer, $z(r)$ is maximal at $R_M^\text{AA}$ and minimal at $R_N^\text{AA}$ and $R_X^\text{AA}$ [96–98]. In AB-stacked TMD heterobilayer, $z(r)$ is maximal (minimal) at $R_N^\text{AB}$ ($R_M^\text{AB}$), while $H_{\perp}^0$ is in between [86, 97]. Here M and X refer to the metal and chalcogen, while R and H represent the AA- and AB-stacking. The super- and subscript denote atoms from the top and bottom layer are aligned locally [93]. The variation of $z(r)$ at different local stacking regions in experiments translates into $\phi' \sim 0$ and $-\pi/2$ for the AA- and AB-stacked heterobilayer, as shown in Figs. 3(a) and 3(b). $\phi$ of the...
moiré potential is usually determined by fitting the continuum model to the first-principal energy bands. It has been reported that $\phi \sim \pi/12$ for AB-stacked MoTe$_2$/WSe$_2$ [86] while $\phi$ for AA-stacked MoTe$_2$/WSe$_2$ is still unclear. Nevertheless, most AA-stacked TMD heterobilayers have a $\phi$ of $\pi/6 \sim \pi/4$ [83, 99] and it is natural to expect AA-stacked MoTe$_2$/WSe$_2$ has $\phi$ in the same range. Because there is a topological phase around $\phi \sim -\pi/3$, as shown in Fig. 1(c), the electric field can drive the topological transition in AB- but not in AA-stacked MoTe$_2$/WSe$_2$. The critical $E_\perp$ for the topological transition can be obtained from Eq. (6) by replacing $\phi$ with the phase of the modified moiré potential in Eq. (7). For $\theta = 0^\circ$, $V_0 = 4.3$ meV, and $z_0 = 0.024$ nm, the topological phase diagrams in terms of $\theta$ and $E_\perp$ are displayed in Figs. S3(c) and S3(d) for the AA- and AB-stacked MoTe$_2$/WSe$_2$, respectively. For the AA-stacked MoTe$_2$/WSe$_2$, no topological phase appears for $\phi$ around $\pi/6 \sim \pi/4$. For the AB-stacked MoTe$_2$/WSe$_2$ with $\phi \sim \pi/12$, a topological phase appears for $E_\perp$ within $0.66 \sim 0.73$ V/nm which is close to $0.68 \sim 0.70$ V/nm observed in the experiment [84].

**Correlated Chern insulator.**—To stabilize a Chern insulator, it is required to break the TRS, which can be achieved by the Coulomb interaction. We project the Coulomb interaction onto the moiré minibands as

$$H = \sum_{n,k,\tau} (E_{n,k,\tau} - \mu) c_{n,k,\tau}^\dagger c_{n,k,\tau} + \frac{1}{2A} \sum_q \rho(q) V_q \rho(-q),$$  

where $c_{n,k,\tau}$ is the annihilation operator of the eigenstate given by $H_1 \ket{\psi_{n,k,\tau}} = E_{n,k,\tau} \ket{\psi_{n,k,\tau}}$. $A$ is the area of the system, and $\mu$ is the chemical potential. $V_q = e^2 \tanh(qd_\perp)/2\varepsilon_0 q$ is the screened Coulomb interaction in a dual-gated setup whose gate distant is $d_\perp \sim 10$ nm [84]. Here $\varepsilon$ is the dielectric constant and $\varepsilon_0$ is the vacuum permittivity. The density operator

$$\rho(q) = \sum_{n,k} \sum_{\tau} A_{n',q}(k,k') c_{n,k,\tau} c_{n,k',\tau}$$

where the form factor $A_{n',q}(k,k') = \langle \psi_{n,k,\tau} | e^{iq\cdot\tau} | \psi_{n',k',\tau} \rangle$ encodes the correlation between states in different bands and at different momenta.

The interacting Hamiltonian Eq. (8) can be solved self-consistently by using the standard Hartree-Fock approximation [93]. To identify the correlated Chern insulator at $\nu = 1$ and quantum valley-spin Hall insulator at $\nu = 2$ in AB-stacked MoTe$_2$/WSe$_2$, we calculate the Hall conductance $G_H$ and spin Hall conductance $G_{SH}$ as a function of $\varepsilon$ under the electric field $E_\perp = 0.69$ V/nm at which the correlated Chern insulator was observed in the experiment [84]. At $\nu = 1$, the Hall conductance drops from $e^2/h$ to 0 at $\varepsilon \sim 21$, as shown in Fig. 4(a). When $\varepsilon < 21$, the system becomes a valley-polarized Chern insulator whose energy bands are shown in Fig. 4(b). Here the blue solid and red dashed bands are from the $\pm K$ valleys, respectively, and the top valence band from the K valley with $C_+ = -1$ is empty. The energy gap $\Delta_\varepsilon$ decreases with $\varepsilon$ and vanishes with $G_H$ at $\varepsilon_0$ above which the valley polarization disappears and the system becomes a normal metal. The energy gap for $\varepsilon = 8$ in Fig. 4(b) is $\Delta_\varepsilon = 2.71$ meV that agrees with the one observed in the experiment [84]. At $\nu = 2$, the spin Hall conductance jumps from 0 to $2e^2/h$ at $\varepsilon \sim 6$ above which the system becomes a quantum valley-spin Hall insulator, as shown in Figs. 4(c) and 4(d). In this case, the top valence bands from $\pm K$ valleys with opposite Chern numbers $C_+ = -C_- = -1$ are empty. The energy gap decreases with $\varepsilon$. The valley polarization only appears at strong interaction for $\varepsilon < 6$, and the top two valence bands from either K or -K valley are empty. Because the two bands from the same valley carry opposite Chern numbers, the system becomes a valley-polarized trivial insulator.

**Discussion and summary.**—We demonstrate a generic mechanism to realize topological moiré minibands by placing massive Dirac fermions in a moiré potential. The revised continuum model can serve as a paradigm to investigate the interplay between electric correlation and nontrivial topology in the moiré system. The broadened topological phases for large $s$ in Fig. 1(c) suggests that the nontrivial topology favors TMD heterobilayers with large twist angle and lattice mismatch whereas small band gap. The phase of the moiré potential also plays a vital role in determining the topological property and can be tuned by the vertical electric field.

A single Dirac cone in lattice model is not allowed when the TRS is present according to the Nielsen–Ninomiya theorem [100]. In MSL, it becomes possible to fold Dirac cones into the MBZ, and label them by the valley index. These Dirac cones with different valley indices are separated by a large momentum, and they do not hybridize at the single particle level in clean systems. With the Coulomb interaction, the
Dirac cone of one valley flavor is populated while that of the other valley remains empty, which results in the spontaneous breaking of TRS. Therefore, the TMD heterobilayer becomes an exciting platform to study the physics of a single massive Dirac cone, where topological bands can be realized. A similar situation for massless Dirac cone can be realized on the surface of 3D topological insulators [101, 102].

In summary, we highlight the importance of the Dirac nature of low-energy states in TMD constituent layers by explicitly demonstrating the existence of topological moiré minibands in TMD heterobilayer MSL. We take the AB-stacked MoTe$_2$/WSe$_2$ heterobilayer as an example and show that a correlated Chern insulator can be stabilized by the Coulomb interaction under a vertical electric field. Our theory provides a mechanism to the electric-field-driven Chern insulating state observed in the TMD heterobilayer and points a direction to design topological moiré materials.

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See Supplemental Materials for (i) local stacking configurations in AA- and AB-stacked TMD heterobilayer, (ii) comparison of the two continuum models in the trivial phase, (iii) Wannier orbitals of moiré minibands, and (iv) details of Hartree-Fock calculations.

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Supplemental Material: Massive Dirac fermions in moiré superlattices: a route toward correlated Chern insulators

AA- AND AB-STACKED TMD HETEROBILAYERS

The lattice structures of AA- and AB-stacked TMD heterobilayers are shown in Figs. S1(a) and S1(b), respectively. In the AA stacking (R stacking), the two layers have the same lattice orientation. There are three local stacking configurations $R^M_\text{M}$, $R^M_\text{X}$, and $R^M_\text{X}$ where the atoms from the top and bottom layers are nearly aligned in the out-of-plane direction, as shown in Fig. S1(a). Here M and X refer to the metal and chalcogen. In the AB stacking (H stacking), the bottom layer is rotated by $180^\circ$ with respect to the top layer and the local stacking configurations $H^M_\text{M}$, $H^M_\text{X}$, and $H^X_\text{X}$ with near interlayer alignment are shown in Fig. S1(b). In both cases, the atomic registry between the two different layers varies periodically due to the lattice mismatch and the three different local stacking configurations can be identified in each moiré unit cell.

COMPARISON OF THE TWO CONTINUUM MODELS IN THE TRIVIAL PHASE

In this section, we focus on the topologically trivial phase and compare the energy bands and Berry curvatures given by the two continuum models in Eqs. (1) and (2) of the main text. Here we set $\theta = 1^\circ$, $\phi = 40^\circ$, and $V_0 = 8$ meV away from the topological phase identified in Fig. 1(d) of the main text. The other model parameters are same as those specified in the main text. The top valence bands from the two different models exhibit excellent agreement with each other, as shown in Fig. S2(a). The corresponding Berry curvatures of the top valence bands from the two different models are shown in Figs. S2(b) and S2(c), respectively. The two Berry curvature profiles agree well with each other. Nevertheless, the Berry curvature profile in S2(b) is strictly antisymmetric, $\Omega(k) = -\Omega(-k)$, due to the exact intravalley TRS of the model in Eq. (1) in the main text, while the Berry curvature profile in S2(c) is approximately antisymmetric.

WANNIER ORBITALS OF MOIRÉ MINIBANDS

In this section, we compare the Wannier orbitals of the moiré minibands from the two different continuum models. In Fig S3, we extract the top two valence bands from Fig. 2(a) of the main text. The red dashed bands are from the continuum model in Eq. (1) and have zero valley Chern numbers, while the blue solid bands are from the continuum model in Eq. (2) and have valley Chern numbers $C_+ = \mp 1$.

For the trivial band given by the continuum model in Eq. (1), the Wannier orbital can be obtained from the Fourier transform of the Bloch wave as

$$W_{n,\tau}(\mathbf{r} - \mathbf{R}) = \frac{1}{\sqrt{N}} \sum_k e^{-i\mathbf{k} \cdot \mathbf{r}} \psi_{n,\mathbf{k},\tau}(r),$$  \hspace{1cm} (S1)

where $\mathbf{R}$ is the moiré superlattice vector and $N$ is number of moiré unit cells. In Fig. S3, we show the Wannier orbital of the top trivial band for $\mathbf{R} = 0$. Here we choose a gauge in which the Bloch wave is real at $H^M_\text{M}$ at the origin. The Wannier center at $H^M_\text{M}$ forms a triangular lattice, as shown in Fig. S4. Therefore, the Coulomb interaction in the trivial moiré miniband can simulate the Hubbard model on a triangular lattice.
FIG. S3. The top two valence bands extracted from Fig. 2(a) of the main text. The red dashed and blue solid bands are from the continuum models in Eq. (1) and (2) of the main text, respectively. The valley Chern numbers of the valence bands are marked in the figure.

FIG. S4. The Wannier orbital of the top valence band (red dashed line) in Fig. S3 whose valley Chern number is $C_+ = 0$. The Wannier center at $H_M^M$ is connected by the black triangular lattice.

On the other hand, the moiré minibands are topologically nontrivial according to the revised continuum model in Eq. (2), and Eq. (S1) is inapplicable to the case with Chern bands due to the Wannier obstruction. In this case, we need to consider the top two valence bands (blue solid lines) in Fig. S3 such that the total Chern number is zero. For the two-band system, the Wannier orbitals can be prepared as

$$W_{1, \tau}(r) = \frac{1}{\sqrt{2N}} \sum_k e^{-ikR} \left[ \psi_{1,k,\tau}(r) + \psi_{2,k,\tau}(r) \right],$$

$$W_{2, \tau}(r) = \frac{1}{\sqrt{2N}} \sum_k e^{-ikR} e^{i\theta_{1,k,\tau}} \left[ \psi_{1,k,\tau}(r) - \psi_{2,k,\tau}(r) \right],$$

(S2)

where $\psi_{1,k,\tau}(r)$ and $\psi_{2,k,\tau}(r)$ are the Bloch waves of the first and second valence band. For the Dirac model in Eq. (2), the Bloch wave is a two-component spinor, i.e., $\psi_{n,k,\tau} = (\psi_{n,k,\tau}^c, \psi_{n,k,\tau}^v)^T$. We fix a gauge such that $\psi_{1,k,\tau}(r)$ is real at $H_M^M$ at the origin. Then we perform another gauge transformation $e^{i\theta_{n,k,\tau}} \psi_{n,k,\tau}(r)$ such that $e^{i\theta_{n,k,\tau}} \psi_{n,k,\tau}(r)$ is real at $H_X^X$ at $r = (a_M/\sqrt{3}, 0)$. Note that $H_M^M$ and $H_X^X$ are the moiré potential minima for holes when $\phi \sim \pi/3$. For $R = 0$, the squared amplitudes of the two Wannier orbitals are shown in Figs. S5 (a) and S5(b). It is easy to show that the two Wannier orbitals are orthogonal. The Wannier centers at $H_M^M$ and $H_X^X$ form a honeycomb lattice and each Wannier center is surrounded by three peaks of wavefunction amplitude maxima. The peculiar three-peak structure of the Wannier orbitals is similar to that in twisted bilayer graphene [S1, S2]. The two moiré minibands with opposite Chern numbers together can realize the Haldane model as that proposed in TMD homobilayers [S3]. Further considering the time-reversal counterparts from two distinct valleys as well as the Coulomb interaction, the system can simulate the Kane-Mele-Hubbard model.

FIG. S5. (a) and (b) The Wannier orbitals for the top two valence bands (blue solid lines) in Fig. S3 whose valley Chern numbers are $C_+ = \mp 1$. The Wannier centers at $H_M^M$ in (a) and at $H_X^X$ in (b) correspond to the A and B sublattices of the white honeycomb lattice.
HARTREE-FOCK CALCULATIONS

Under the standard Hartree-Fock approximation, the mean-field Hamiltonian reads

\[ H_{MF} = \sum_{n,k,\tau} (E_{n,k,\tau} - \mu + V_{n,k,\tau}^H + V_{n,k,\tau}^F) c_{n,k,\tau}^\dagger c_{n,k,\tau}, \quad (S3) \]

where the Hatree and Fock terms are

\[ V_{n,k,\tau}^H = \sum_{n',k',q} \frac{V_q}{A} \Lambda_{n,n'}^{(\tau)}(k,k',q) \Lambda_{n',n}^{(\tau)}(k',k,-q) \langle c_{n',k',\tau}^\dagger c_{n',k',\tau} \rangle, \]

\[ V_{n,k,\tau}^F = -\sum_{n',k',q} \frac{V_q}{A} \Lambda_{n,n'}^{(\tau)}(k,k',q) \Lambda_{n',n}^{(\tau)}(k',k,-q) \langle c_{n',k',\tau}^\dagger c_{n',k',\tau} \rangle. \quad (S4) \]

The form factor \( \Lambda_{n,n'}^{(\tau)}(k,k',q) \) and the screened Coulomb potential \( V_q \) are defined in the main text. The mean-field Hamiltonian is solved self-consistently numerically. Because the bandwidth of the top valence band is larger than the gap to the next valence band, it is insufficient to consider only the top one. To guarantee the convergence of the top valence band, we retain the topmost six valence bands from each valley in the numerical calculations and solve the mean-field Hamiltonian self-consistently at zero temperature.

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