Electronic Supplementary Information (ESI)

Tuning Band Gaps of BN Nanosheets and Nanoribbons via Interfacial Dihalogen Bonding and External Electric Field

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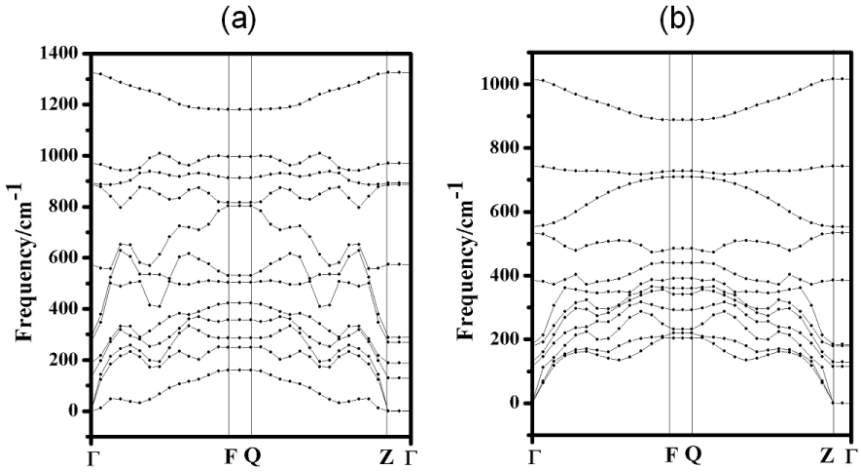

Fig. S1 Phonon dispersion structure of monolayer fluoro-BN (a) and chloro-BN (b).

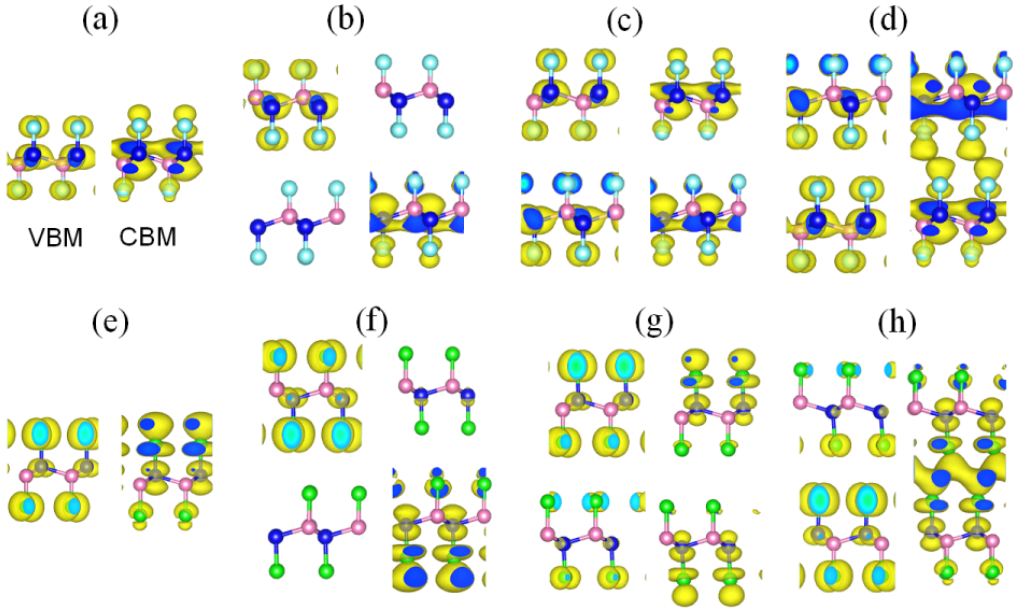

Fig. S2 Partial charge densities of VBM (left) and CBM (right) states at the Γ point for monolayer fluoro-BN (a), AB-stacked bilayer fluoro-BN with interlayer B-F···F-N (b), B-F···F-B (c), and N-F···F-N (d) connections. (e) to (h) correspond to the VBM and CBM distributions of monolayer chloro-BN, AB-stacked bilayer chloro-BN with interlayer B-Cl···Cl-N, B-Cl···Cl-B, and N-Cl···Cl-N connections, respectively.

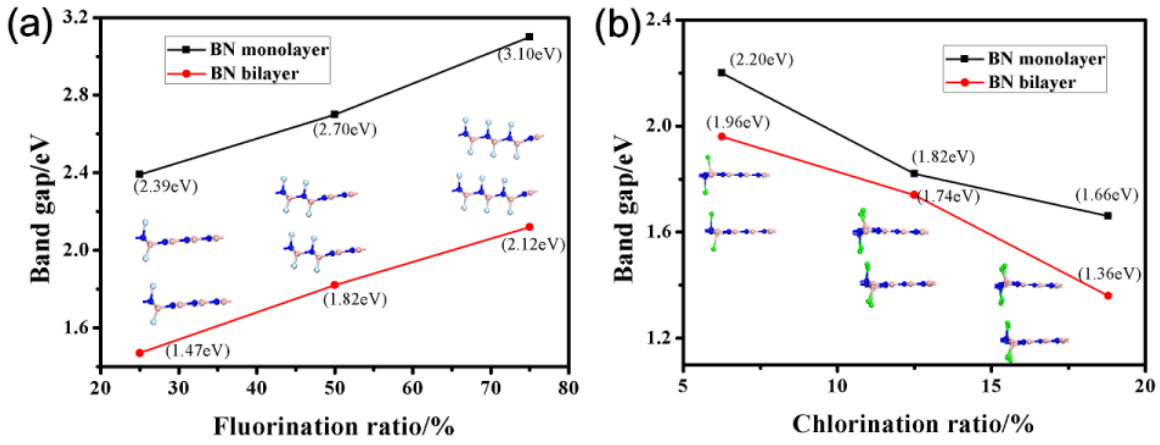

Fig. S3 The band gap of partially fluorinated (a) and chlorinated (b) BN monolayers and bilayers as a function of fluorination or chlorination ratio, and the bilayer structures corresponding to different ratios are shown in the inset.

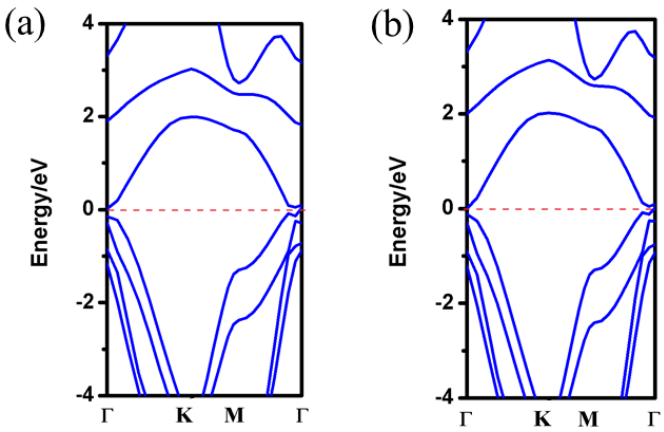

Fig. S4 Band structure of hybrid fluoro-BN/chloro-BN bilayer based on HSE06 computations with a mixing parameter of 0.2 (a) and 0.15 (b), respectively.