Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information:

Novel Two-Dimensional Tetrahexagonal Boron Nitride with Sizable bandgap and Sign-Tunable Poisson's Ratio

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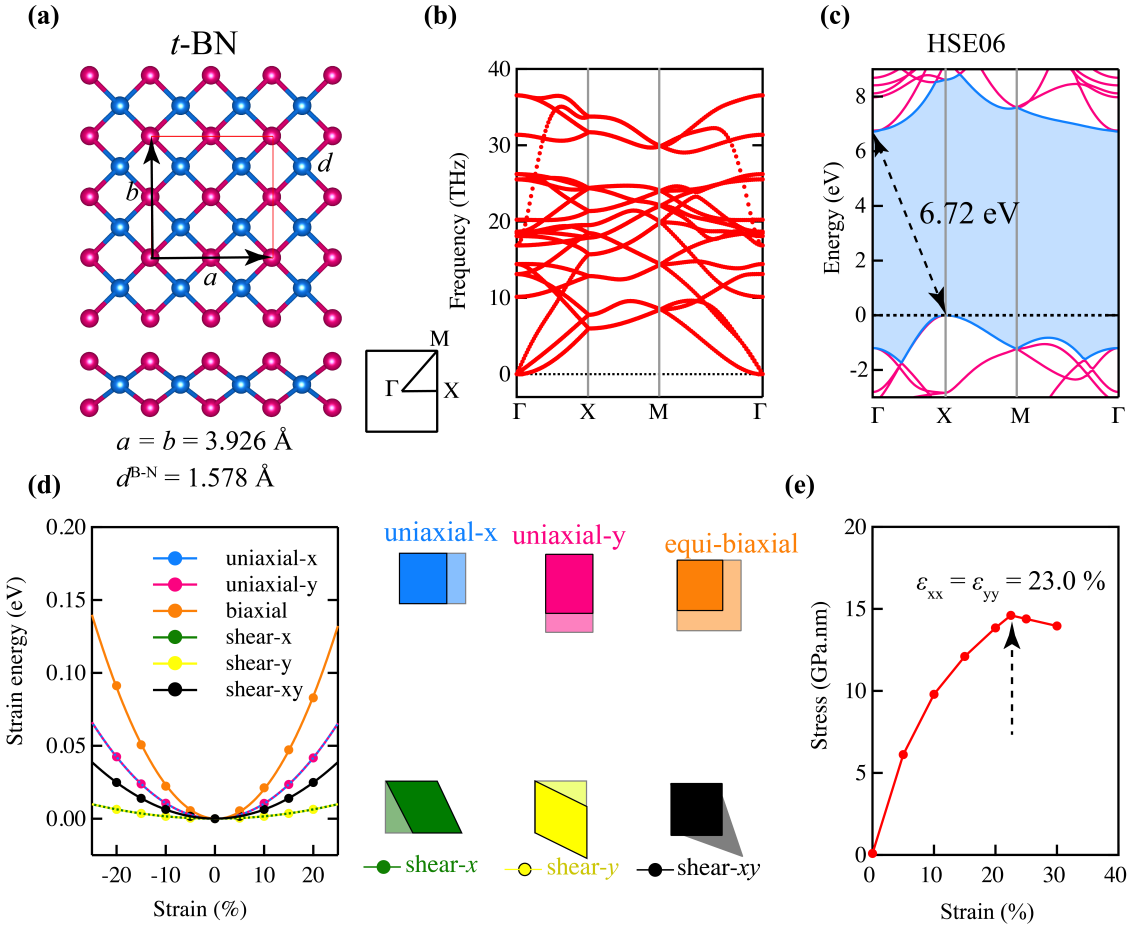
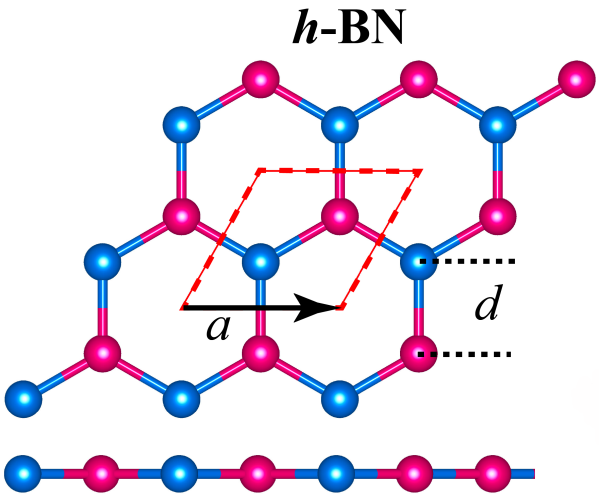


Figure S1: (a) Optimized atomic structure, (b) phonon band dispersions along with the high symmetric k points given by the 2D rectangular Brillouin zone (inset), (c) electronic band structure obtained from the HSE06 hybrid functional method, and (d) strain energy as a function of various strains of t-BN. The Fermi level energy in (c) is set to zero (depicted by the black dashed line). Blue and pink spheres in (a) refer to B and N atoms, respectively. (e) Stress-strain curve for equi-biaxial tensile strain of t-BN.



$a^{\mathrm{PBE}} = 2.513$ Å

$d^{\mathrm{PBE}} = 1.451$ Å

$a^{\mathrm{LDA}} = 2.490$ Å

$d^{\mathrm{LDA}} = 1.437$ Å

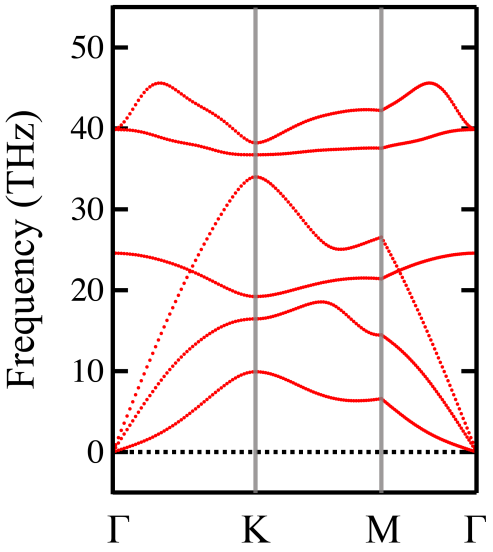


Figure S2: Optimized atomic structure (upper panel) and phonon band dispersions (lower panel) of hexagonal BN (h-BN). The lattice constant a and bond length d obtained from the LDA and PBE functional level are depicted inset of the Figure S2.

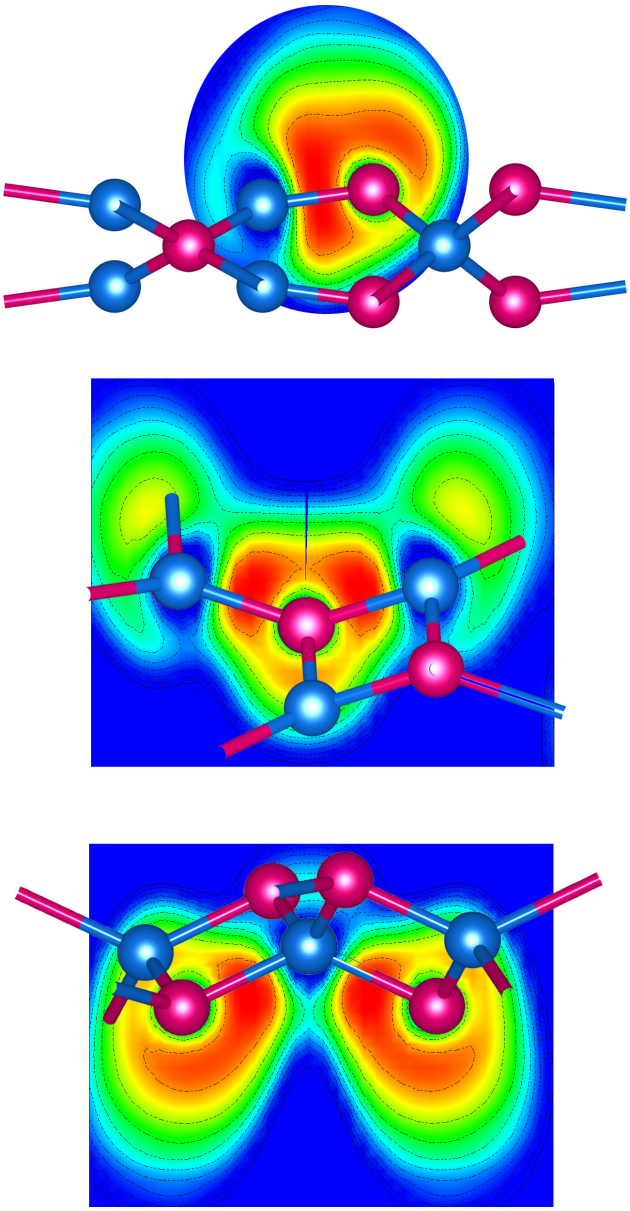


Figure S3: Electron local function (ELF) of *th*-BN. The specific 2D-slice projections are chosen to show the bonds between 3-fold coordinated B and N atoms (B^3-N^3) (upper panel), between 3-fold coordinated B and 4-fold coordinated N atoms (B^3-N^4) (middle panel), and between 4-fold coordinated B and 3-fold coordinated N atoms (B^4-N^3) (lower panel). The ELF is dimensionless, and has a range from 0 (in blue color) to 1 (in red color). ELF=1 means highly localized and bounded electrons, while ELF=0 means lack of electron.

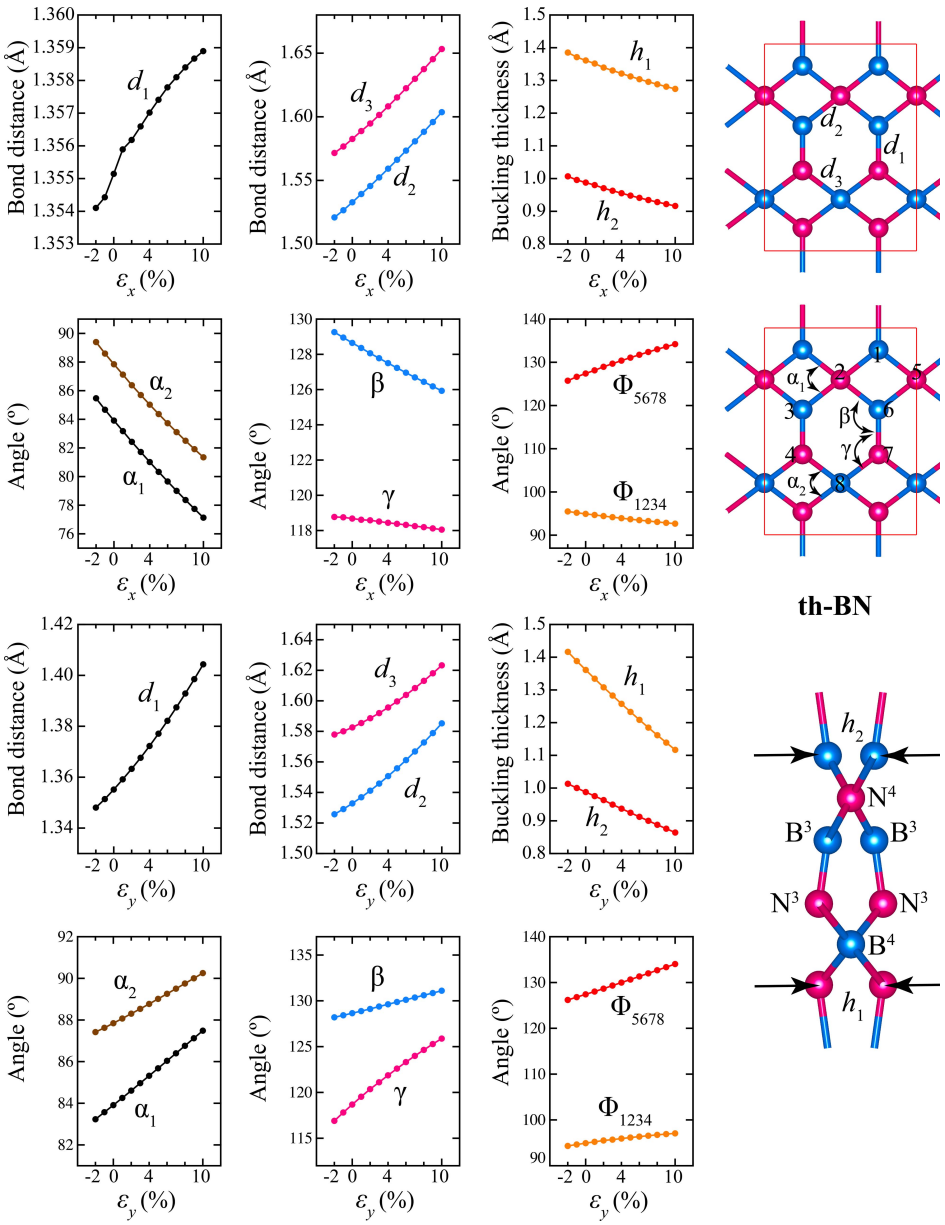


Figure S4: The variation of bond length d_1, d_2, and d_3, buckling height h_1 and h_2, bond angles, and dihedral angles for *th*-BN with respect to zigzag strain (ε_x) and armchair strain (ε_y).

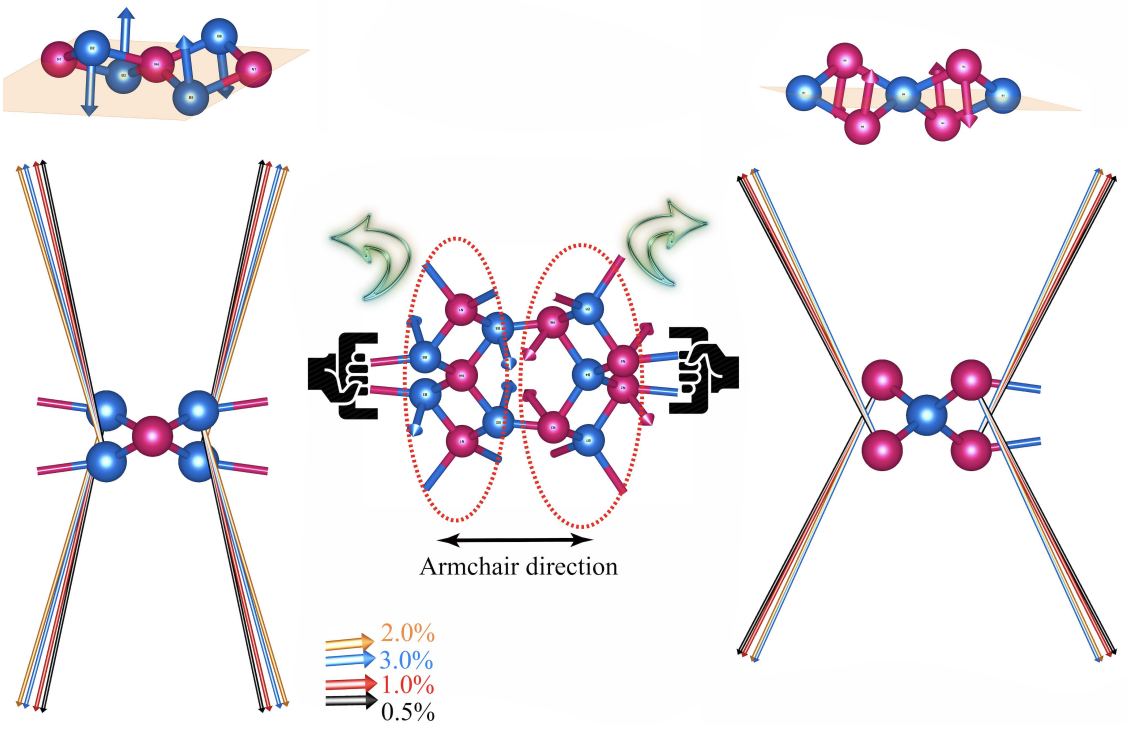


Figure S5: The moving atom directions of *th*-BN when subjected to various armchair strains ranging from 0.5 to 3.0%. Sky blue and pink balls represent B and N atoms, respectively.

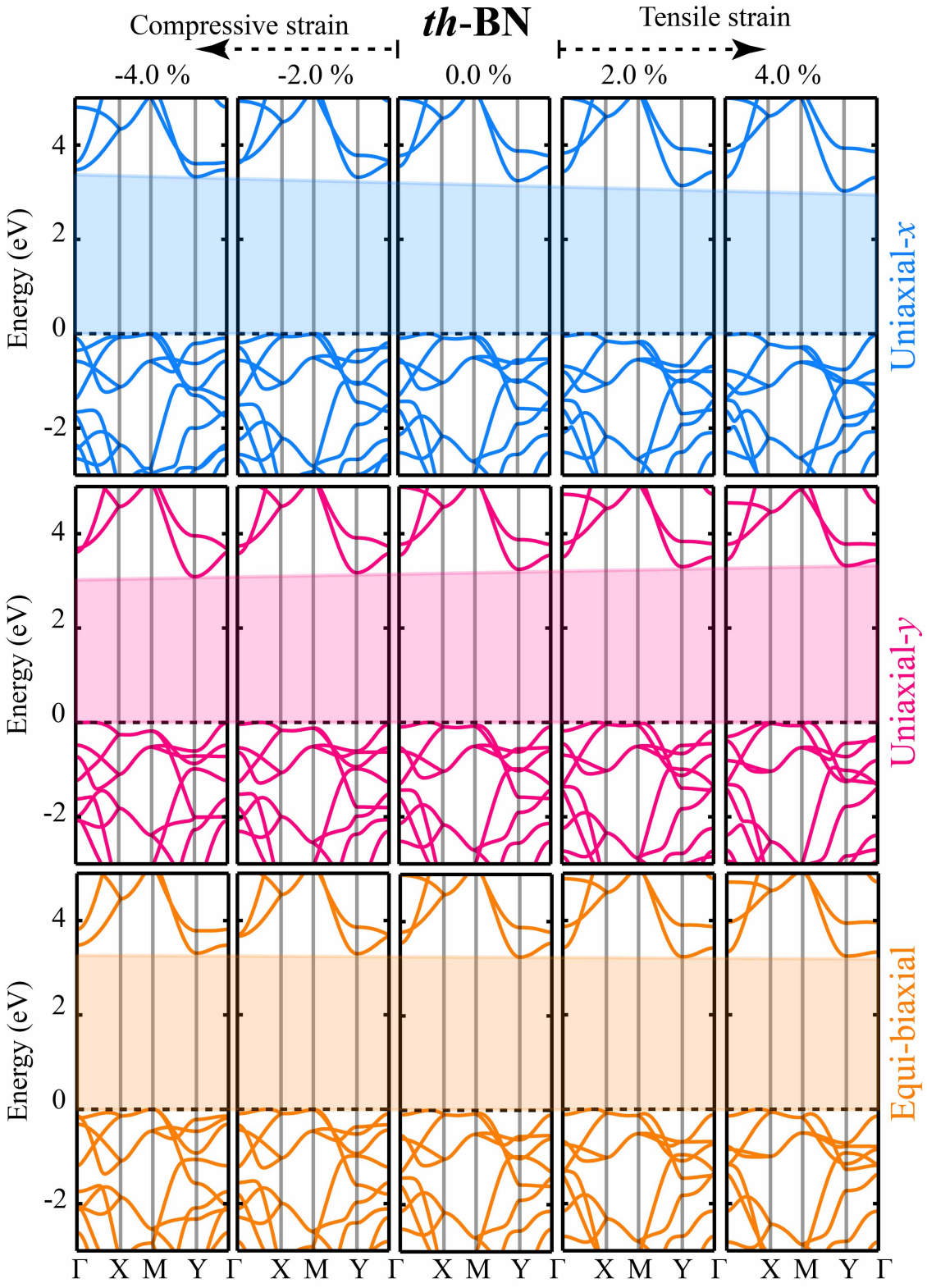


Figure S6: The HSE06 hybrid functional electronic band structures of *th*-BN when subjected to zigzag, armchair, and equi-biaxial compressive and tensile strains ranging from -4% to 4%.

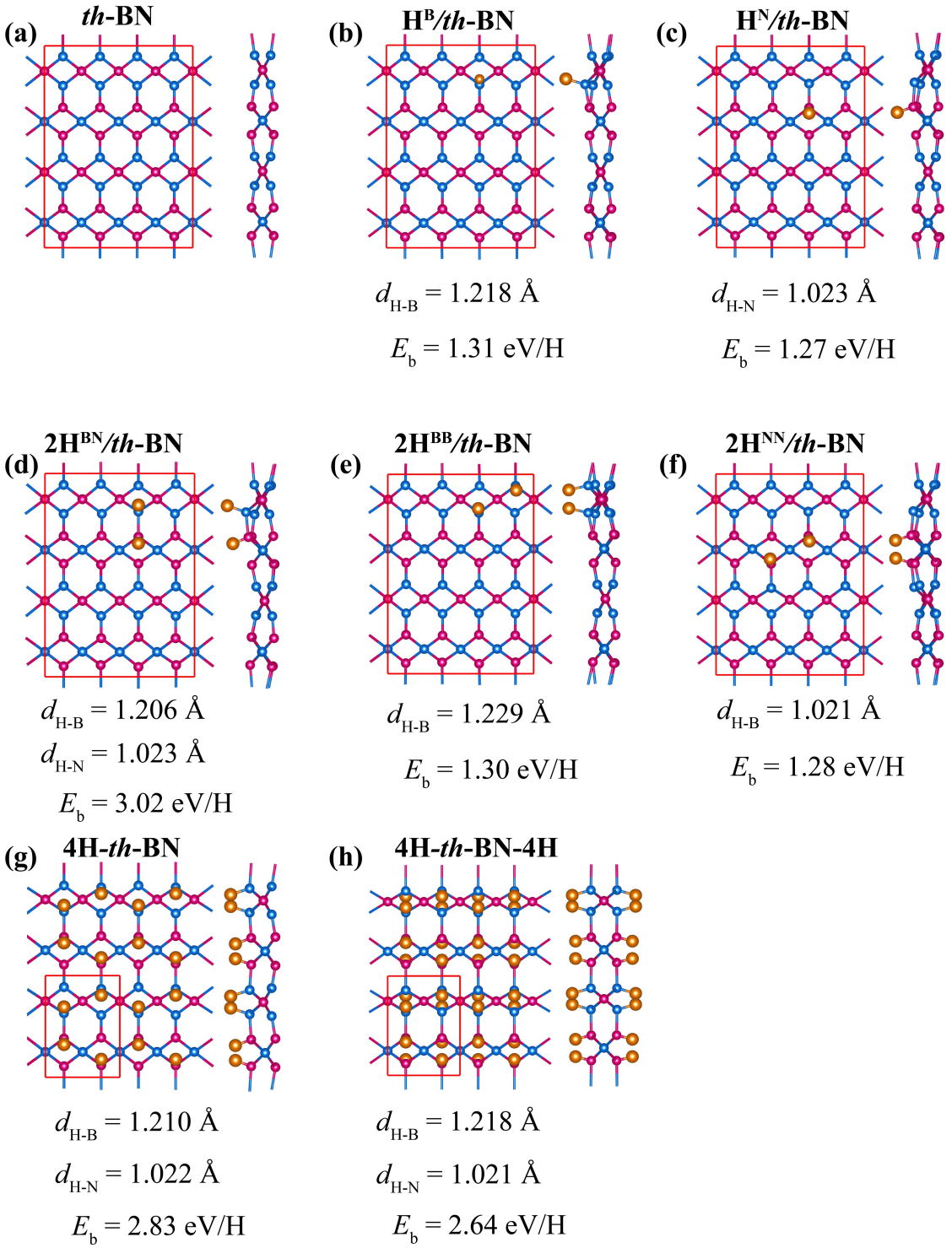


Figure S7: Optimized atomic structures of *th*-BN and its hydrogenated derivatives. The bond length between hydrogen atom and its adsorbed atom (B or/and N), and the calculated H binding energy values are depicted inset of the Figure S7.