Supplemental Information

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(i) The calculated results show that the resultant binding of a graphene/BN bilayer is a delicate balance between short-range Pauli's repulsive forces and long-range vdW attractive forces. For the equilibrium separation of the AB-stacked system, the magnitude of the Pauli's repulsive forces is larger in the AA-stacked system relative to that of the AB-system. As a result, the equilibrium spacing for the AA stacked bilayer is always higher than that of AB stacked bilayer leading to a smaller binding energy for the AA-stacked system.

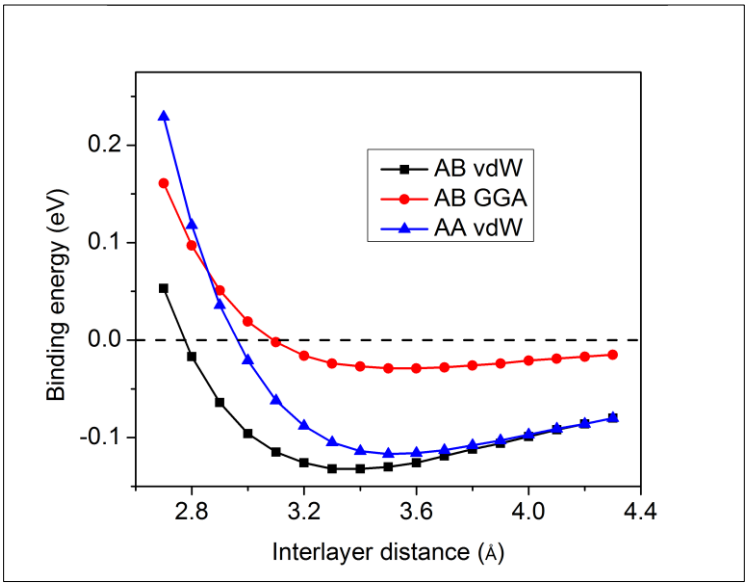

Figure S1: (Color online) The calculated energy surface of the graphene/BN bilayer for AA and AB Stacking configurations.

For the AB-stacked bilayer, the GGA-DFT results (red line) show a very weak bonding between the graphene and BN layers yielding a binding energy of -0.03 eV associated with the equilibrium separation of 3.5 Å. The vdW-DFT results find the binding energy of -0.13 eV with the equilibrium separation of 3.3 Å. Note that the vdW functional form properly describes the long-range dispersive interactions for the graphene/BN bilayer system.

It has been argued that the long-range vdW interaction has a minimal dependence on the stacking format between two graphene layers or between two BN layers [56]. This is what we

find in Figure S1 for the interlayer spacing of 4 Å and beyond where the energy values of both AA and AB stacking configurations superimpose each other. For the smaller interlayer spacing, Fig S1 shows the presence of a larger Pauli's repulsion for the AA stacking relative to that for the AB stacking. It is due to topoly of the stacking configurations: near-neighbor distance in the AA stacking is smaller that in the AB stacking for the same interlayer sepataion of the bilayer sysytem.

(ii)

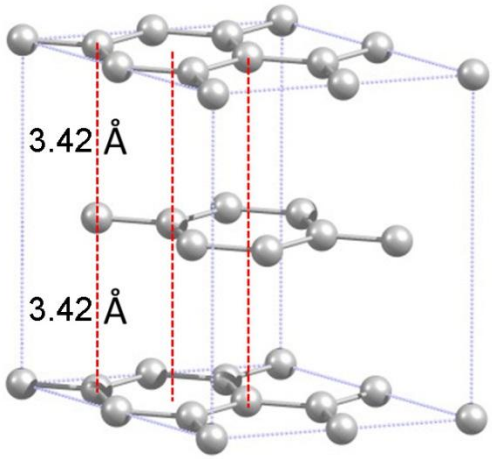

Figure S2: (Color online) A schematic diagram of the ABA stacked trilayer graphene calculated at the vdW-DFT level of theory. The gray spheres represent carbon atoms.

(iii) The differences between the ABA stacked trilayer graphene and graphene/BN/graphene systems can be attributed to dissimilarity of the constituent layers, though the layers are stacked in a same order. The constituent bilayers (i.e. graphene/BN and graphene/graphene) have the similar long-range vdW attractive forces acting on each-other at larger interlayer distances, whereas the short-range Pauli's repulsive forces acting on the graphene/graphene bilayer is larger than that of graphene/BN bilayer due to differences in the effective atomic volume of C in graphene and B and N in the BN lattice (Figure S3).

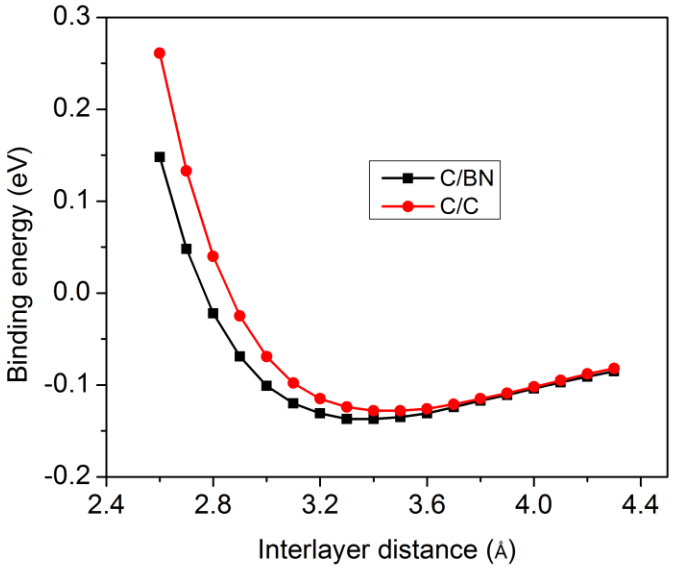

Figure S3: (Color online) The calculated energy surface of the AB-stacked graphene and graphene/BN bilayer systems.

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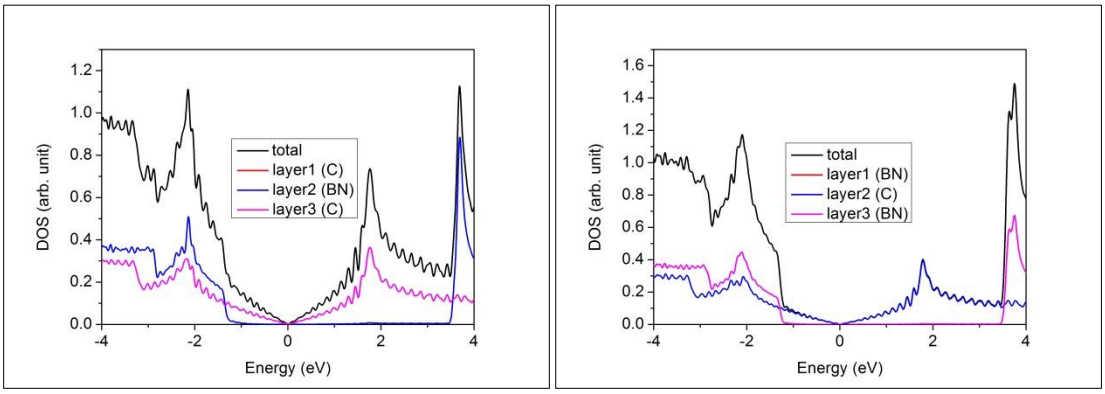
(i) The projected density of states (PDOS) of the considered trilayer systems are given in Figure S4. It shows that the constituent graphene contribute to states near Fermi energy, whereas states associaed with BN are far from Fermi energy.



(a) graphene/BN/graphene (b) BN/graphene/BN/

Figure S4: (Color online) The projected desnity of states (PDOS) of the ABA-stacked graphene/BN/graphene and BN/graphene/BN/ trilayers. Zero is aligned to Fermi energy of the system.

(ii) The local density of states (LDOS) near the Fermi energy ($E_f \pm 0.6$ eV) are given in Figure S5. The LDOS is formally the DOS weighted by the amplitude of the corresponding wave functions at different points in space, and is a function of both energy and position. Figure S2 shows that the bands near the Fermi energy solely originate from graphene in the graphene/BN/graphene and BN/graphene/BN/ trilayers.

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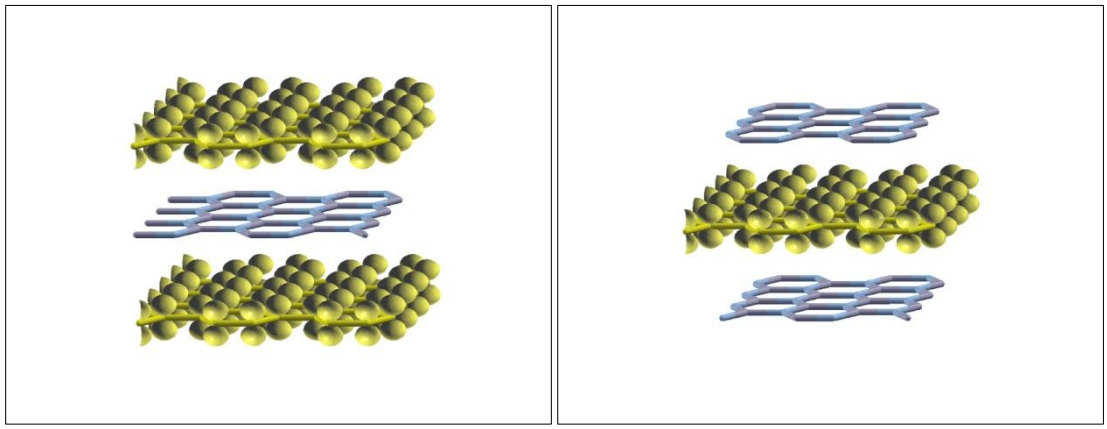

(a) graphene/BN/graphene (b) BN/graphene/BN/

Figure S5: (Color online) The local desnity of states (LDOS) of the ABA-stacked graphene/BN/graphene and BN/graphene/BN/ trilayers. Zero is aligned to Fermi energy of the system.