Supporting Information

Tunable doping and band gap of graphene on functionalized hexagonal boron nitride with hydrogen and fluorine

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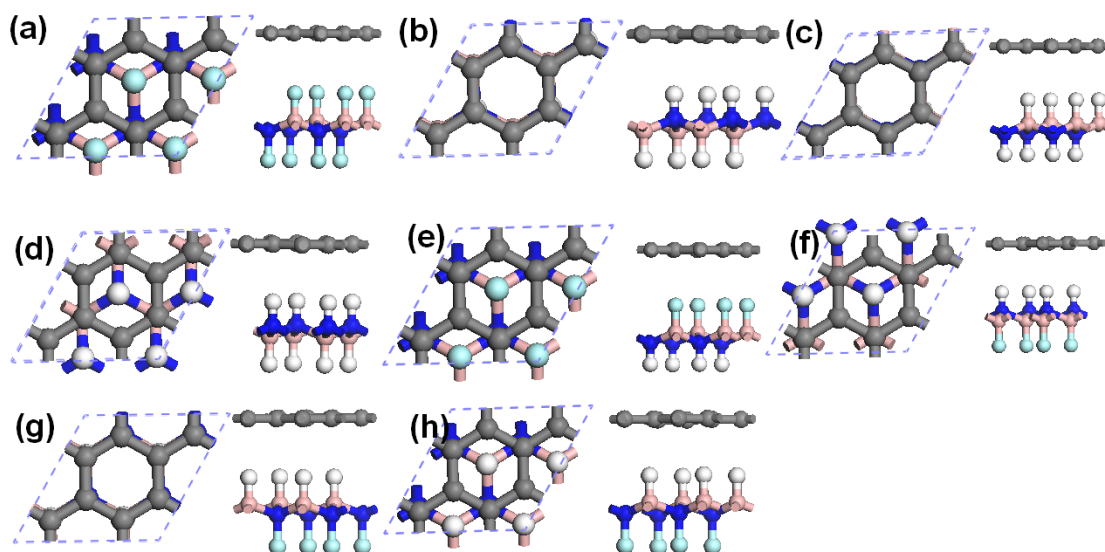[*] *E-mail address:* tsb1980@xmu.edu.cn,   yujianping402871@sina.com

Figure S1. Structures (top and side view) of graphene supported on the hydrogenated and fluorinated h-BN with different configurations. (a) G/B-FBNF, (b) G/N-HBNH, (c) G/B-HBNH, (d) G/Nh-HBNH, (e) G/Fh-FBNH, (f) G/Hh-FBNH, (g) G/H-HBNF, and (h) G/Hh-HBNF.
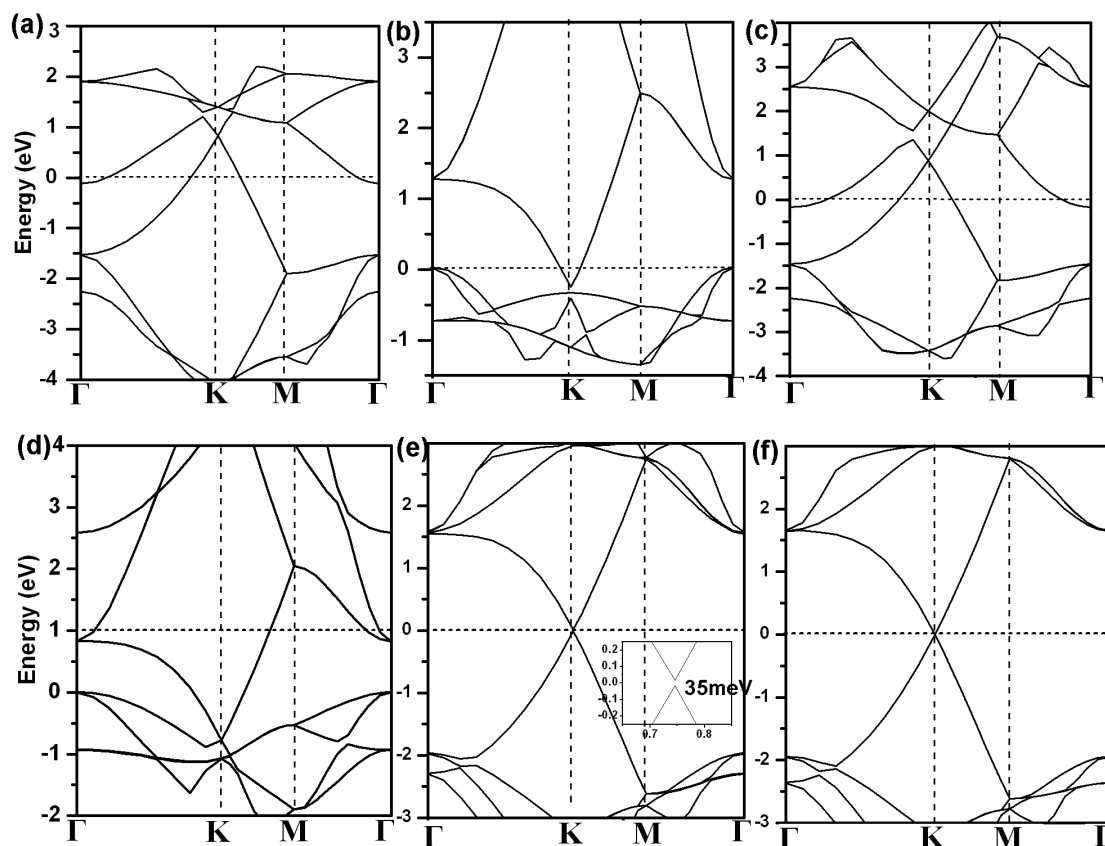

Figure S2. Band structures of (a) G/Bh-FBNF, (b) G/Nh-HBNH, (c) G/Fh-FBNH, (d) G/Hh-FBNH, (e) G/H-HBNF, and (f) G/Hh-HBNF. The Fermi level is set to 0.
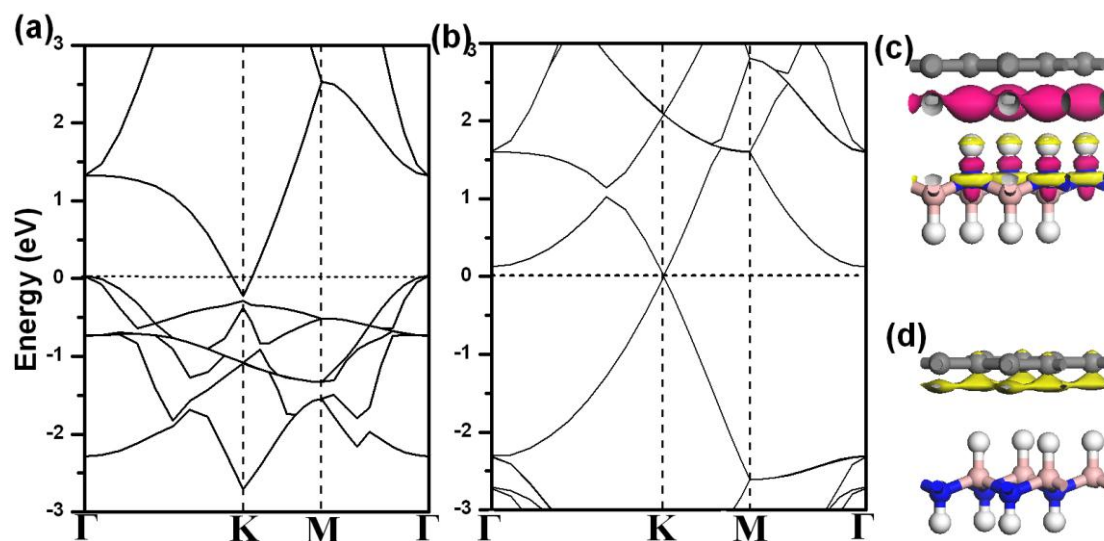
Figure S3. Band structures (a, b) and charge density difference (c, d) of hybrid structures G/N-HBNH and G/B-HBNH, respectively. The red and yellow areas in (c) and (d) denote electron accumulation and depletion, respectively, and isosurfaces are 0.003 e/Å^3. The Fermi level is set to 0.
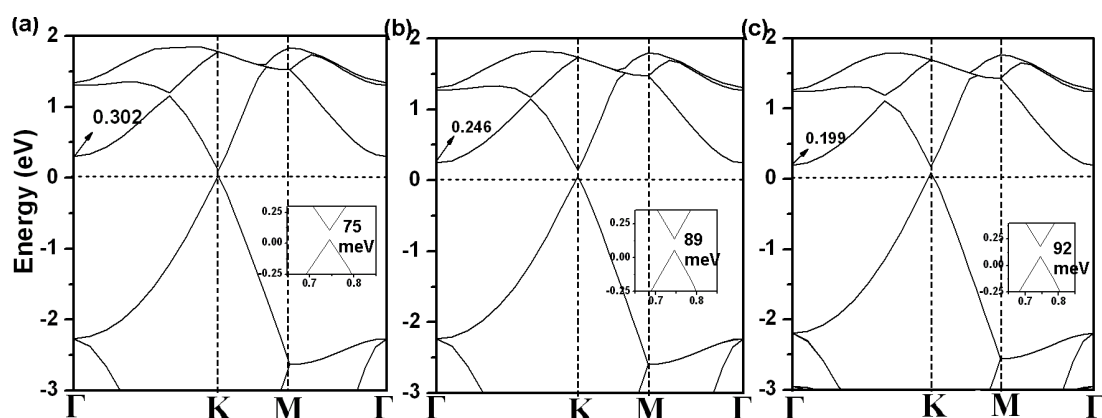

Figure S4. Band structures of G/F-HBNF with the electric field of (a) 0.2, (b) 0.3, and (c) 0.4 V/Å, respectively. The arrows in (a)-(c) show the energy level of the lowest unoccupied state (LUS) at Γ point with respect to the Fermi level. The Fermi level is set to 0.