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RESEARCH ARTICLE

Moiré flat bands of twisted few-layer graphite

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Supporting Information

Campare—In the main text, we show the moiré bands of the A+ABA, BA+ABA and ABA+ABA in the Fig. 2. Note that there are two remaining configurations of tFL-graphite with $N = 3$, *i.e.*, AB+ABA and BAB+ABA as shown in Fig. S1. Their moiré bands are given in Fig. S2. The only difference between AB+ABA and BA+ABA is the relative orientation of the vdW layers, and their moiré band structures are slightly different. For example, for the AB+ABA [Fig. S2 (b)], two low energy bands (the blue line and the black line) are touching at Γ point, while there is an observable gap in BA+ABA [Fig. 2 (f) of the main text]. The moiré bands of ABA+ABA and BAB+ABA configurations are also slightly different at the γ point.

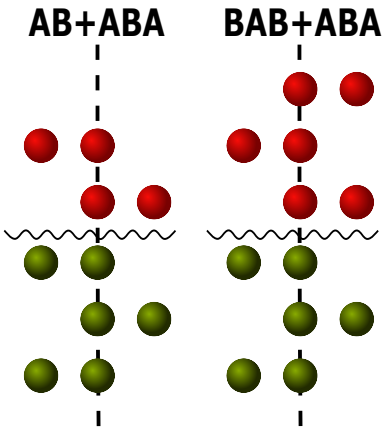

FIG. S1: Side view of tFL-graphite configurations: AB+ABA, BAB+ABA.

Unit of the DOS—In order to give an intuitive impression about the order of magnitude of the DOS in the tFL-graphite [see Fig. 2 of the main text], we replot the bands and DOS of A+ABA in Fig. S3, where the unit of DOS is given.

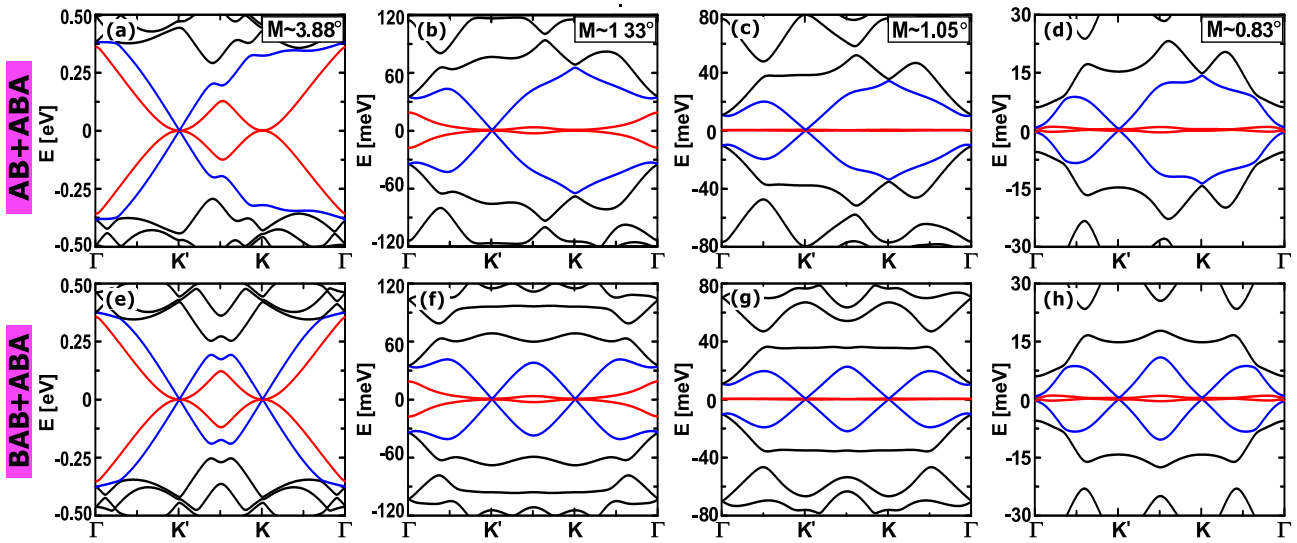

FIG. S2: (a-d) and (e-h) are the moiré bands of the AB+ABA and BAB+ABA, respectively. (a,e) are calculatedat $\theta = 3.88°$. (b,f) are calculated at $\theta = 1.33°$. (c,g) are calculated at $\theta = 1.05°$. (d,h) are calculated at $\theta = 0.83°$. Minimal model is used and the parameters are the same as Fig. 2 of the main text.

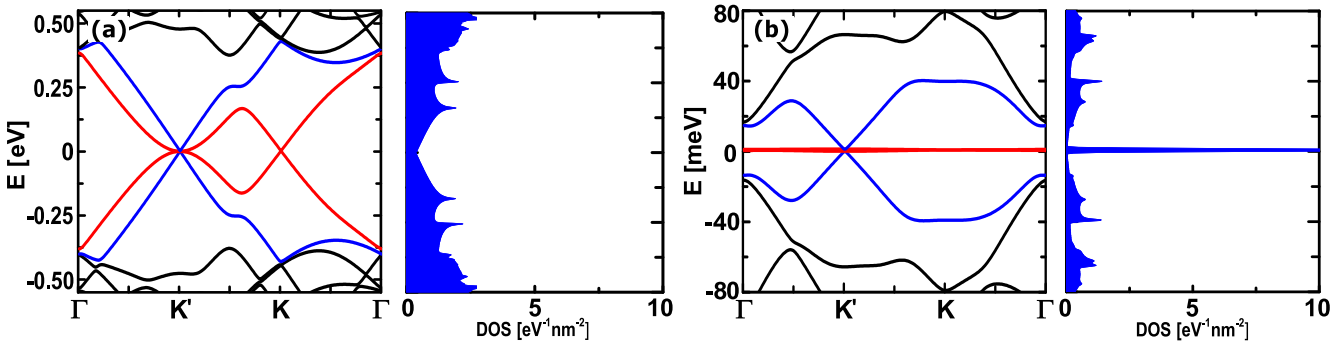

FIG. S3: (a) and (b) are the moiré band (and DOS) of the A+ABA at $\theta = 3.88°$ and $\theta = 1.05°$, respectively. Minimal model is used.

Moiré bands calculated with full parameters model—In Fig. 2 of the main text, the moiré bands are calculated with minimal model, where the influence of the remote hopping γ_3 and γ_4 are not considered. Here, we give some results based on full parameters model in Fig. S4, in order to illustrate the more realistic situations. Fig. S4 (a-b) are for A+ABA, (c-d) are for AB+ABA and (e-f) are for ABA+ABA. The first (second) row in Fig. S4 is at $\theta = 1.33°$ ($1.05°$). First of all, due to the remote hopping, the flat bands become dispersive but their bandwidth are still very small (red solid lines). Meanwhile, the two flat bands are separated in energy, *e.g.*, see Fig. S4 (c,d). Second, a twist angle dependent gap at the Dirac point of the linear bands is induced by γ_3 and γ_4 (blue solid lines). In Fig. S4, the dashed lines are the moiré bands with $\xi = 1$.

Tunable valley Chern number—In Fig. 3 of the main text, we show that, in ABA+ABA and BAB+ABA, a proper perpendicular electric field can give rise to four isolated nearly flat bands, which have nonzero valley Chern number. The valley Chern number is calculated by the standard formula $C_n = \int_{mBZ} d^2\boldsymbol{k}\Omega_n(\boldsymbol{k})/2\pi$, where n is the band index. The Berry connection is

$$\Omega_n(\vec{k}) = -2\sum_{n\neq n'} \mathrm{Im}[\frac{\langle u_n|\frac{\partial H}{\partial k_x}|u_{n'}\rangle\langle u_{n'}|\frac{\partial H}{\partial k_y}|u_n\rangle}{(E_{n'}-E_n)^2}], \tag{S1}$$

where $|u_n\rangle$ is the moiré superlattice Bloch state, and E_n is the corresponding eigenvalue.

Such topological flat bands can also be realized in AB+ABA and BA+ABA tFL-graphite, which is shown in Fig. S5. Fig. S5 (a) is the moiré bands of AB+ABA under an electric field $V = 20$ meV at $\theta = 1.33°$, where the valley Chern

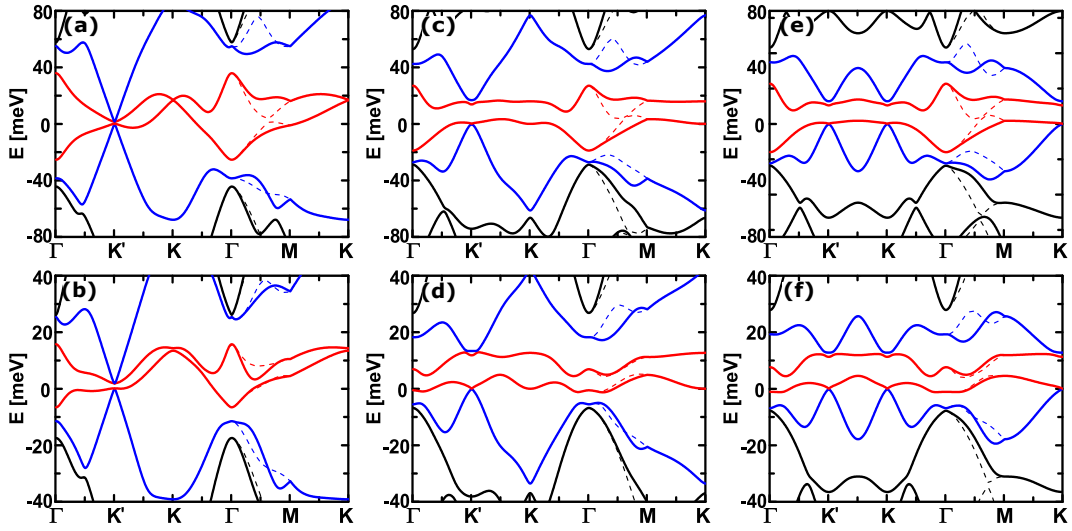

FIG. S4: Moiré bands calculated with full parameter model. (a-b) are for A+ABA, (c-d) are for AB+ABA and (e-f) are for ABA+ABA. (a), (c), (e) are calculated at $\theta = 1.33°$, and (b), (d), (f) are calculated at $\theta = 1.05°$. $\gamma_0/\gamma_1/\gamma_3/\gamma_4$ = 2610/360/283/138 meV.

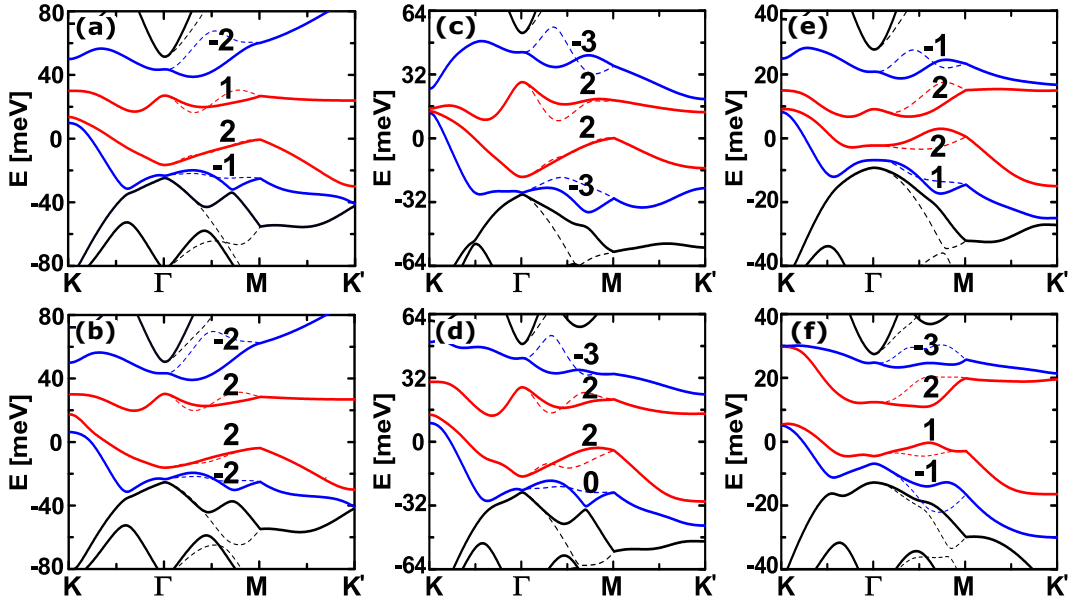

FIG. S5: Moiré bands and valley Chern number in the presence of perpendicular electric field. (a) AB+ABA with $V = 20$ meV and $\theta = 1.33°$. (b) BA+ABA with $V = 20$ meV and $\theta = 1.33°$. (c) ABA+ABA with $V = 10$ meV and $\theta = 1.33°$. (d) ABA+ABA with $V = 20$ meV and $\theta = 1.33°$. (e) ABA+ABA with $V = 10$ meV and $\theta = 1.05°$. (f) ABA+ABA with $V = 20$ meV and $\theta = 1.05°$. The full parameter model is used. Valley Chern numbers are denoted by black numbers and the dashed lines are the moiré bands with $\xi = 1$.

number of each band is denoted by the black number. That of BA+ABA is given in Fig. S5 (b) with $V = 20$ meV and $\theta = 1.33°$. We see that, though AB+ABA and BA+ABA have similar band structure, but their valley Chern number are different.

The valley Chern number depends on the twist angle and the perpendicular electric field. As an example, we calculate the moiré bands and the valley Chern number of ABA+ABA with various potential difference [V=10, 20 meV] and different twist angle [$\theta = 1.33°$, $1.05°$], see in Fig. S5 (c-f). Similar phenomenon has been reported in the twisted multilayer graphene with rhombohedral stacking, see Ref. [33-35, 40, 45] of the main text.

Note that in thicker tFL-graphite with $N > 3$, we can not get isolated moiré bands even if a perpendicular electric field is applied , and thus there is no well defined valley Chern number for a single moiré band.

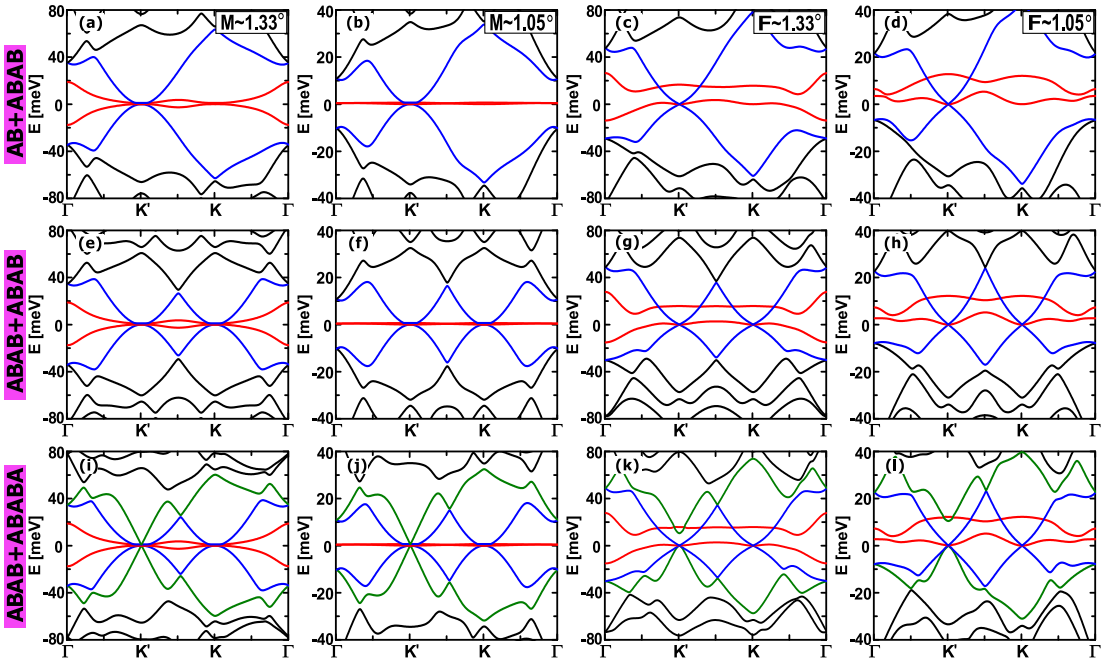

FIG. S6: (a-d), (e-h) and (i-l) are the moiré bands of the AB+ABAB, ABAB+ABAB and ABAB+ABABA, respectively. (a, e, i) are calculated with the minimal model at $\theta = 1.33°$; (b, f, j) are calculated with minimal model at $\theta = 1.05°$; (c, g, k) are calculated with full parameter model at $\theta = 1.33°$; (d, h, l) are calculated with full parameter model at $\theta = 1.05°$. The parameters are the same as the Fig. 4 of the main text.

Moiré bands of several related tFL-graphites—In the main text, we have studied the moiré bands of thicker tFL-graphites with $N > 3$. Several typical examples are given in Fig.4, *i.e.*, BA+ABAB, BABA+ABAB, BABA+ABABA. Note that there are several tFL-graphite configurations closely related to these examples, *i.e.*, AB+ABAB, ABAB+ABAB, ABAB+ABABA, where the only difference is the relative orientation of the vdW layers. For comparison, we plot the moiré bands of these related tFL-graphites in Fig. S6.

Electric field influence on the moiré bands—In Fig. 3 of the mian text, we show that a perpendicular electric field can significantly change the moiré bands in the cases of $N = 3$. Actually, a perpendicular electric field also can dramatically modify the moiré bands when $N > 3$. Two examples, *i.e.*, AB+ABAB, ABAB+ABAB, are given in Fig. S7. As a comparison, we first plot the moiré bands of AB+ABAB and ABAB+ABAB with zero electric field at $\theta = 1.05°$ in Fig. S7 (a) and (c), respectively (red lines). Then, an electric field with $V = 20$ meV is applied, and the corresponding moiré bands are given in Fig. S7 (b) and (d), see the blue lines. We see that the band shape, as well as the DOS, is significantly changed by the applied electric field.

Wave function of the flat band—As show in Fig. S8 below, we plot the wave functions of the flat band in A+ABA tFL-graphite. We can see that the wave functions mainly distribute on both sides of the twisted interface (twisted layers), and there is almost no distribution far away from the twisted layers.

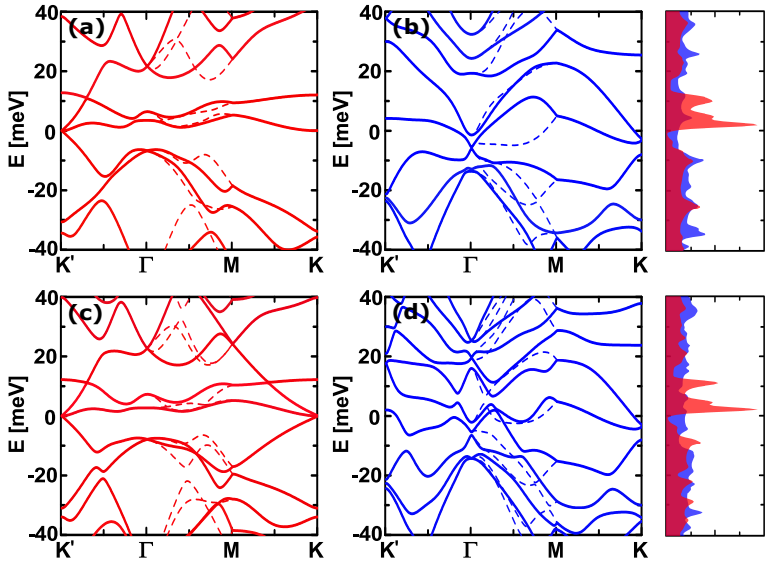

FIG. S7: (a) is the moiré bands of the AB+ABAB with zero electric field at $\theta = 1.05°$ (red), and (b) is that with $V = 20$ meV (blue). (c) is the moiré bands of the ABAB+ABAB with zero electric field at $\theta = 1.05°$ (red), and (b) is that with $V = 20$ meV (blue). The right column is the corresponding DOS, where red is for zero electric field and blue is for finite electric field. Full parameter model is used: $\gamma_0/\gamma_1/\gamma_3/\gamma_4 = 2610/360/283/138$ meV.

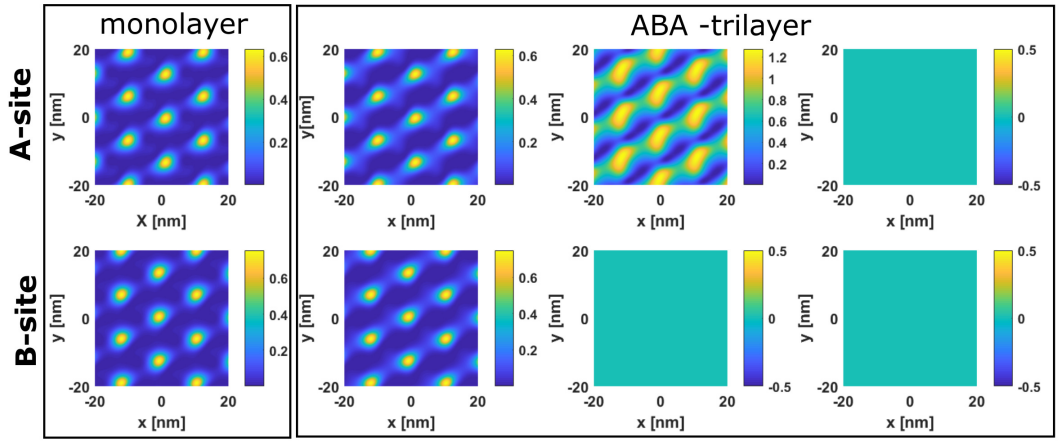

FIG. S8: The wave functions of the flat band in A+ABA tFL-graphite.