

Supporting Information

Enhancing the energetic and magnetic stability of atomic hydrogen chemisorbed on graphene by (non)compensated B-N pairs

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Fig. S1

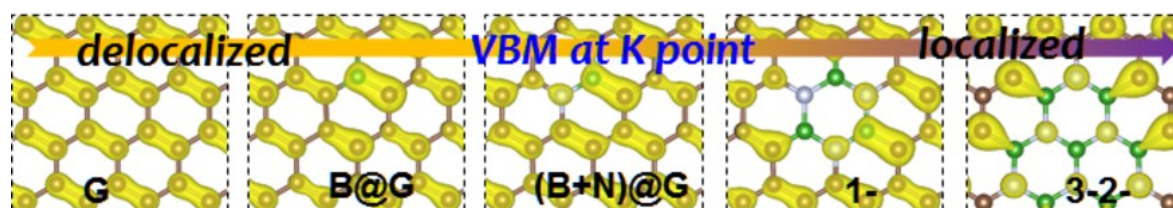


Figure S1. The changing trend of partial charge of VBM at Brillouin K point, including both compensated and noncompensated G, B@G, (B+N)@G, 1- and 3-2-. The isosurface is set to $0.0016 \text{ e}/\text{\AA}^3$.

Fig. S2

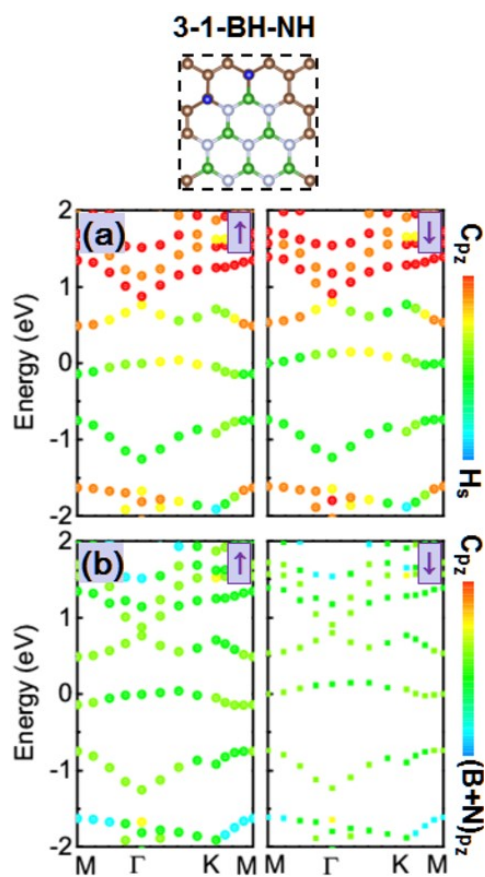


Figure S2. For noncompensated doping 3-1-BH-NH, (a) spin polarized projected bands for weights of Cp_z and adsorbate H_s , while (b) for weights of Cp_z and doped $(B+N)p_z$.

Fig. S3

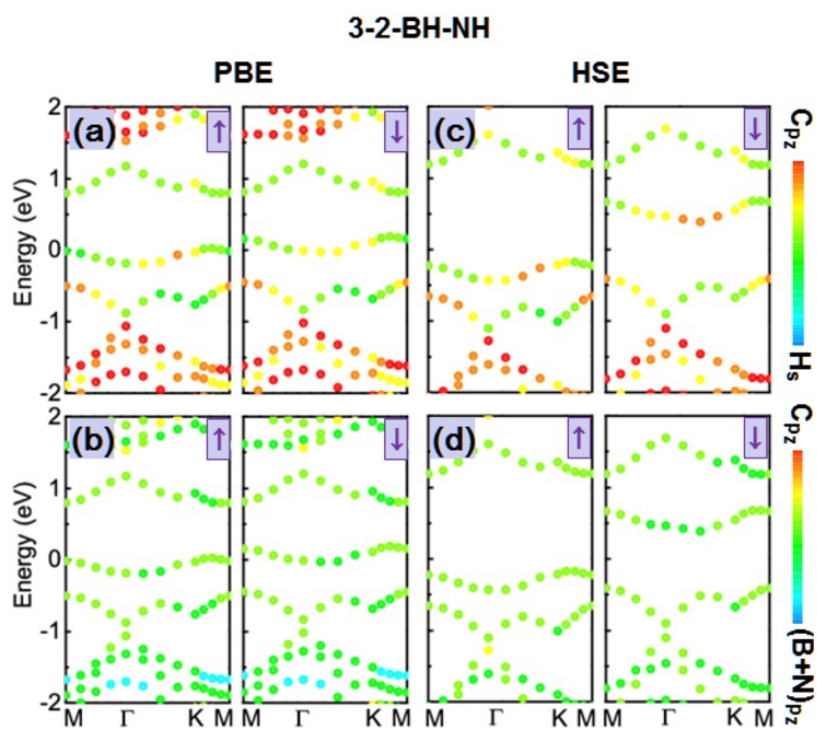


Figure S3. For 3-2-BH-NH, spin polarized projected bands calculated by PBE and HSE functionals. (a), (c) for weights of Cp_z and adsorbate $H s$, while (b), (d) for weights of Cp_z and doped $(B+N) p_z$.