Supplementary Information:

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

Mehmet Emin Kilic* and Kwang-Ryeol Lee*

Computational Science Center, Korea Institute of Science and Technology, Seoul 136-791, Republic of Korea

E-mail: mekilic@kist.re.kr; krlee@kist.re.kr
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.
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 ($\varepsilon_x$) and armchair strain ($\varepsilon_y$).
Figure S5: The moving atom directions of \textit{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 \textit{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.