Electronic Supplementary Material (ESI) for Nanoscale.

A Promising Way to Open an Energy Gap in Bilayer Graphene

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The method of getting the electrostatic potential

Taking bilayer graphene (BLG) as an example, we calculated the electrostatic potential of the unit cell and get a file named LOCPOT. Then we calculated the mean value in the x, y plane, and plotted its distribution along the z-direction, as shown in Figure S1. From Figure S1, the vacuum level is +2.030eV. And the Fermi level of the BLG is -2.285eV from our calculation. The work-function of the material can be calculated by subtracting the Fermi level from the vacuum level. In the manuscript, we use the opposite values of the work-functions as the electrostatic potential of different materials. As a result, the electrostatic potential of BLG is -4.315eV.

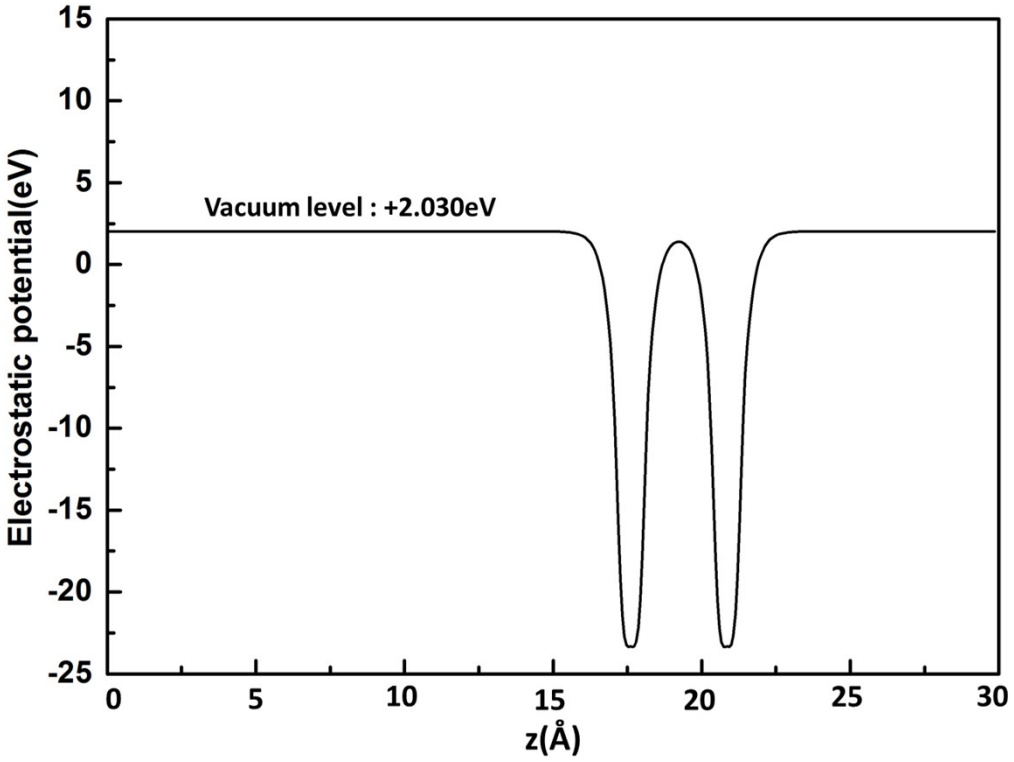

Figure S1. The electrostatic potential of BLG. The horizontal axis stands for the direction perpendicular to the layers, the vertical axis stands for the electrostatic potential.

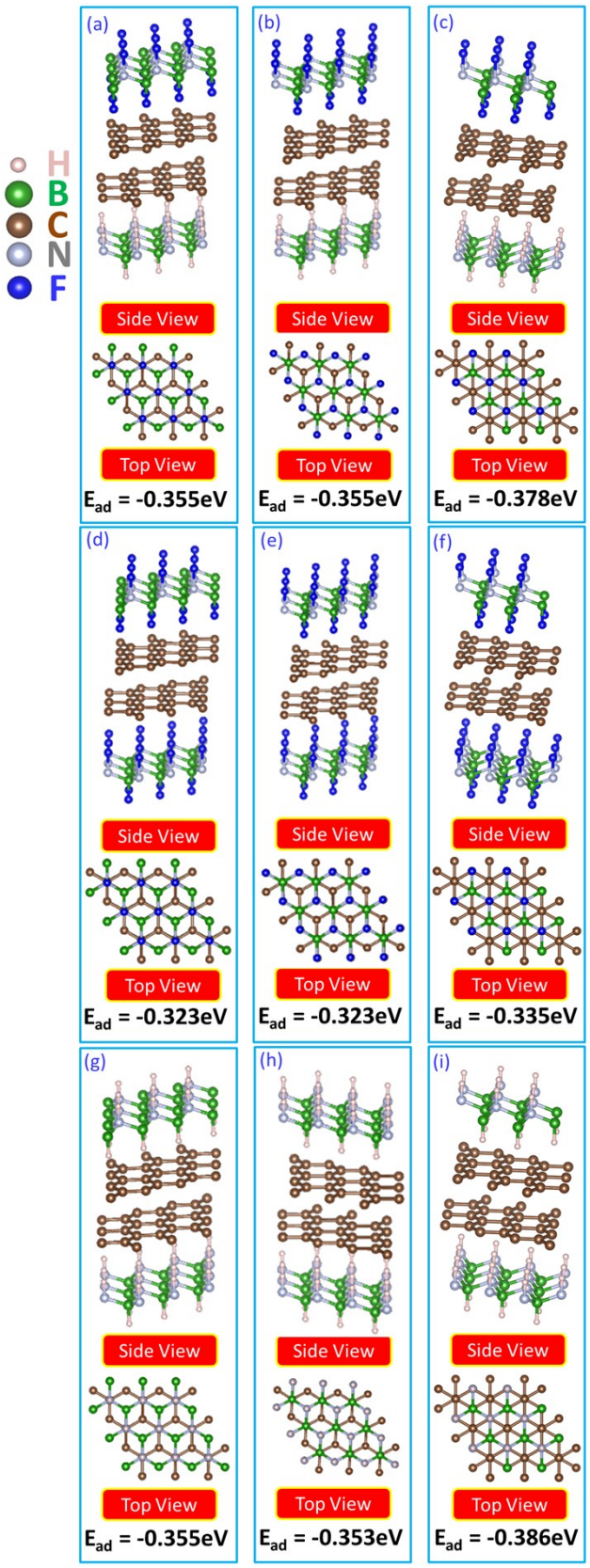

Figure S2. The top and side view of different stacking patterns of sandwich like systems. The hydrogen, boron, carbon, nitrogen, fluorine atoms are in light red, green, brown, grey and blue, respectively.

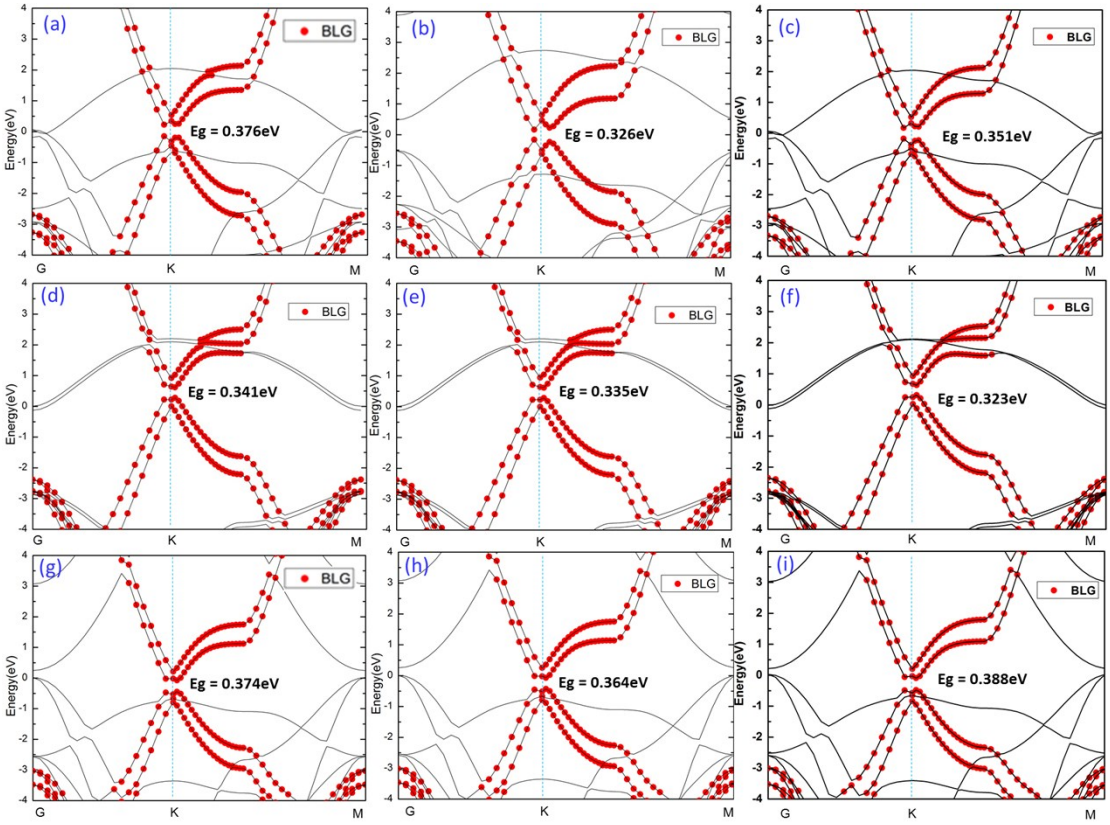

Figure S3. The band structures of the different stacking patterns corresponding to the structures in Figure S1. The red spheres stand for the projected band structures of BLG. The solid lines stand for the band structures of the whole system. The Fermi level has been shifted to zero.

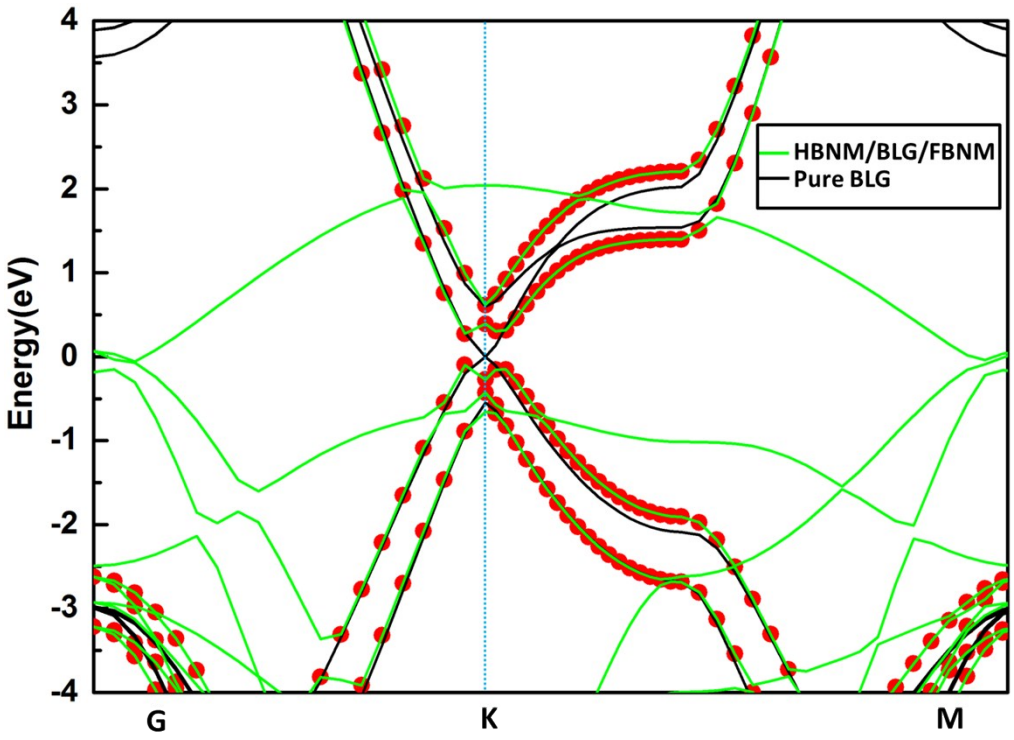

Figure S4. The band structures of HBNM/BLG/FBNM (the green line) and pure BLG (the black line). The red spheres stand for the projected band structures of BLG in structure HBNM/BLG/FBNM. And the calculated carrier's mobility of sandwiched BLG in structure HBNM/BLG/FBNM and pure BLG is 1.9×10^6 m/s and 2.7×10^6 m/s.

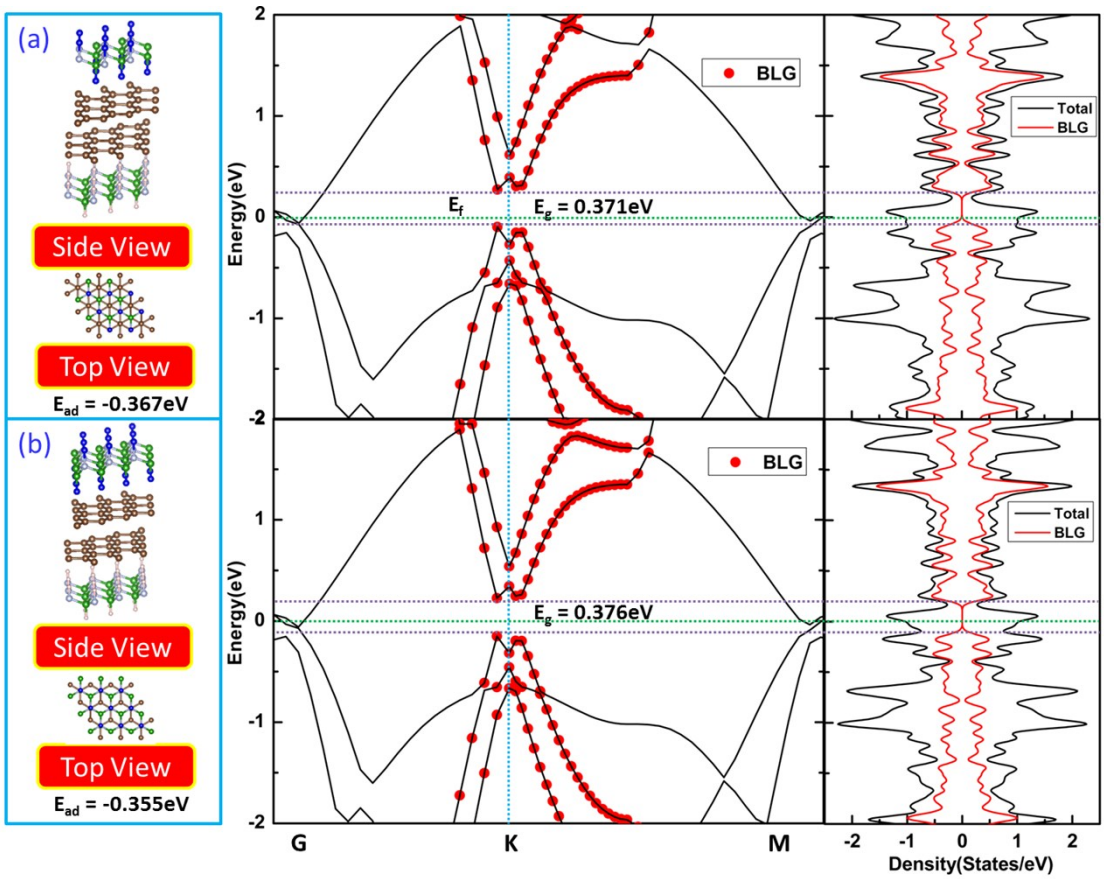

Figure S5. The band structures and the density of states (DOS) of the different stacking patterns. The red spheres stand for the projected band structures of BLG. The solid lines stand for the band structures of the whole system. The Fermi level has been shifted to zero and represented by green dotted line. The total DOS of the whole system and the projected DOS of BLG are represented by the black and red line, respectively.

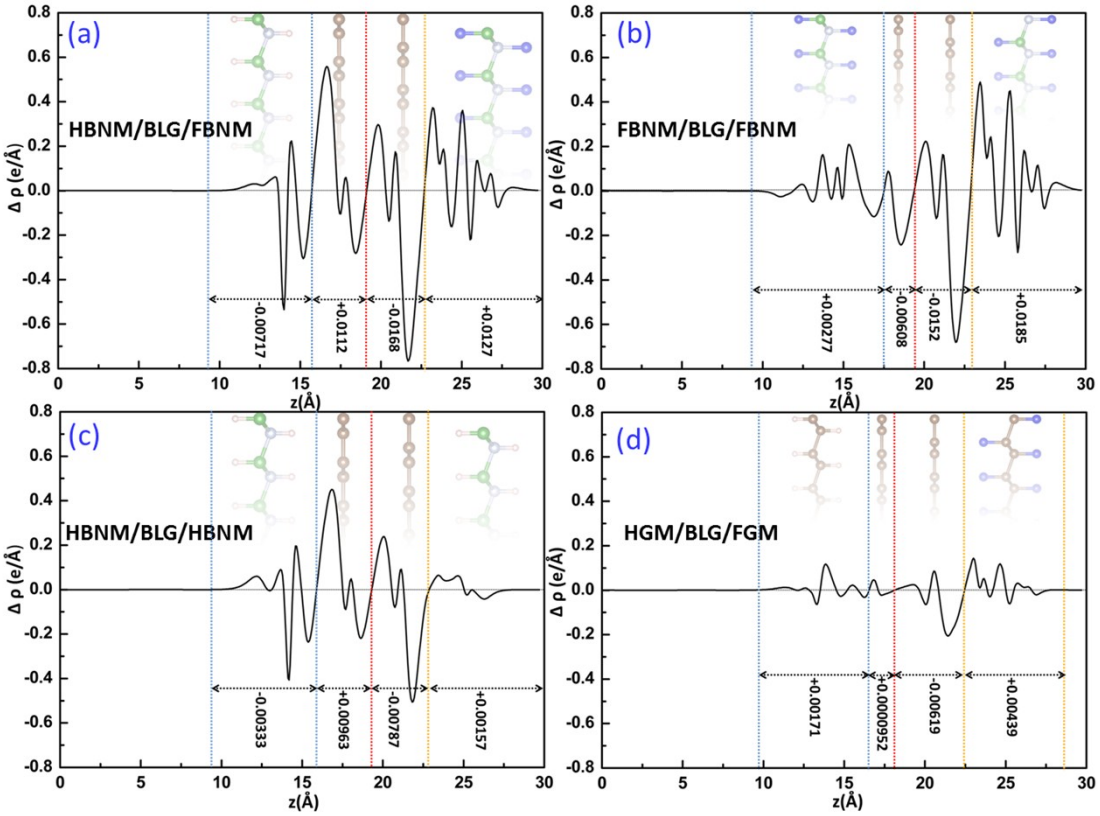

Figure S6. The integrated differential charge along *z-axis* of the supercell for (a) HBNM/BLG/FBNM, (b) FBNM/BLG/FBNM, (c) HBNM/BLG/HBNM, (d) HGM/BLG/FGM structures. The positive and negative numbers represent charge accumulation and depletion with respect to isolated BLG and substrates. The location of different layers is separated by different dot-lines.

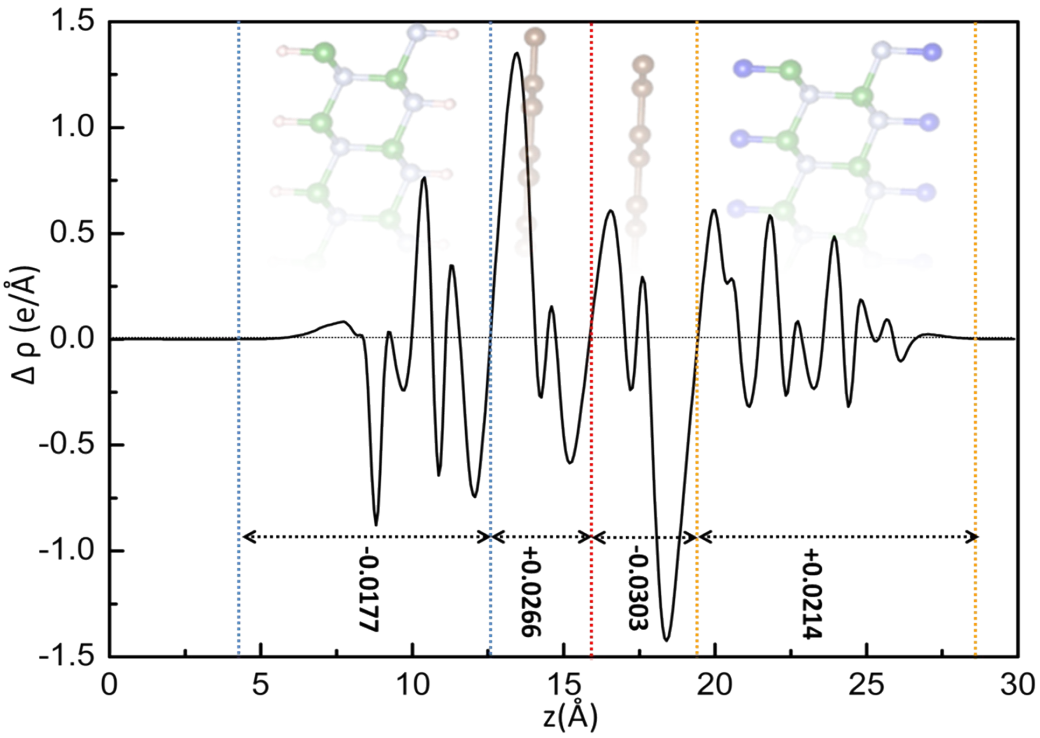

Figure S7. The integrated differential charge along *z-axis* of the supercell for HBNB/BLG/FBNB structure. The positive and negative numbers represent charge accumulation and depletion with respect to isolated BLG and substrates. The location of different layers is separated by different dot-lines.

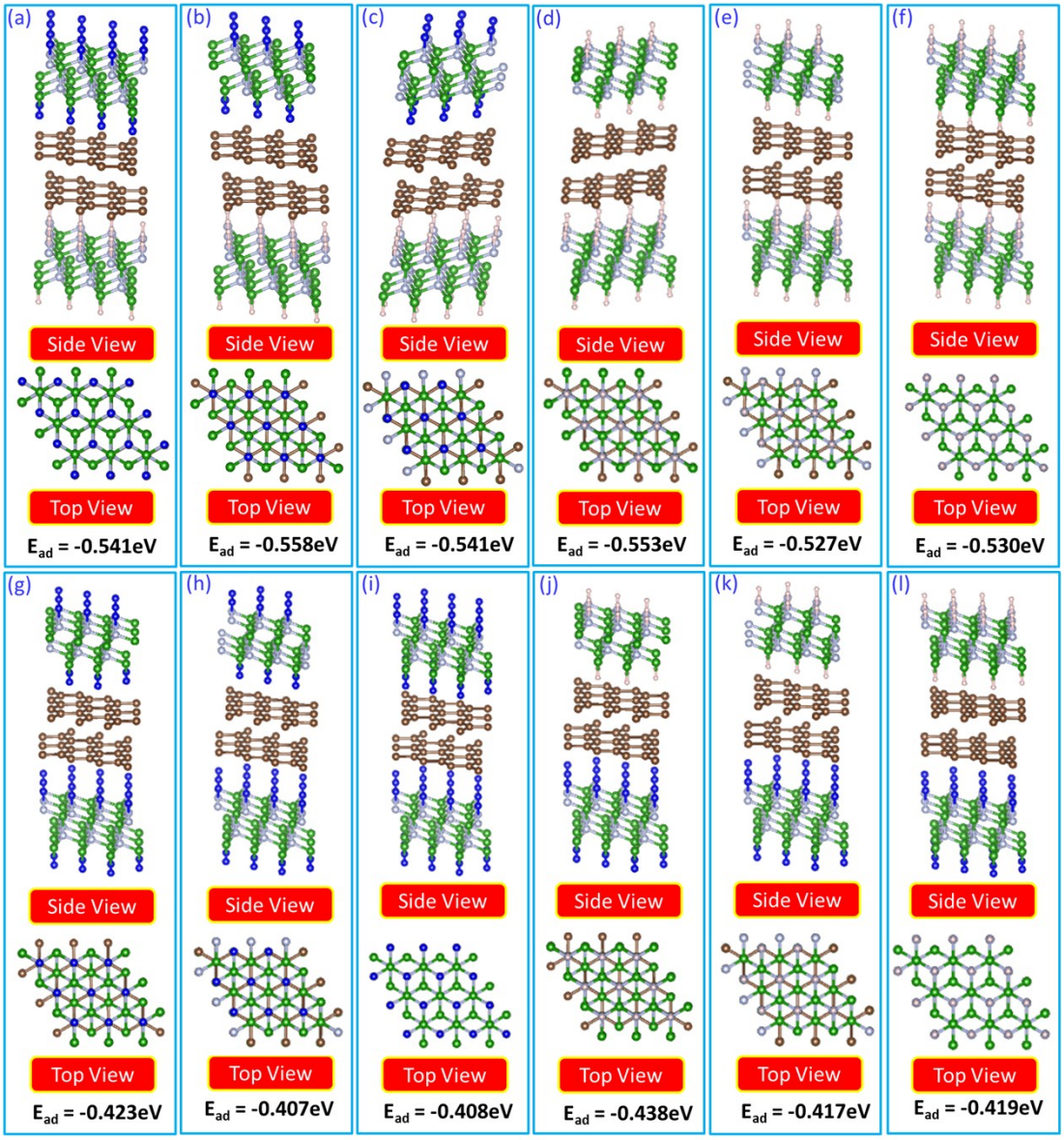

Figure S8. The top and side view of different stacking patterns of sandwich like systems. The hydrogen, boron, carbon, nitrogen, fluorine atoms are in light red, green, brown, grey and blue, respectively.

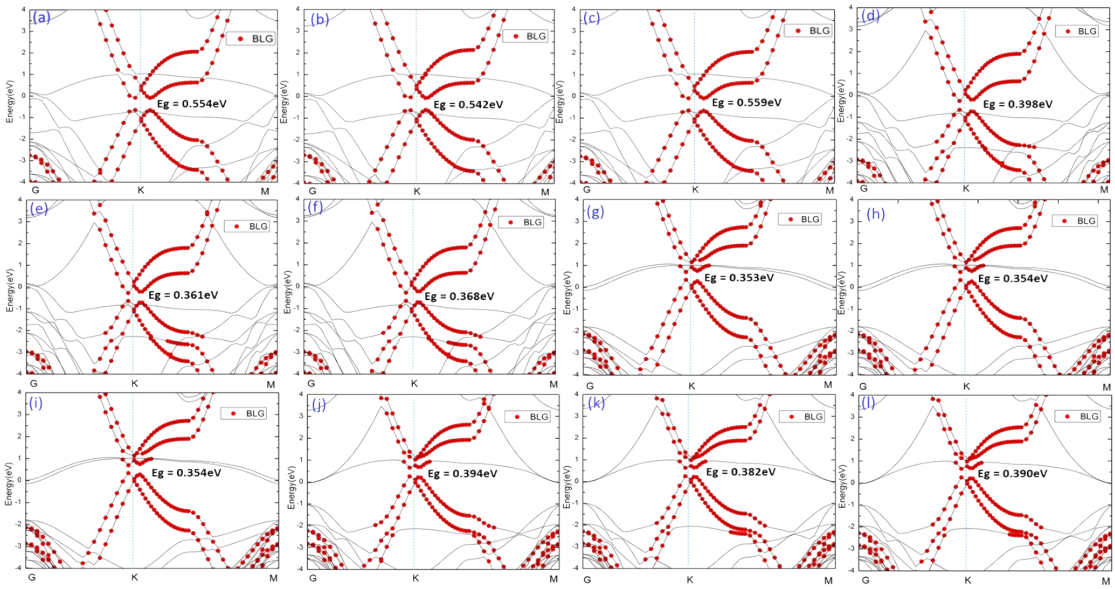

Figure S9. The band structures of the different stacking patterns corresponding to the structures in Figure S5. The red spheres stand for the projected band structures of BLG. The solid lines stand for the band structures of the whole system. The Fermi level has been shifted to zero