Supplementary Information for

Valley-selective circular dichroism and high carrier mobility of graphene-like BC_6N

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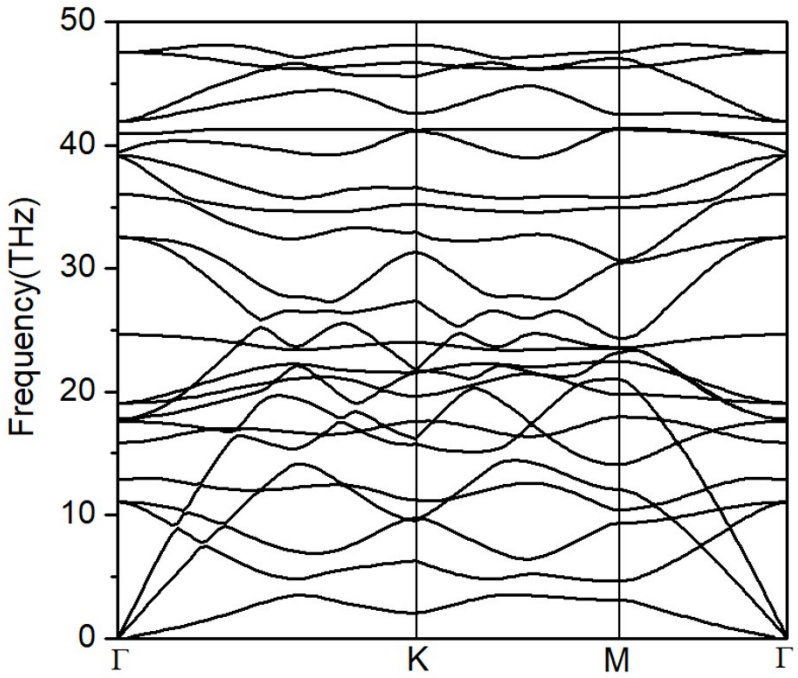


Figure S1. Phonon spectrum of g-BC_6N monolayer calculated from first-principles

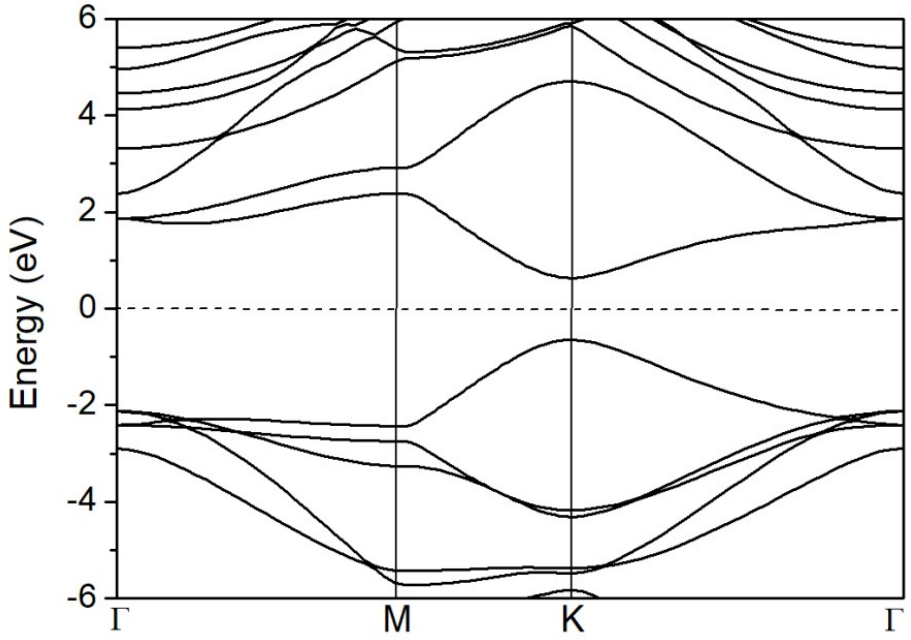
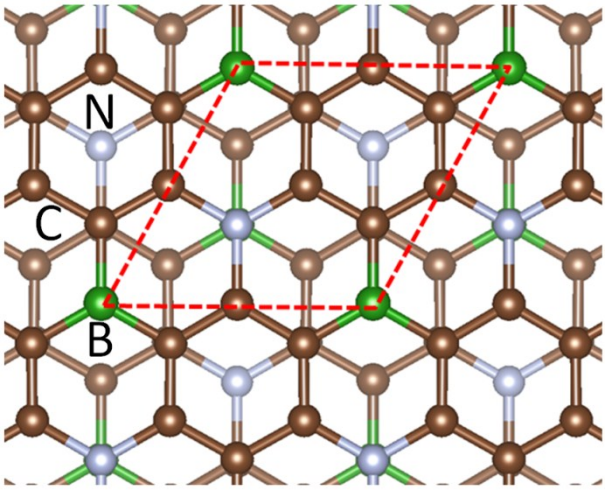
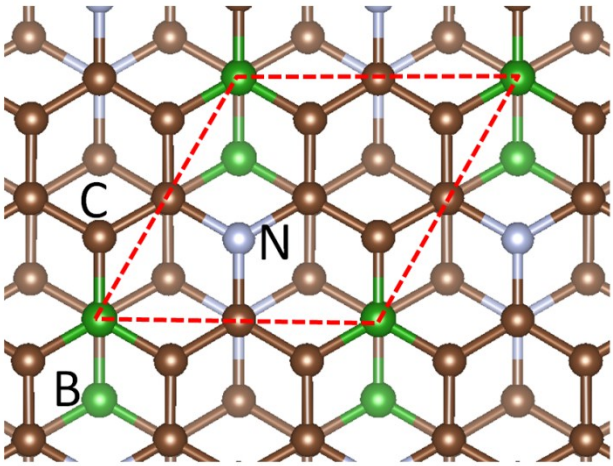


Figure S2. Electronic band structure of g-BC_6N monolayer calculated by using DFT-PBE. The energy at the Fermi level is set to zero. The direct band gap at the K point is about 1.276 eV, which is smaller than that (1.833 eV) obtained from the HSE06 functional.

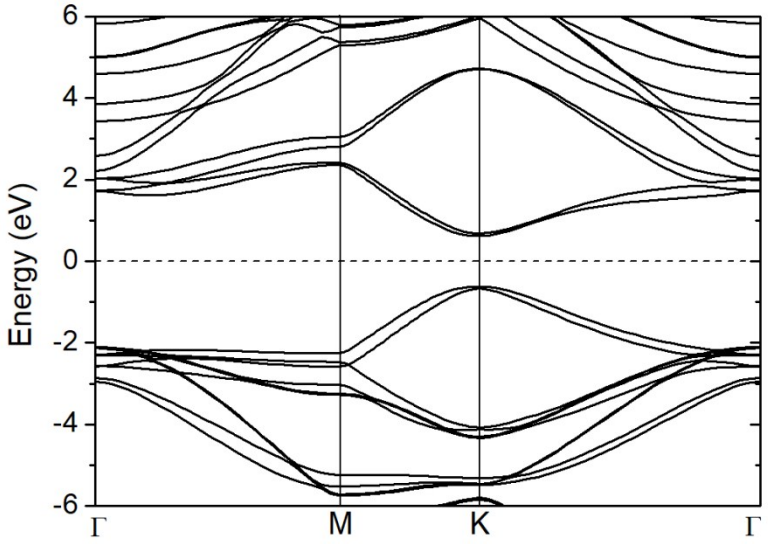


(a) AB-I

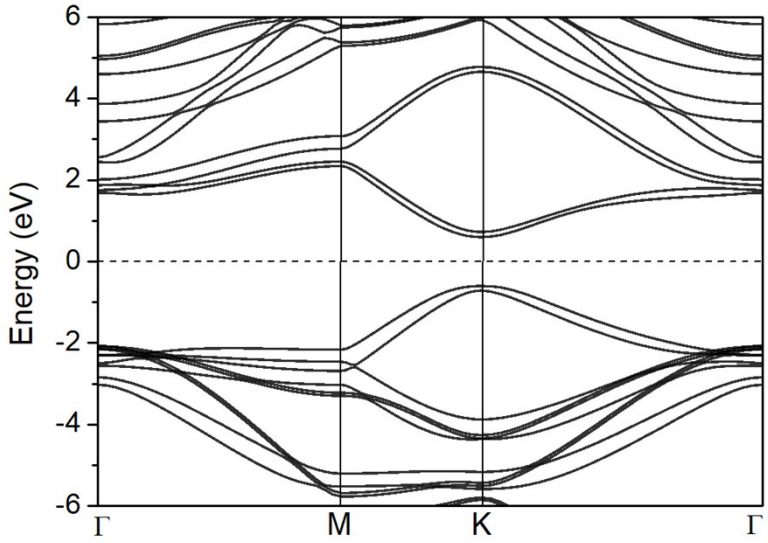


(b) AB-II

Figure S3. Two stable staking patterns of g-BC_6N bilayer. (a) AB-I, (b) AB-II. The two patterns are almost energetically degenerate with AB-I slightly stable than AB-II by about 0.58×10^{-4} eV/atom. The interlayer distance is about 3.50Å. The VDW interaction energy between the two layers is about 16.4 meV/ $Å^2$.



(a) AB-I



(b) AB-I

Figure S4. Electronic band structure of g-BC_6N bilayers calculated by using DFT-PBE. The energy at the Fermi level is set to zero. The direct band gap at the K point are about 1.251 eV for AB-I and 1.202 eV for AB-II, both of which are smaller than that (1.276 eV) for monolayer obtained by using the same strategy.

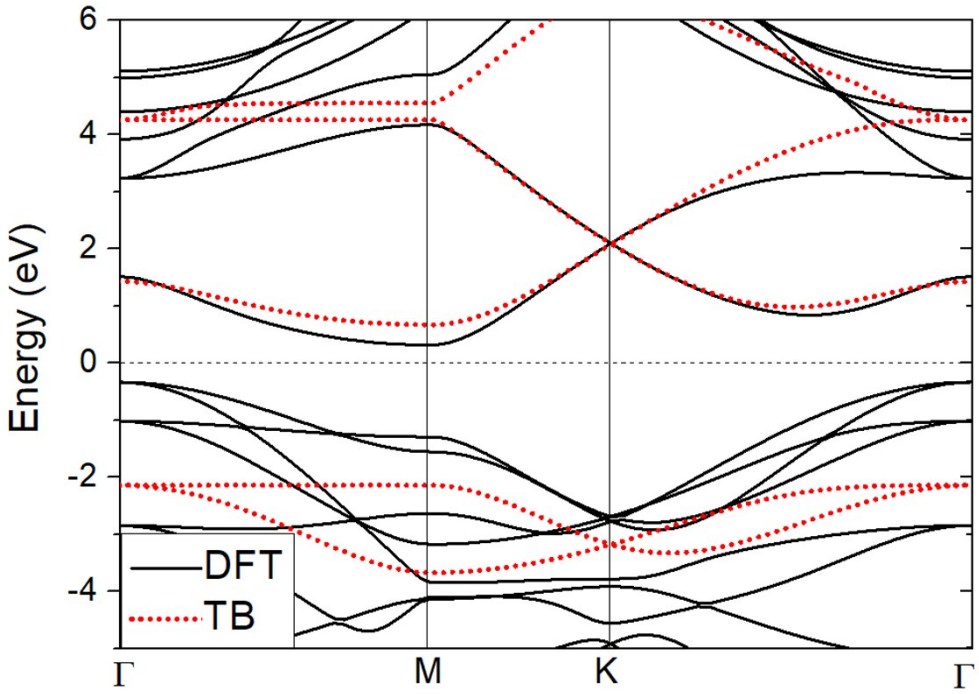


Figure S5. The electronic band lines of g-B_3C obtained at the DFT-PBE level (solid lines) and TB model (dotted lines). The parameters employed in the TB models are t_1=-3.2 eV, t_2=t_3=-2.0 eV, ε_1= ε_2= 2.35 eV. The onsite energy of carbon atom is set to zero.

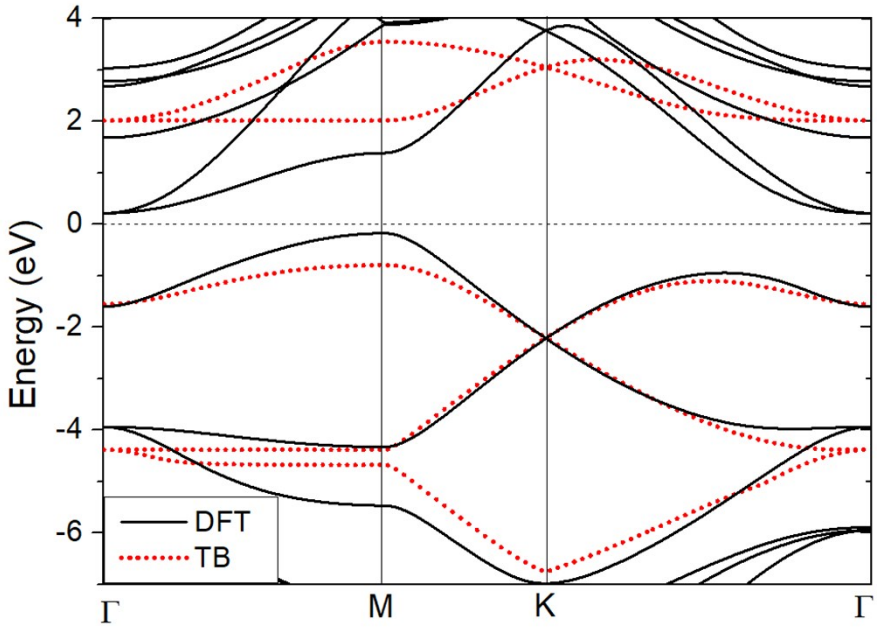


Figure S6. The electronic band lines of g-C_3N obtained at the DFT-PBE level (solid lines) and TB model (dotted lines). The parameters employed in the TB models are t_1=-3.2 eV, t_2=t_3=-2.0 eV, ε_1= ε_2= -2.35 eV. The onsite energy of carbon atom is set to zero.