Emerging flat bands in large-angle twisted bi-layer graphene under pressures

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1. Definition of $\Delta q$.

There are 148 carbon atoms in the 9.4°-TBG model. We divide 148 carbon atoms into 26 groups, based on the P321 symmetry of the cell, as shown in Fig. S2, the symmetrical unique carbon atoms are drawn with same color. There are 6 carbon atoms in the first 24 groups, and 2 carbon atoms in the last 2 groups. Then the bader charge is calculated and averaged. The average value $A_i$ ($i=1,2,3,...,26$) of each group can be obtained. Thus, $\Delta q$ is defined as:

$$\Delta q = q_{\text{max}} - q_{\text{min}}$$

Where $q_{\text{max}}$ is the maximum value and $q_{\text{min}}$ is the minimum value among $A_i$.

Fig. S2 The schematic show of 26 groups of carbon atoms in 9.4°-TBG model, the carbon atoms in one group are drawn with same color.
Fig. S3 (a) and (b) are PCD of the bottom conduction band for 9.4°-TBG at pressures of 0 GPa and 75.52 GPa, respectively. The dashed line indicates the unit cell of 9.4°-TBG. The iso-surface value is $6 \times 10^{-4} \text{ e/Bohr}^3$.

Fig. S4 (a), (b), (c), (d) are band structures under different pressures for twist angle 9.4°.
Fig. S5 (a), (b), (c), (d) are band structures under different pressures for twist angle 13.2°.

Fig. S6 (a), (b), (c), (d) are band structures under different pressures for twist angle 21.8°.
Fig. S7 (a), (b), (c), (d) are band structures under different pressures for twist angle 27.8°.

Fig. S8 The relationship between IDOS and pressure with different twisting angles.