Electronic Supplementary Material (ESI) for Nanoscale.

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

Liangbing Ge[a], Kun Ni[ab*], Xiaojun Wu[a], Zhengping Fu[ac], Yalin Lu[ac], Yanwu Zhu[ab*]

[a]*Hefei National Research Center for Physical Sciences at the Microscale, & CAS Key Laboratory of Materials for Energy Conversion, & Department of Materials Science and Engineering, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China*

[b]*i-ChEM (Collaborative Innovation Center of Chemistry for Energy Materials), University of Science and Technology of China, Hefei, Anhui 230026, P. R. China*

[c]*Anhui Laboratory of Advanced Photon Science and Technology, University of Science and Technology of China, Hefei 230026, P. R. China*

Email: nikun@ustc.edu.cn; zhuyanwu@ustc.edu.cn

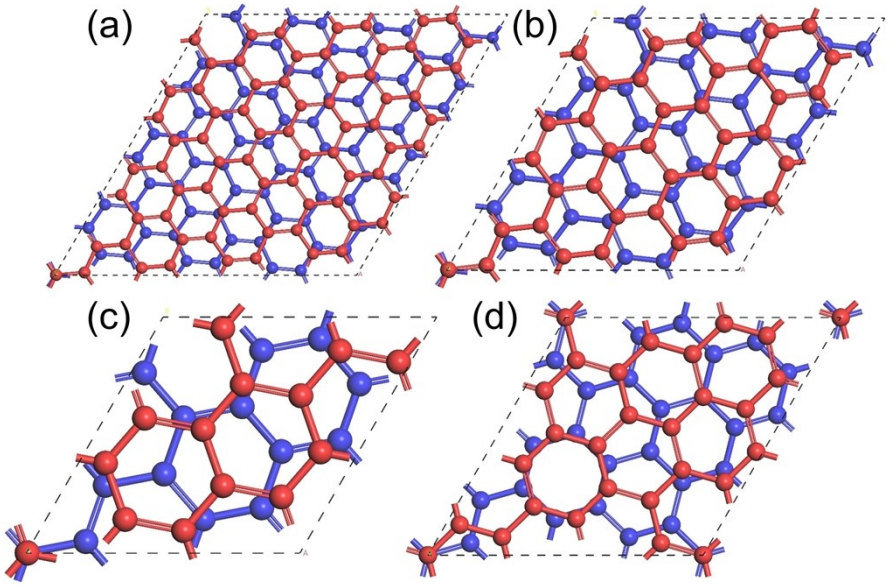

Fig. S1 (a), (b), (c), (d) are geometry models with twist angles of 9.4°, 13.2°, 21.8° and 27.8°, respectively. Two different layers in TBG are colored by red and blue, respectively.

1.Definition of ∆q.

There are148 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, Δq is defined as:

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

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

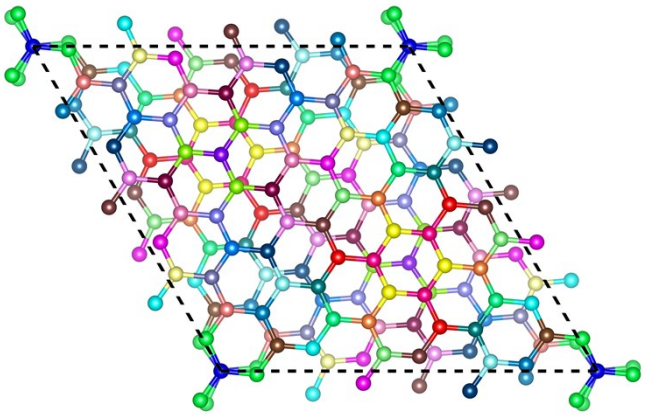

Fig. S2 The schematic show of 26 groups of carbon atoms in 9.4°-TBG model, the carbon atoms in one group are drawn with same color.

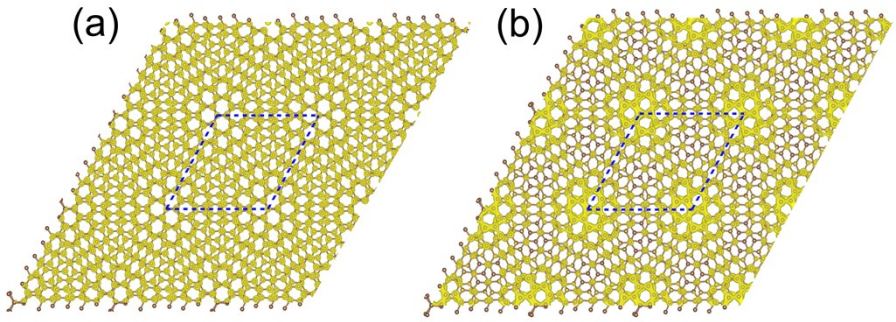

Fig. S3 (a) and (b) are PCD of the bottom conduction band for 9.4°-TBG at pressures of 0 GPa and 75.52 GPa, respectively. The dashed line indicates the unit cell of 9.4°-TBG. The iso-surface value is $6x10^{-4}$ e/Bohr^3.

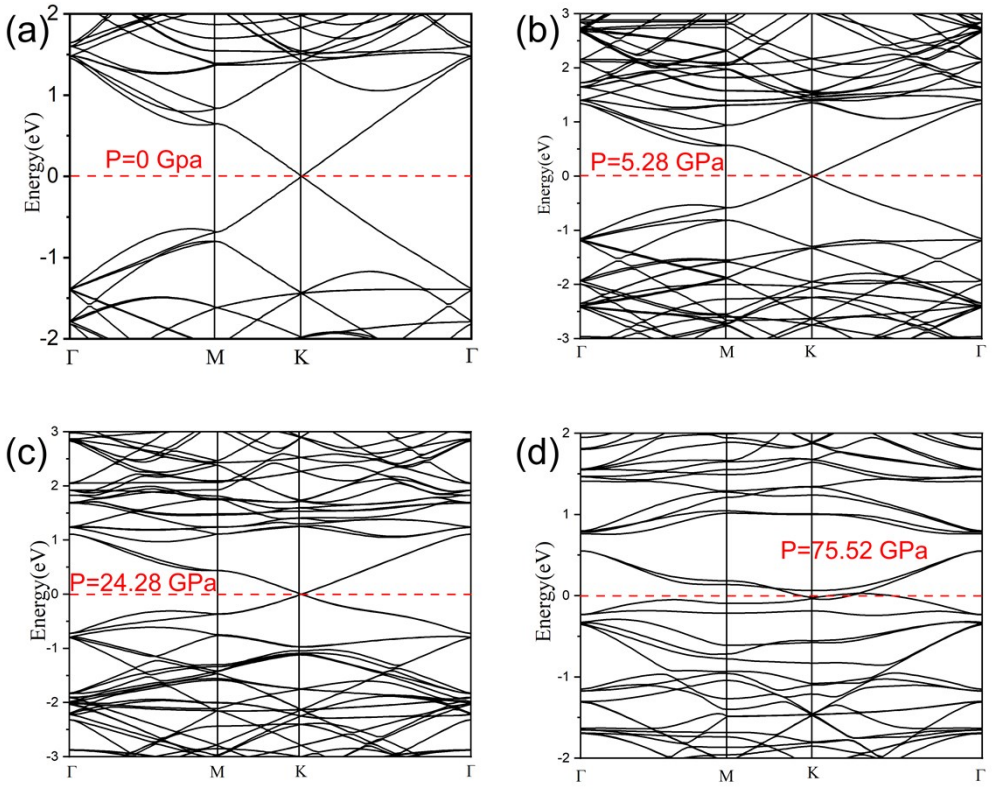

Fig. S4 (a), (b), (c), (d) are band structures under different pressures for twist angle 9.4°.

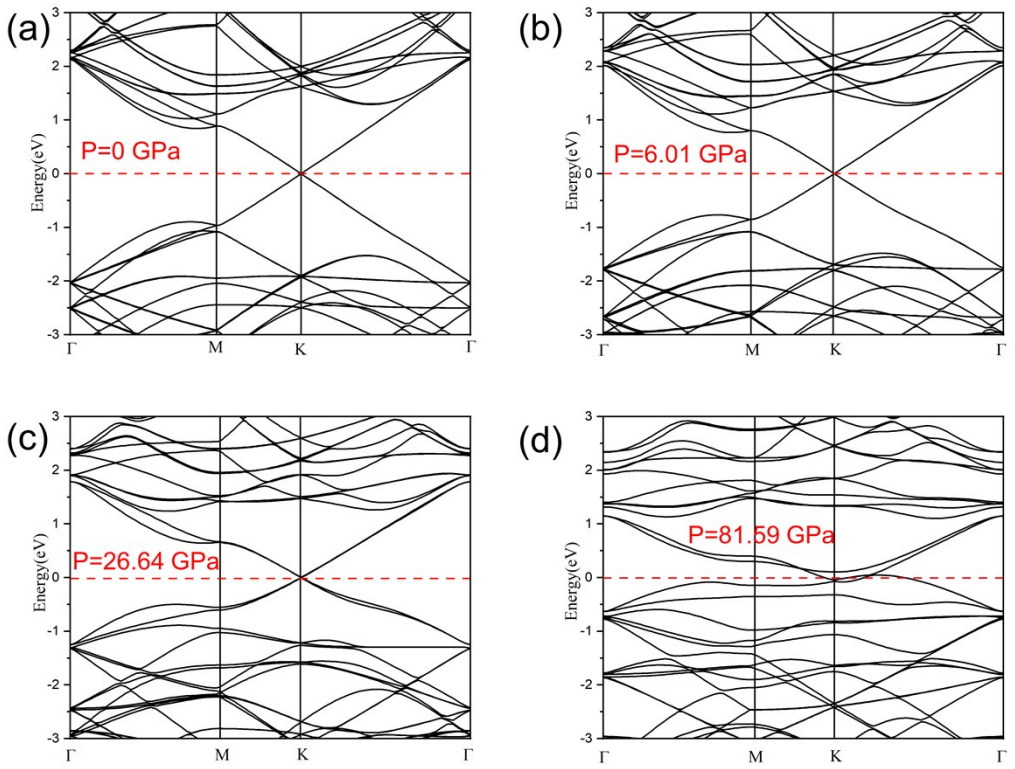

Fig. S5 (a), (b), (c), (d) are band structures under different pressures for twist angle 13.2°.

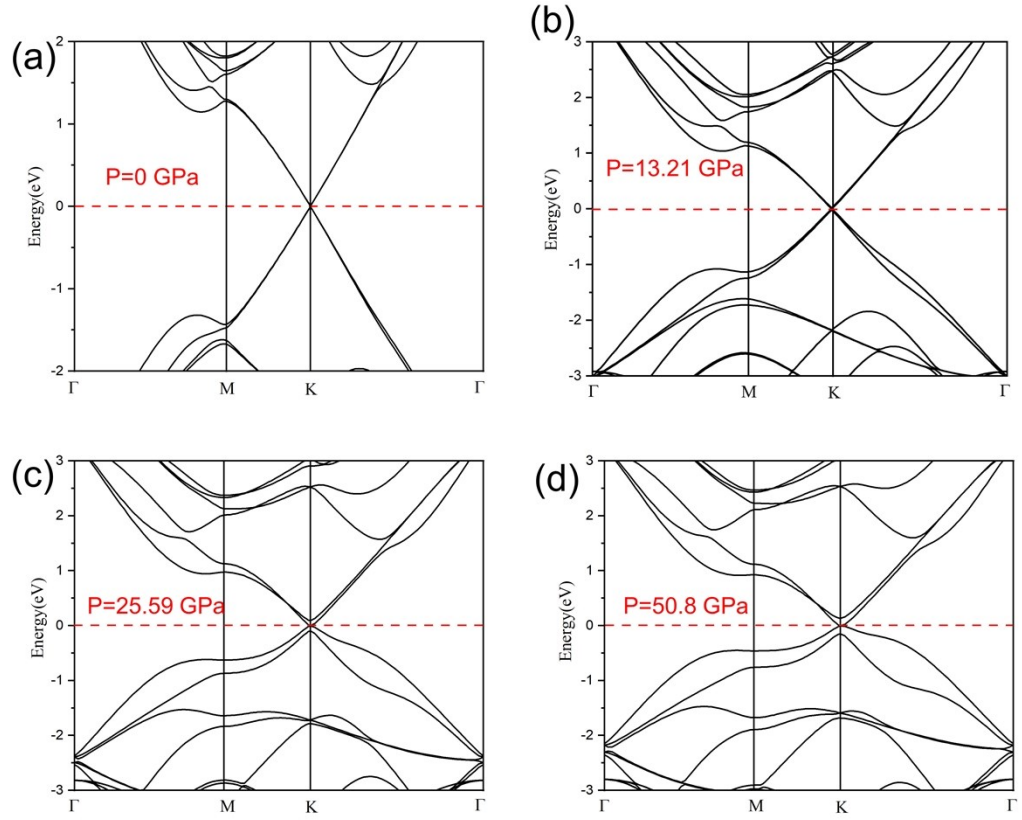

Fig. S6 (a), (b), (c), (d) are band structures under different pressures for twist angle 21.8°.

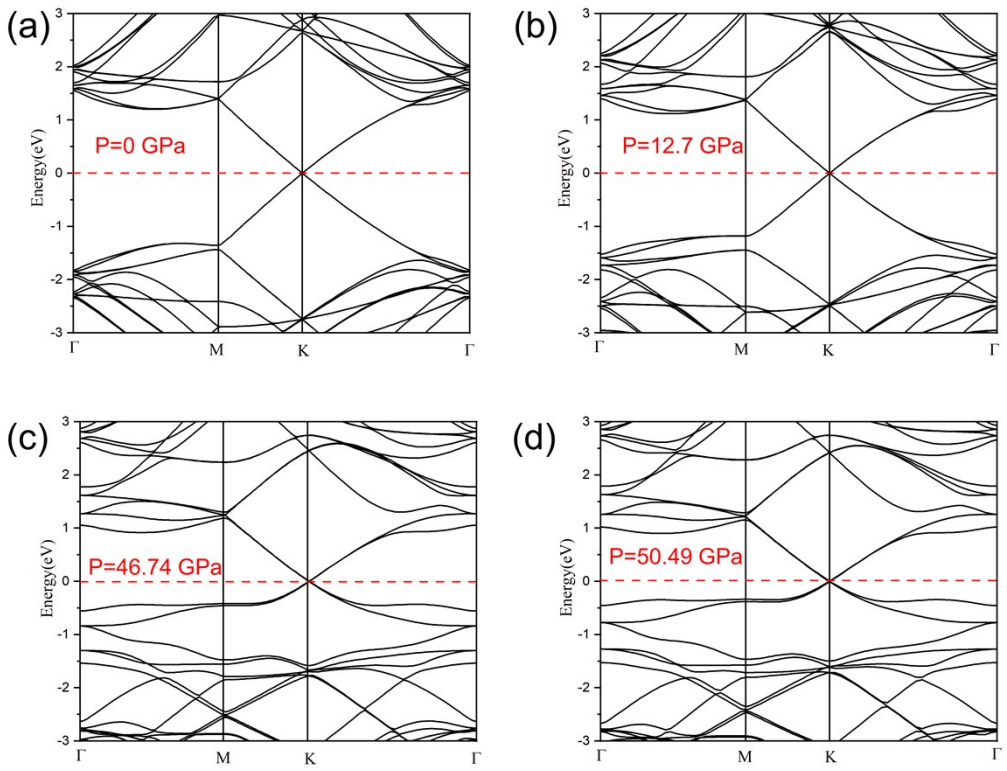

Fig. S7 (a), (b), (c), (d) are band structures under different pressures for twist angle 27.8°.

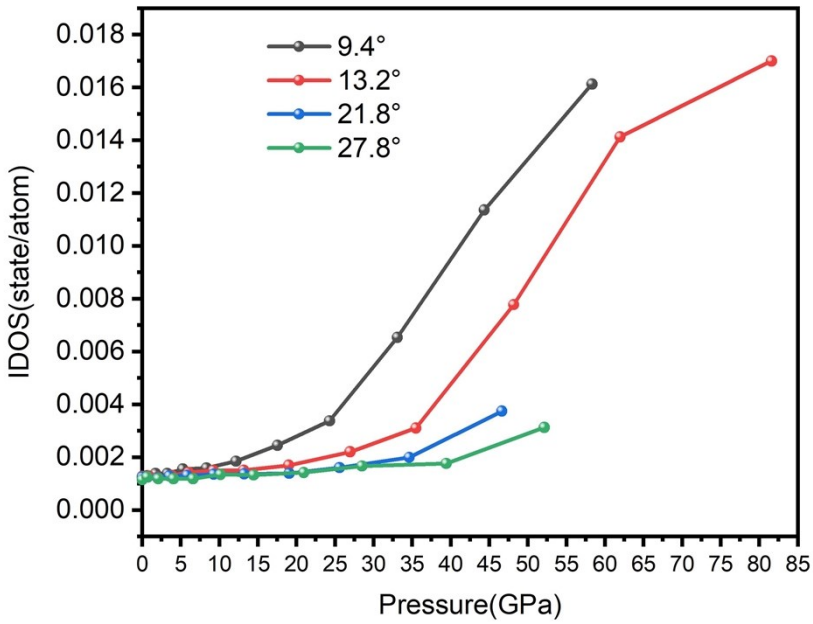

Fig. S8 The relationship between IDOS and pressure with different twisting angles.