Supplementary Information

Energetics of hexagonal boron nitride nanostructures: edge dependence and truncation effect

Xiaoxiao Fu[a], Ruiqin Zhang*[a]

To validate the reliability of the results obtained by SCC-DFTB, structures and $E/n_{B\text{-}N}$ evaluation for reprehensive models are calculated by DFT method additionally with LDA exchange-correlation functional available in SIESTA program. As shown in Figure S1 and S2, both the relaxed structures and the trend of energy obtained by DFT method show very similar results with those obtained using SCC-DFTB method.

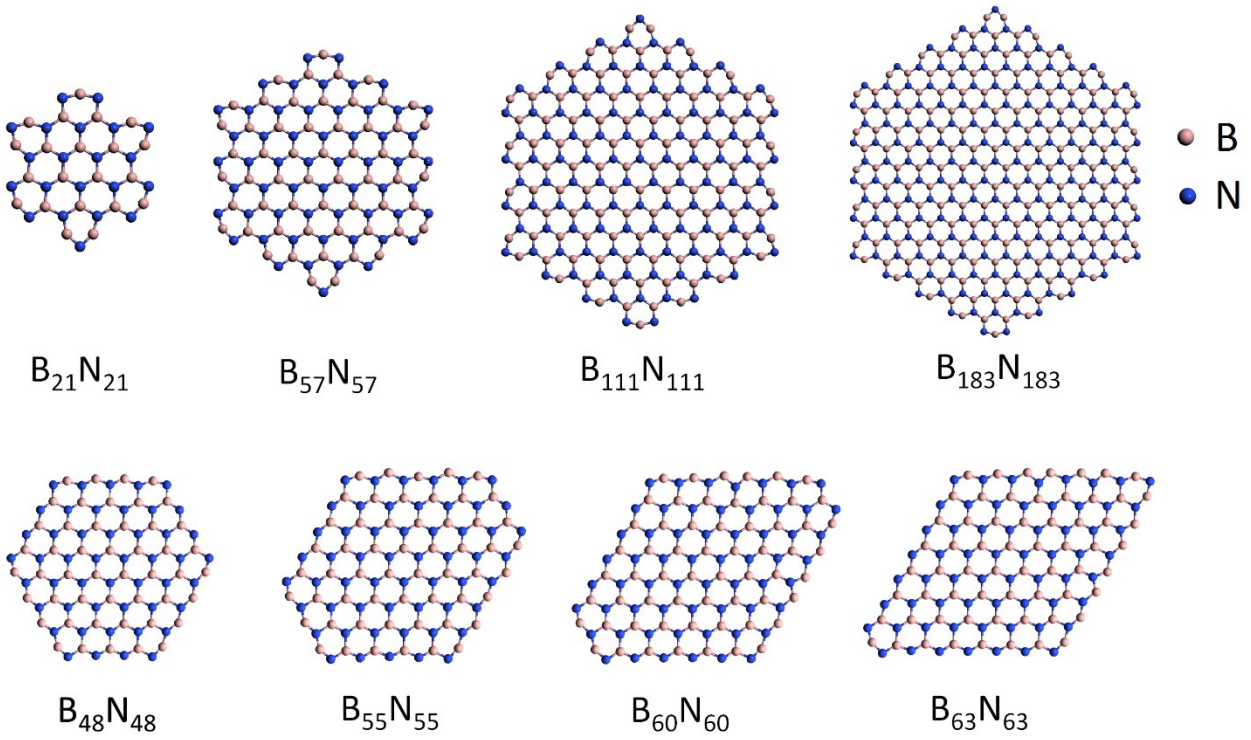

Figure S1 Relaxed structures of hexagonal models with armchair edges, and 8×8 rhombic series (from intact to truncated models) with alternating B- and N-rich zigzag edges by DFT method with LDA exchange-correlation functional.

[a] *Department of Physics and Materials Science, City University of Hong Kong, Hong Kong SAR, China. Email: aprqz@cityu.edu.hk*

There is a small discrepancy of the DFT results and SCC-DFTB results in the relative energy of $B_{55}N_{55}$ and $B_{60}N_{60}$ as shown in Figure S2. This is caused by the small difference of relaxed structures by DFT method and SCC-DFTB method, where we employed high-level-precision calculation by DFT method (Basis size is DZP for both B and N atoms; Mesh cutoff is 300.0 Ry; and Energy shift is 100 meV) compared with that performed SCC-DFTB using Slater-Koster files (parameter details: exchange-correlation functional is LDA; basis involves 2s and 2p shells; and repulsive potential is generated referring to the data of $B_3N_3H_6$ borazine system obtained by PBE/DZVP/GEN-A2* within Ab-initio code). Except the negligible discrepancy in energy discussed above, the main conclusion remains the same. These results demonstrated that SCC-DFTB method is reliable in revealing the energetics and morphologies of the h-BN nanosheets in our work.

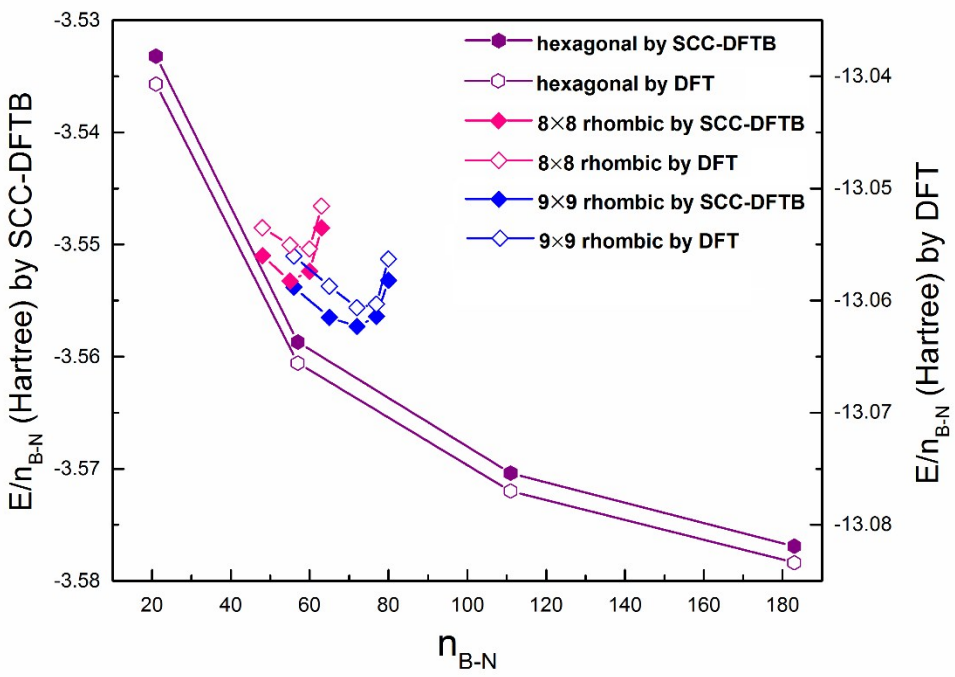

Figure R2 $E/n_{B\text{-}N}$ values of B-N pair numbers in hexagonal h-BN nanosheets with armchair edges with continuously increasing lengths (denoted by the purple hexagonal symbol) and in various rhombic nanosheets (denoted by the square symbols), calculated by SCC-DFTB and DFT method.