Supplementary Information

Electronic structures and quantum capacitance of twisted bilayer graphene with defects based on three-band tight-binding model

Baojuan Xin[a], Kaixin Zou[a], Dayong Liu[b], Boyan Li[c], Hong Dong[a], Yahui Cheng[a], Hui Liu[a], Liang-Jian Zou[d], Feng Luo[e], Feng Lu[a, *], Wei-Hua Wang[a, *]

[a] *Department of Electronic Science and Engineering, and Tianjin Key Laboratory of Efficient Utilization of Solar Energy, Nankai University, Tianjin 300350, China*

[b] *Department of Physics, School of Sciences, Nantong University, Nantong 226019, China*

[c] *National Institute of Clean-and-Low-Carbon Energy, and Beijing Engineering Research Center of Nano-structured Thin Film Solar Cells, Beijing 102211, China*

[d] *Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei 230031, China*

[e] *School of Materials Science and Engineering, Nankai University, Tianjin 300350, China*

[*]Authors to whom correspondence should be addressed: lufeng@nankai.edu.cn; whwangnk@nankai.edu.cn

1. Side view and partial density of states of C atoms with next-nearest neighboring C vacancies in 4×4 graphene supercell

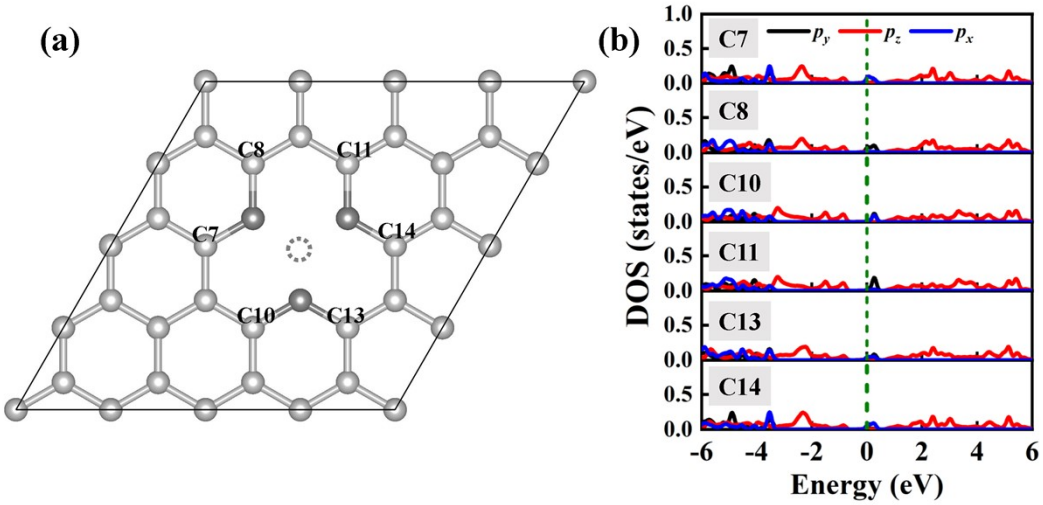

Fig. S1 (a) Side view of graphene supercell with V_C, in which the C atoms with NNN V_C are labeled as 7, 8, 10, 11, 13 and 14. (b) PDOS of C atoms with NNN V_C.

2. The configurations and electronic structures of tBLG with three types of randomly and one type of uniformly distributed C vacancies

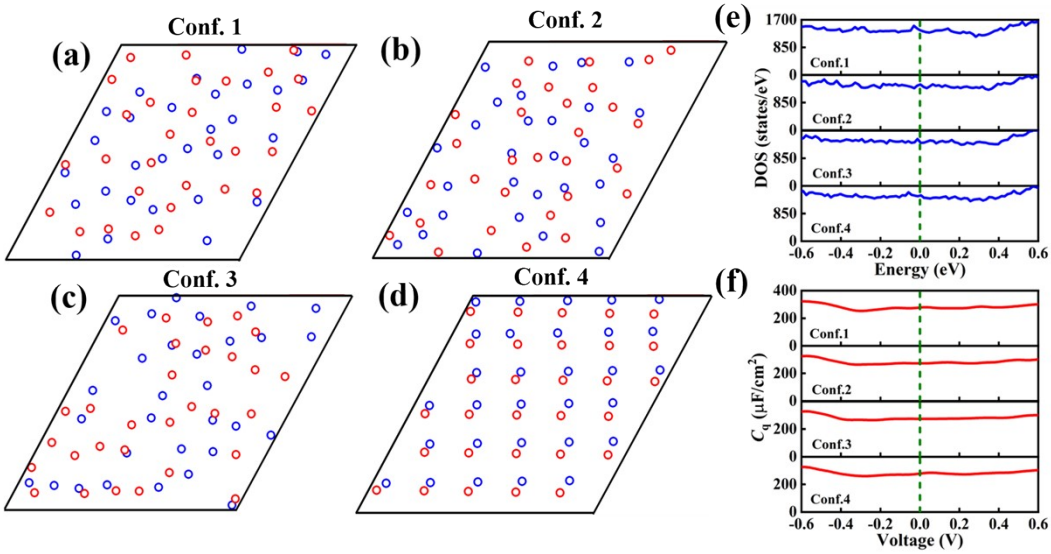

Fig. S2 (a), (b) and (c) Randomly distributed configurations of V_C, (d) uniformly distributed configuration of V_C in tBLG with the defect concentration of 1%. The blue and red circles represent the possible position of the V_C in the top and bottom layers, respectively. Here, the criterion is that the distance between two possible V_C positions is larger than 4*a*, where *a* denotes the lattice constant of graphene. (e) The DOS and (f) quantum capacitance of four V_C configurations in (a-d) of tBLG with the defect concentration of 1%, where blue and red lines represent DOS and quantum capacitance respectively.

3. Zoomed in band structures of tBLG with C vacancies

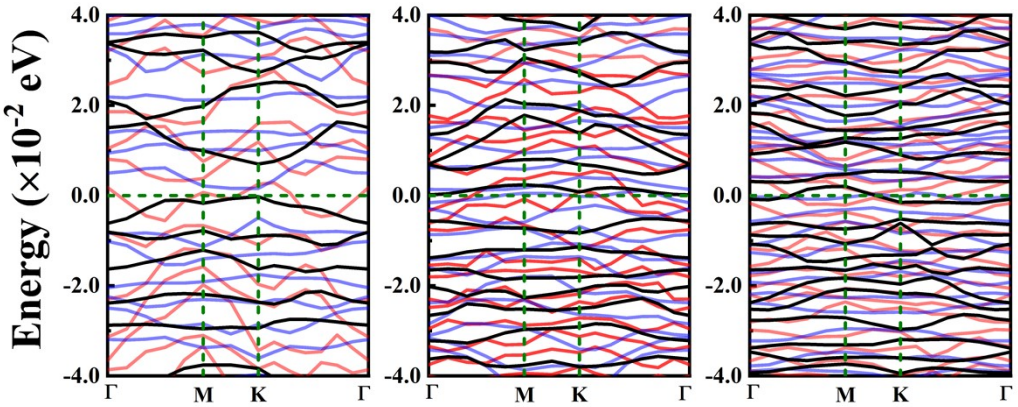

Fig. S3 Zoomed in band structures of tBLG with three-band tight binding model at the C vacancies concentration of 1%, 2% and 3% with the uniformly distributed vacancy configurations.

4. The DOS and quantum capacitance of BLG and tBLG with 0% and 2% C vacancies

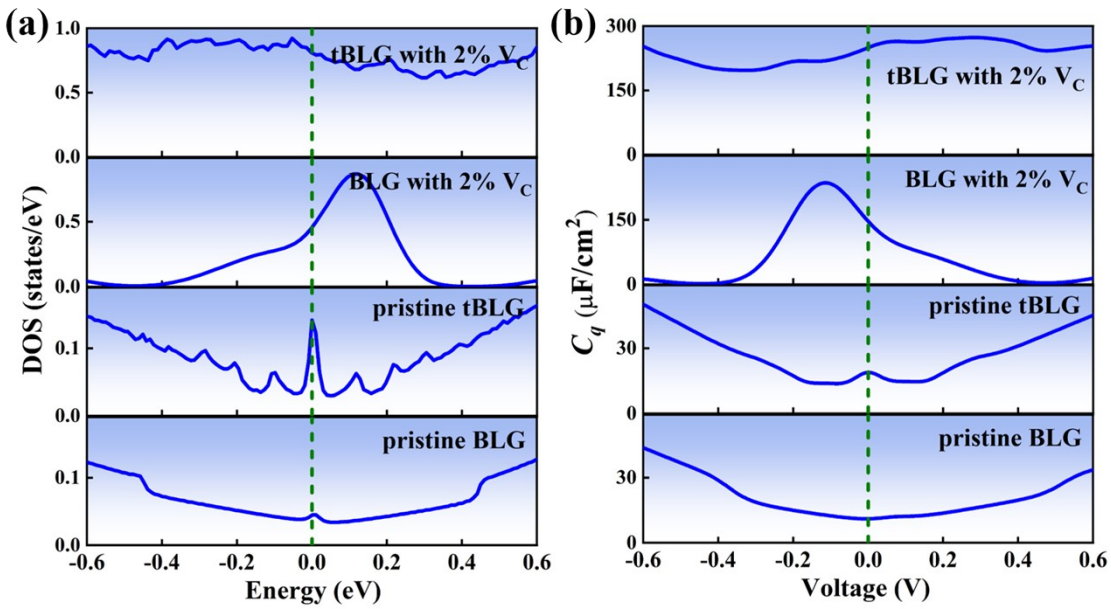

Fig. S4 Density of states corresponding to pristine BLG unit cell size in (a) and quantum capacitance in (b) of pristine BLG, pristine tBLG, BLG with V_C concentration of 2%, and tBLG with V_C concentration of 2%, respectively.