

Supplemental Information

First-principles study on shape of intrinsic hBN island nucleated during CVD initial growth on Cu(111)

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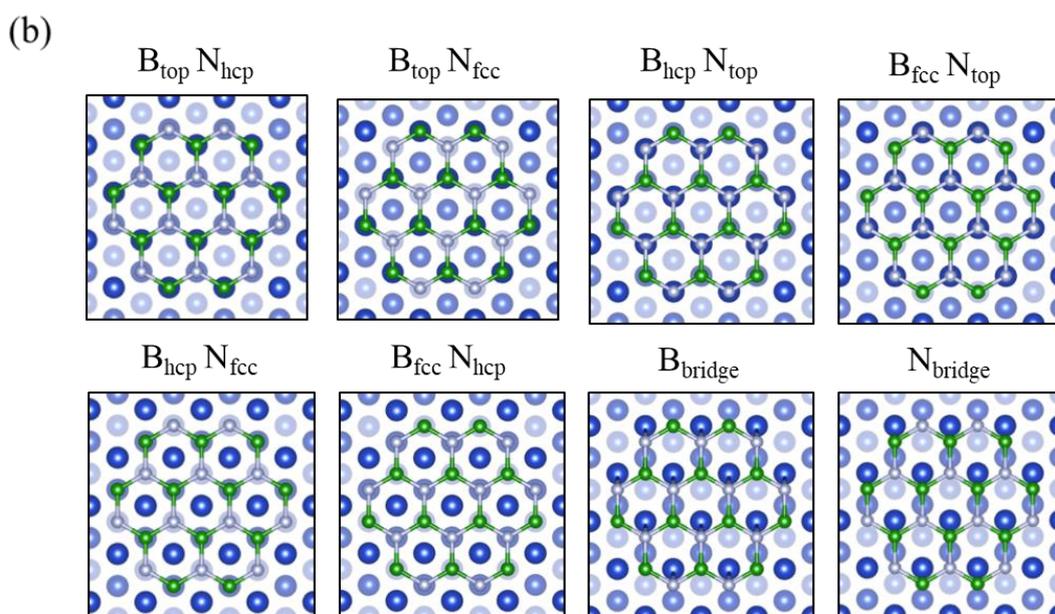
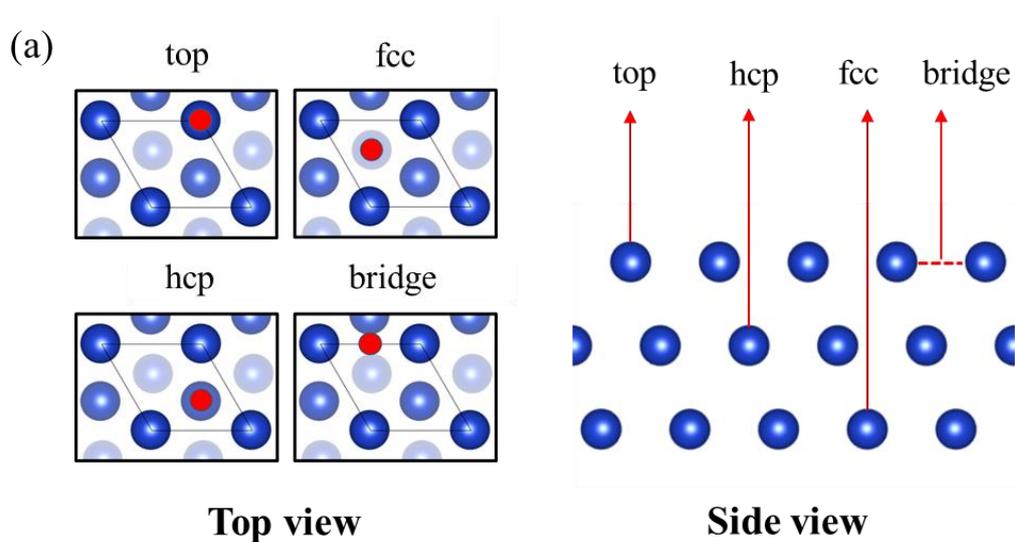


Figure S1. Type of adsorption sites and hBN configuration patterns on the Cu(111) surface. (a) Adsorption sites of top, hcp, fcc and bridge seen from top (left) and side (right) views. The grid line represents Cu(111) 1×1 size. (b) Top views of initial structures without structural optimization of eight different hBN configuration patterns on the Cu(111) surface. The configurations are named with composed elements and abbreviations of adsorption sites. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

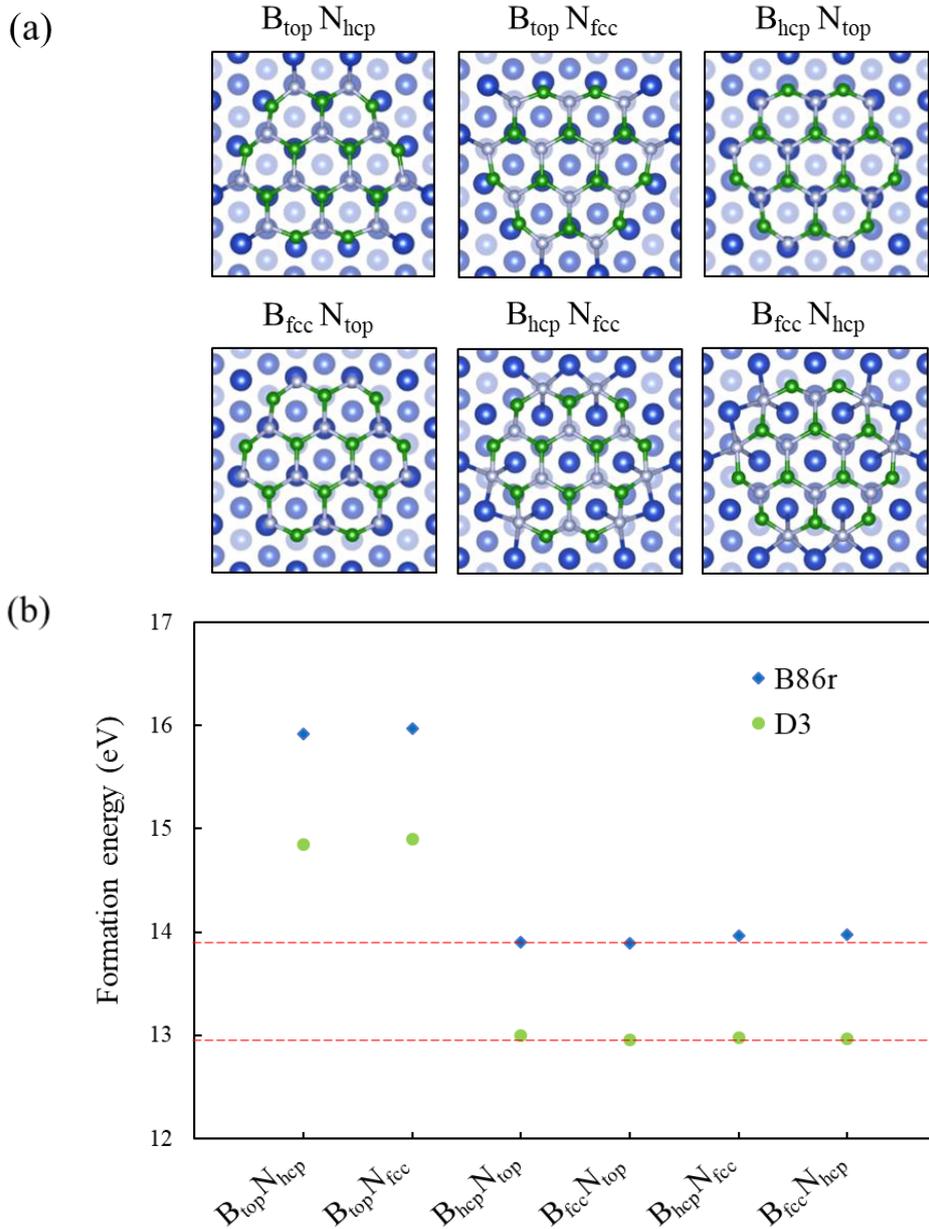
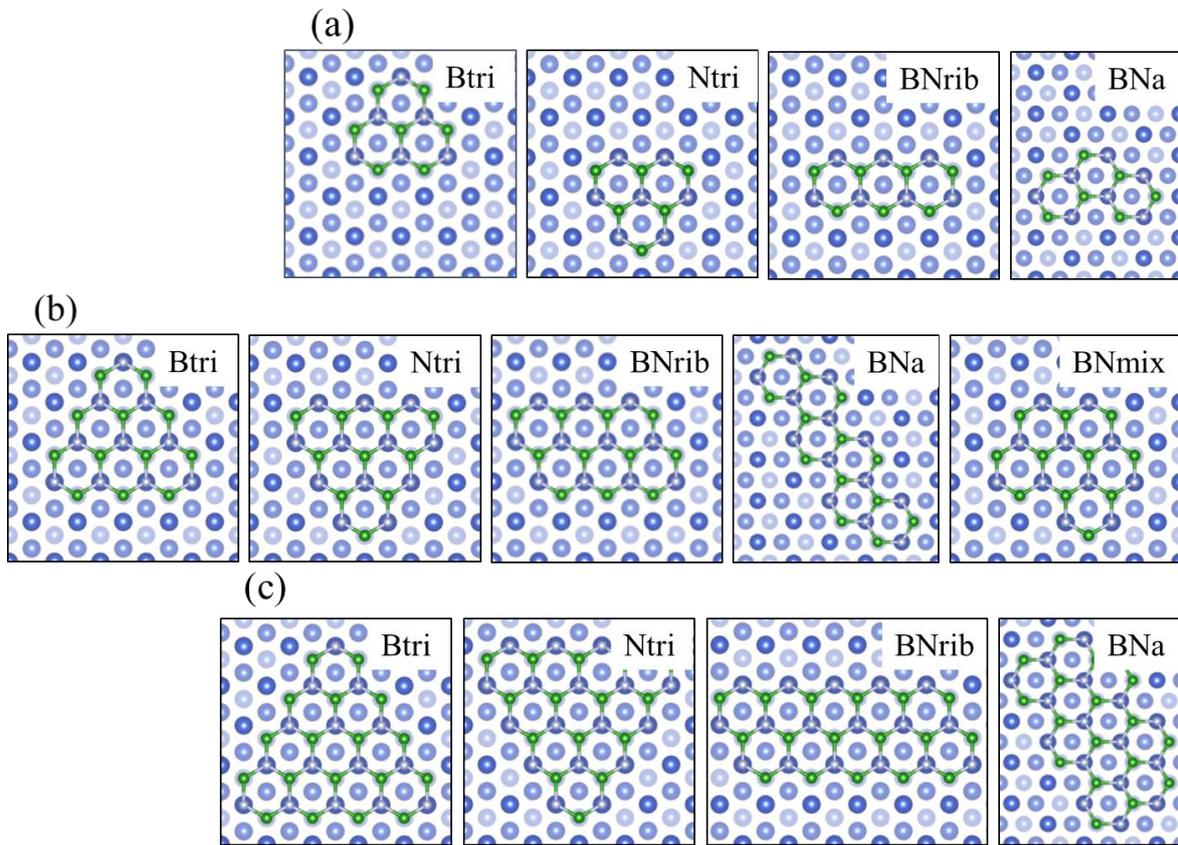


Figure S2. Adsorption site dependence of hBN on Cu(111) surface. (a) Top views of optimized structures of six different hBN configuration patterns on the Cu(111) surface, calculated with B86r. B_{bridge} and N_{bridge} became $B_{\text{hcp}}N_{\text{top}}$ and $B_{\text{fcc}}N_{\text{top}}$, respectively, through structural optimization. (b) Formation energies of hBN on Cu(111) surface as the function of configuration pattern. The configurations are named with composed elements and abbreviations of adsorption sites. Calculations using B86r show that the $B_{\text{fcc}}N_{\text{top}}$ is the most stable, only 0.006 eV lower than the next most stable configuration, $B_{\text{hcp}}N_{\text{top}}$. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.



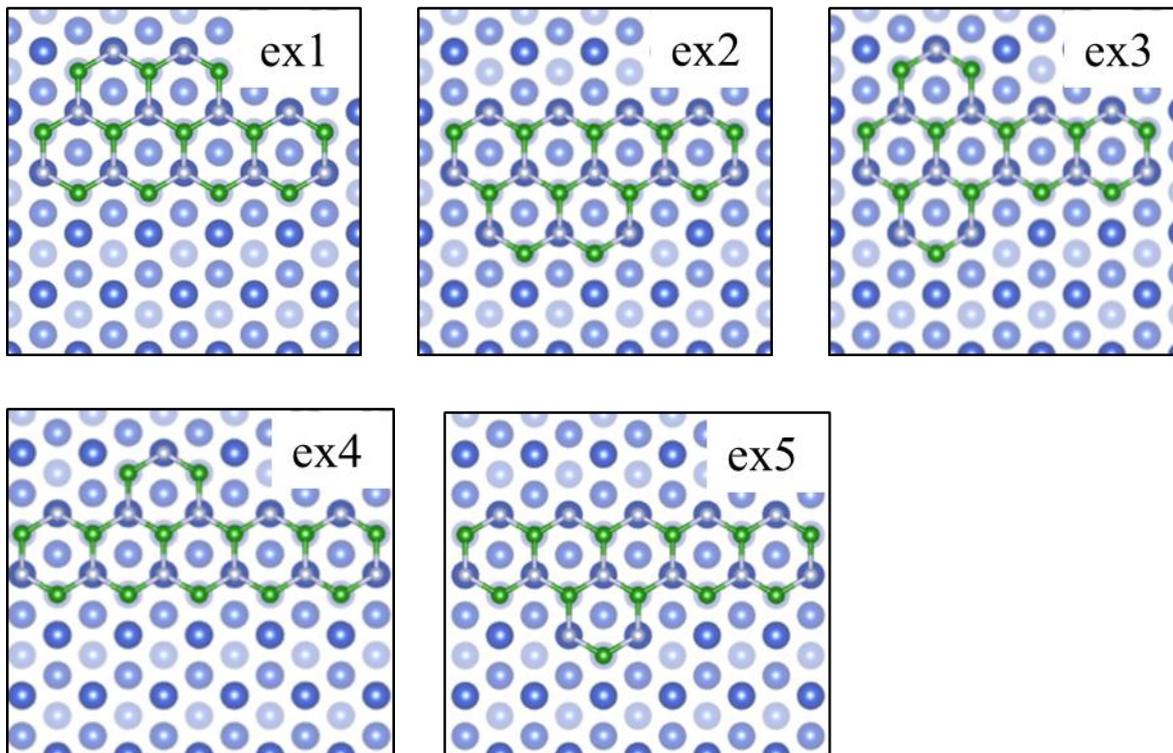


Figure S4. Top views of initial structures of ex1-ex5 of hBN islands with 6 six-membered rings. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

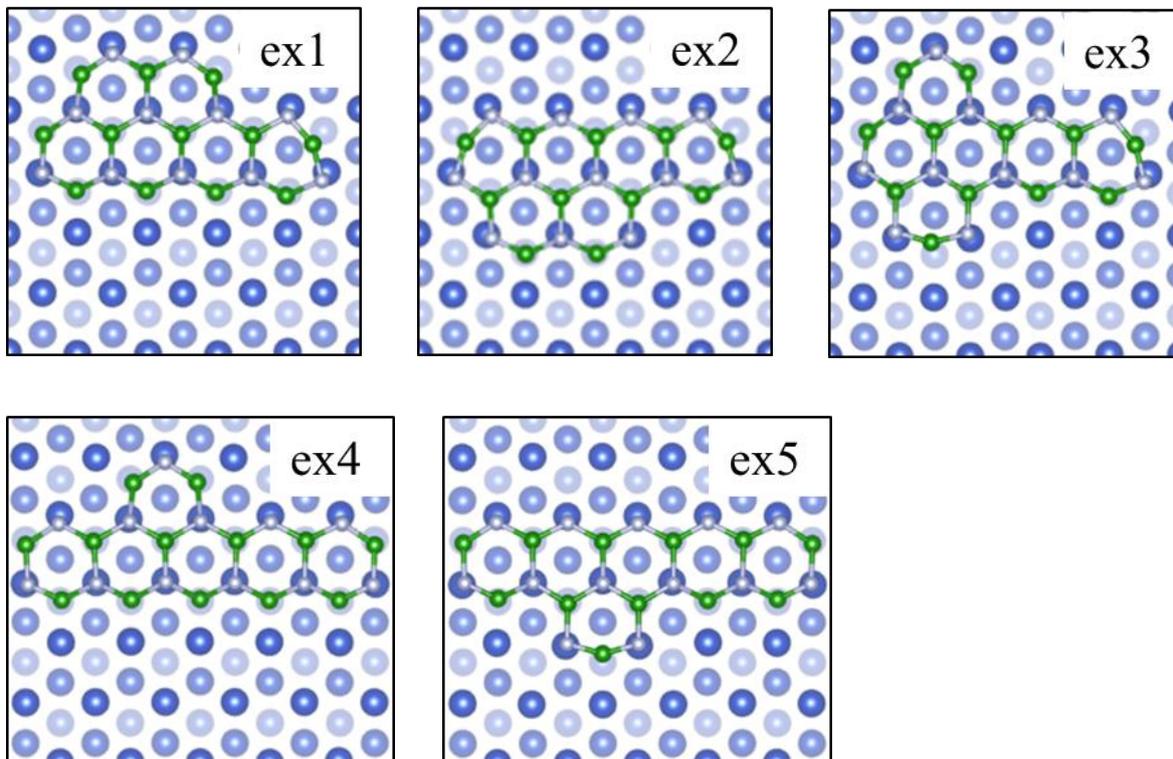


Figure S5. Top views of optimized structures of ex1-ex5 hBN islands with 6 six-membered rings, calculated with B86r. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

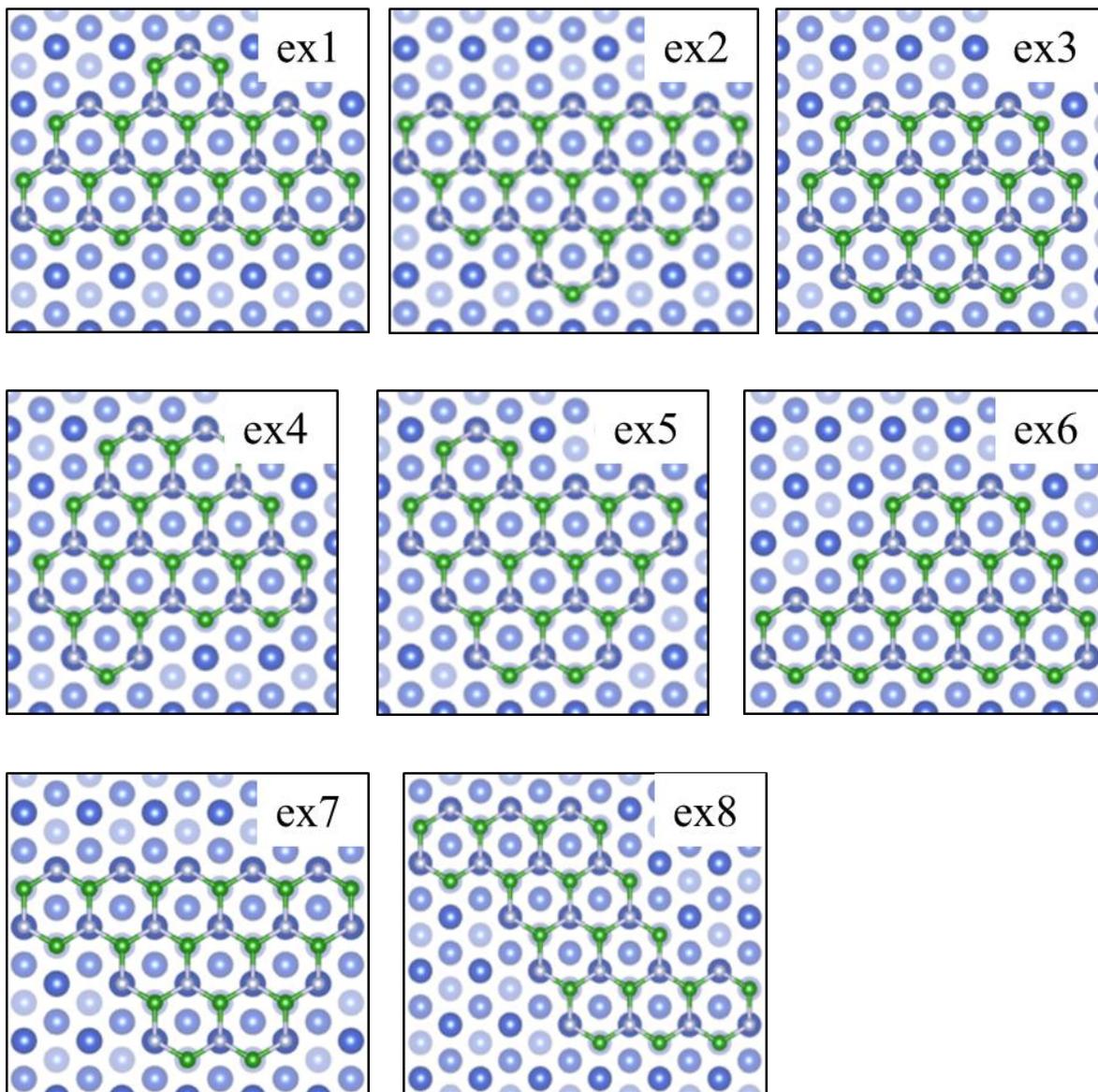


Figure S6. Top views of initial structures of ex1-ex8 hBN islands with 10 six-membered rings. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

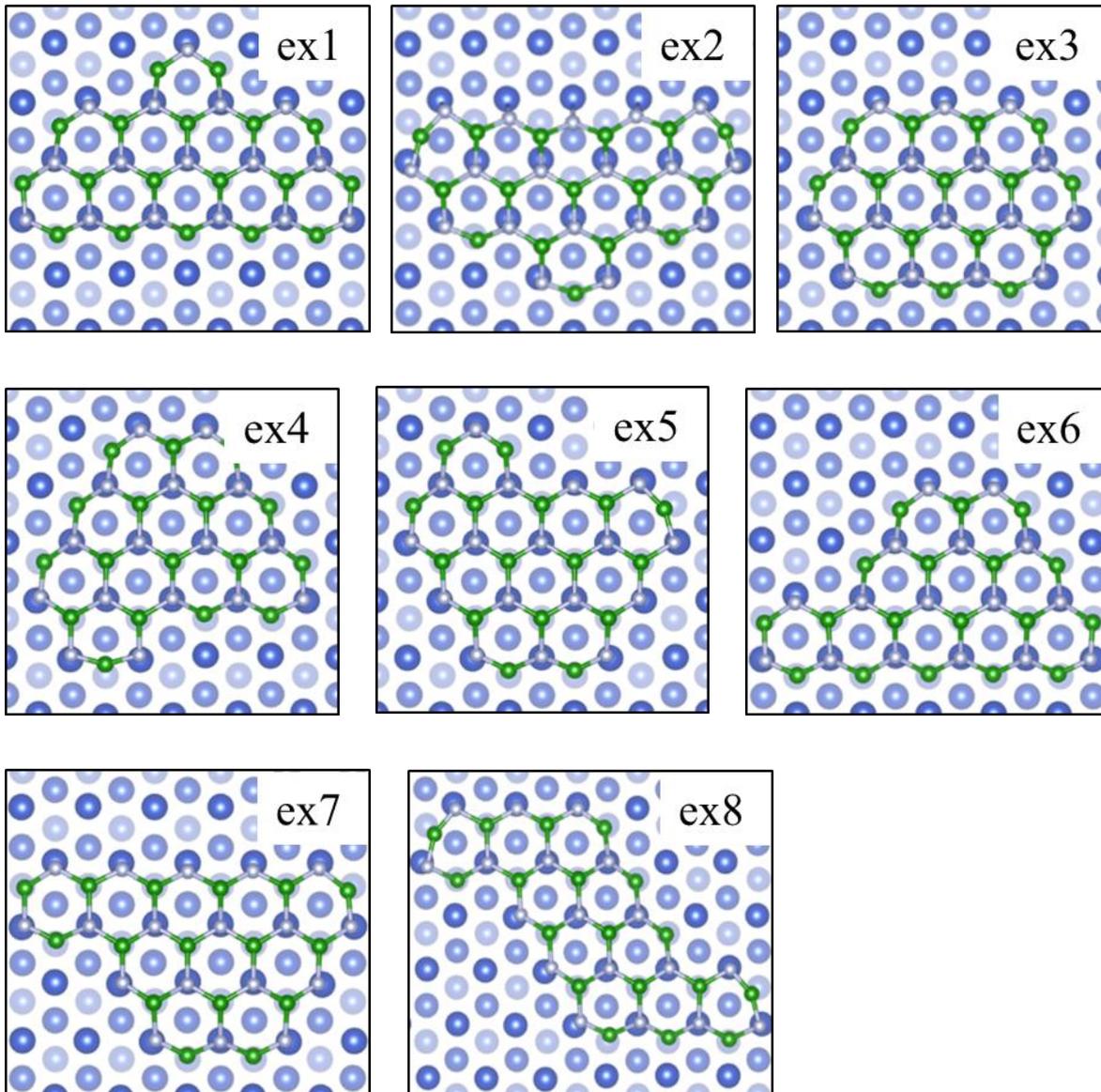


Figure S7. Top views of optimized structures of ex1-ex8 hBN islands with 10 six-membered rings, calculated with B86r. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

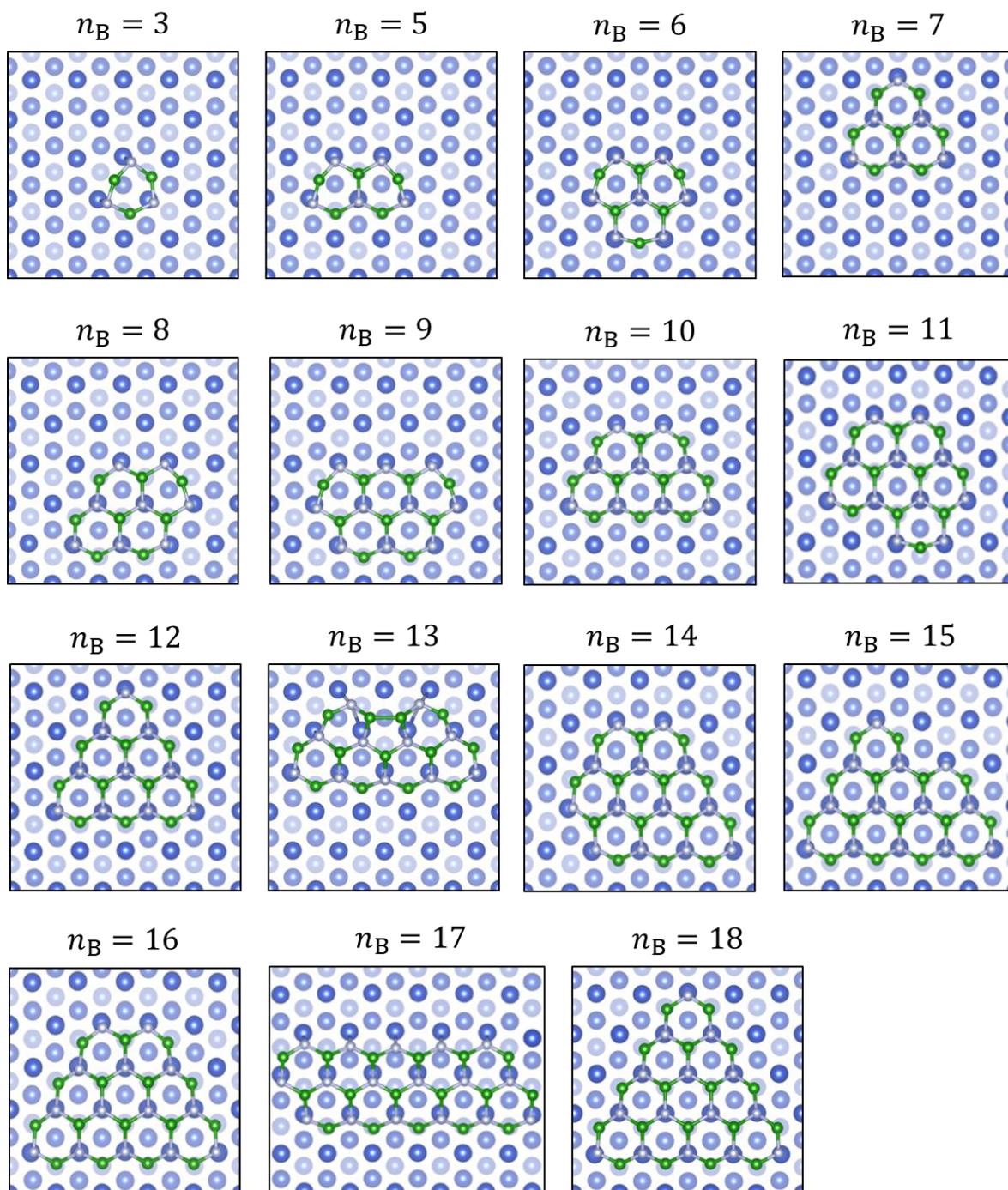


Figure S8. Top views of the most stable structures for each n_B , in the B-rich case. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

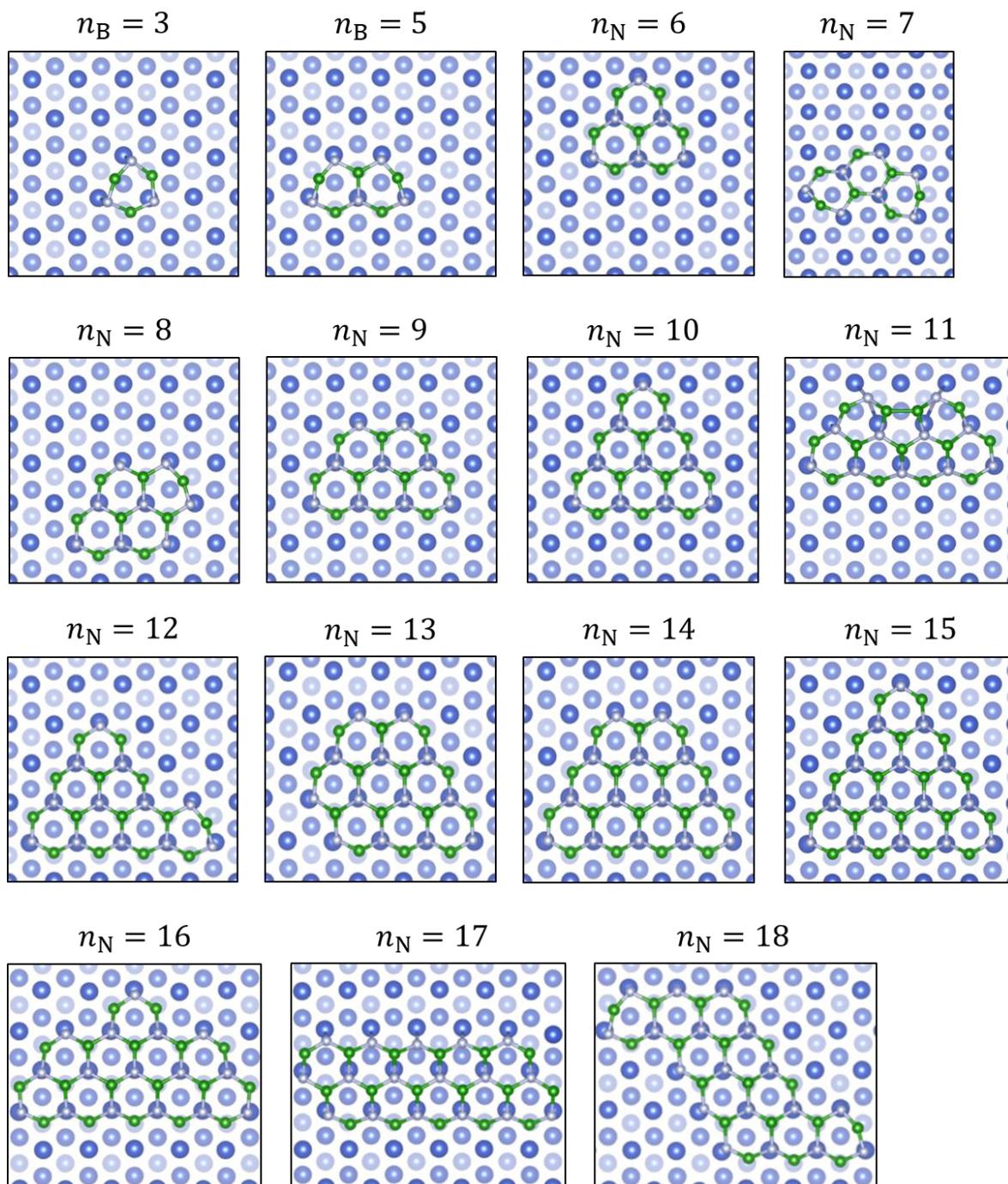


Figure S9. Top views of the most stable structures for each n_N , in the B-rich case. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

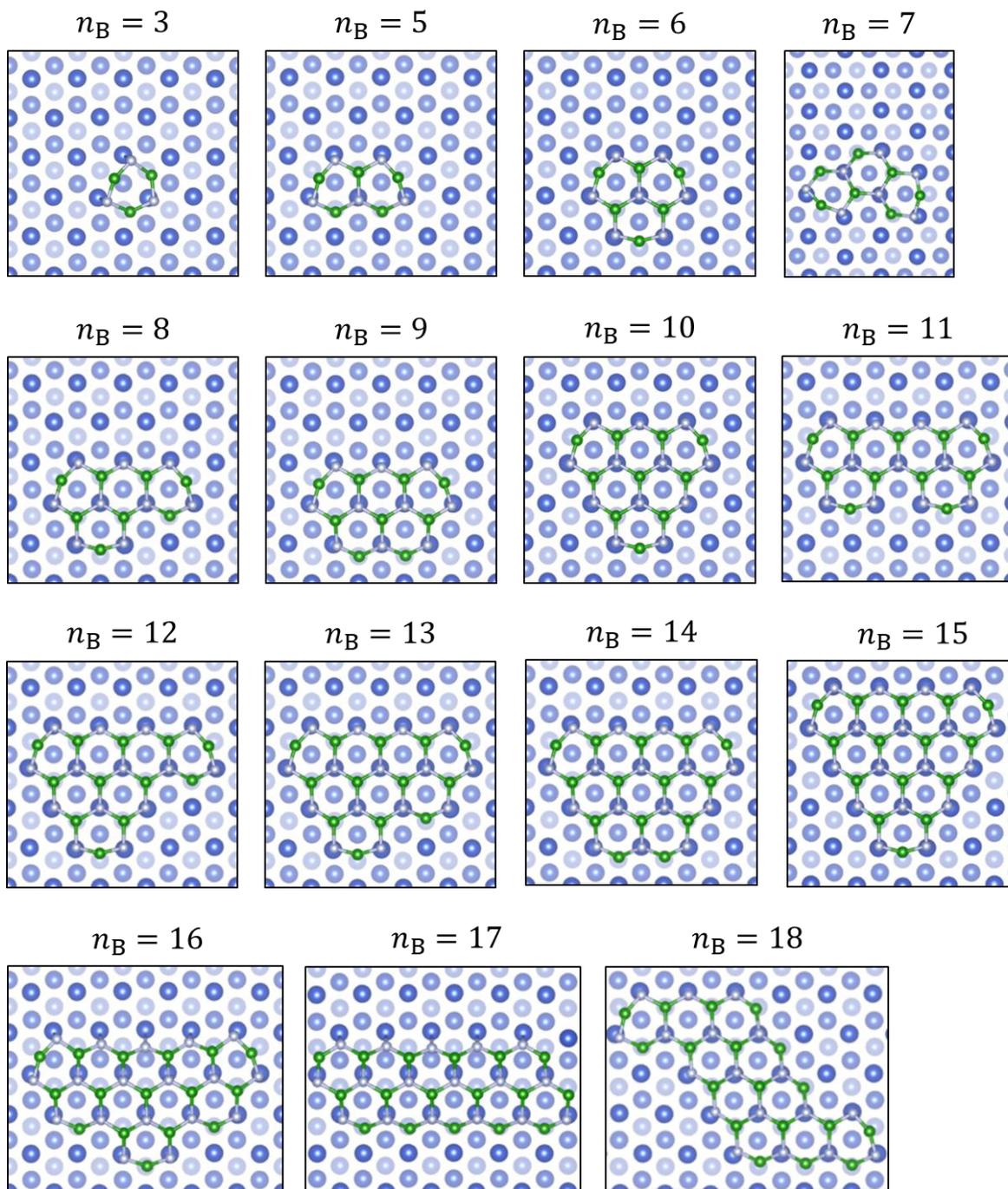


Figure S10. Top views of the most stable structures for each n_B , in the N-rich case. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

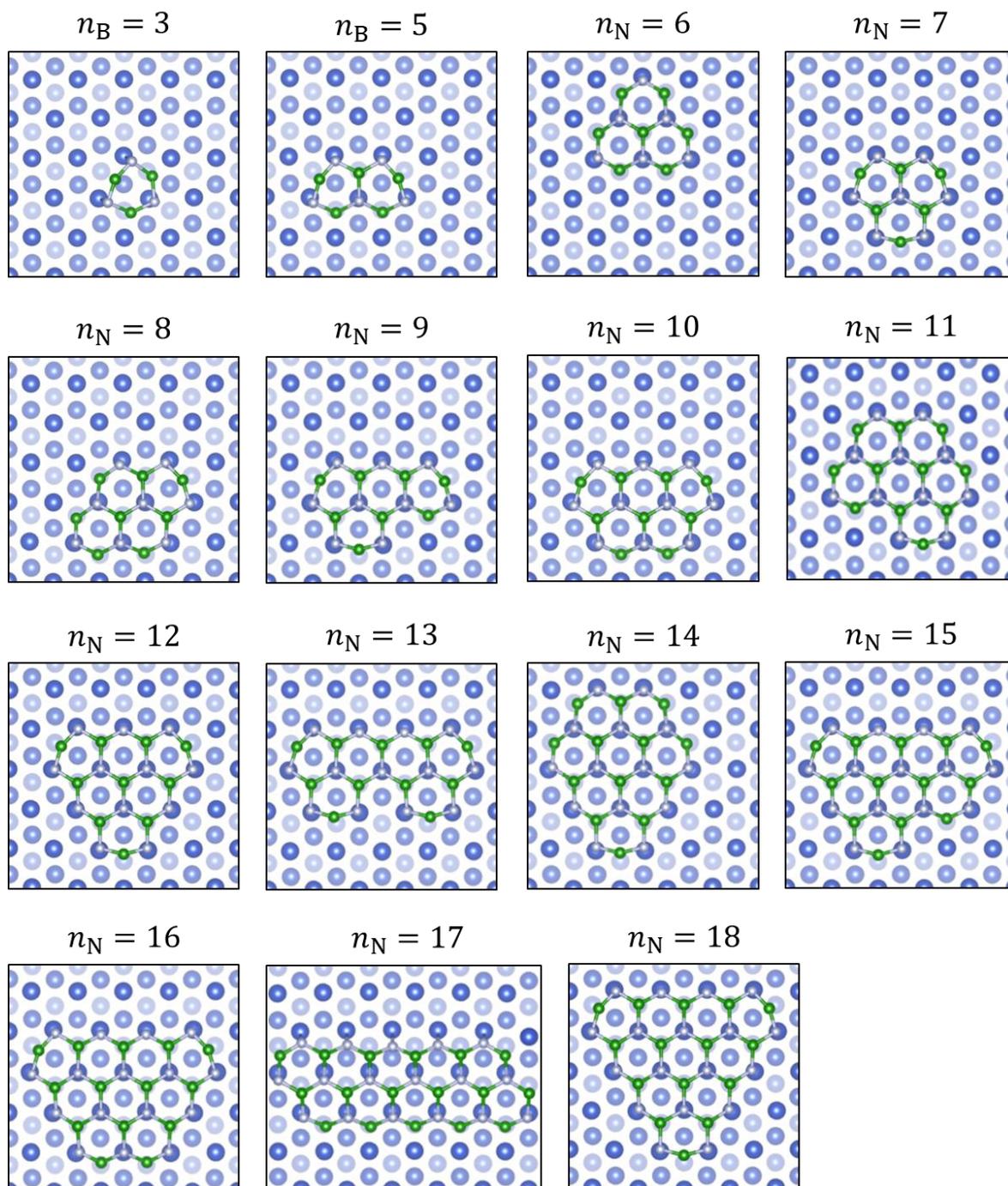


Figure S11. Top views of the most stable structures for each n_N , in the N-rich case. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

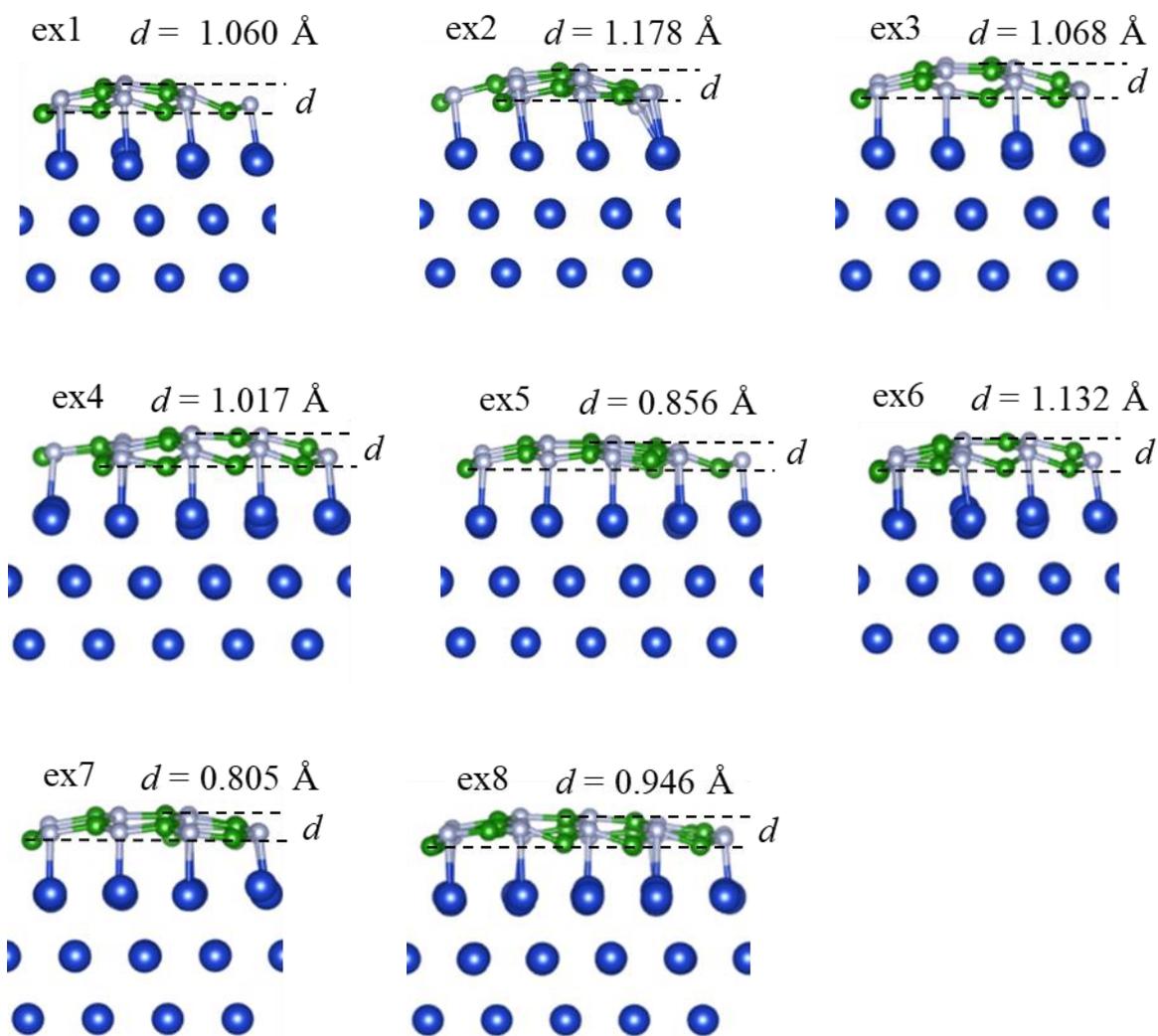


Figure S12. Side views of optimized hBN islands (ex1-ex8) with 10 six-membered rings, calculated with B86r. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

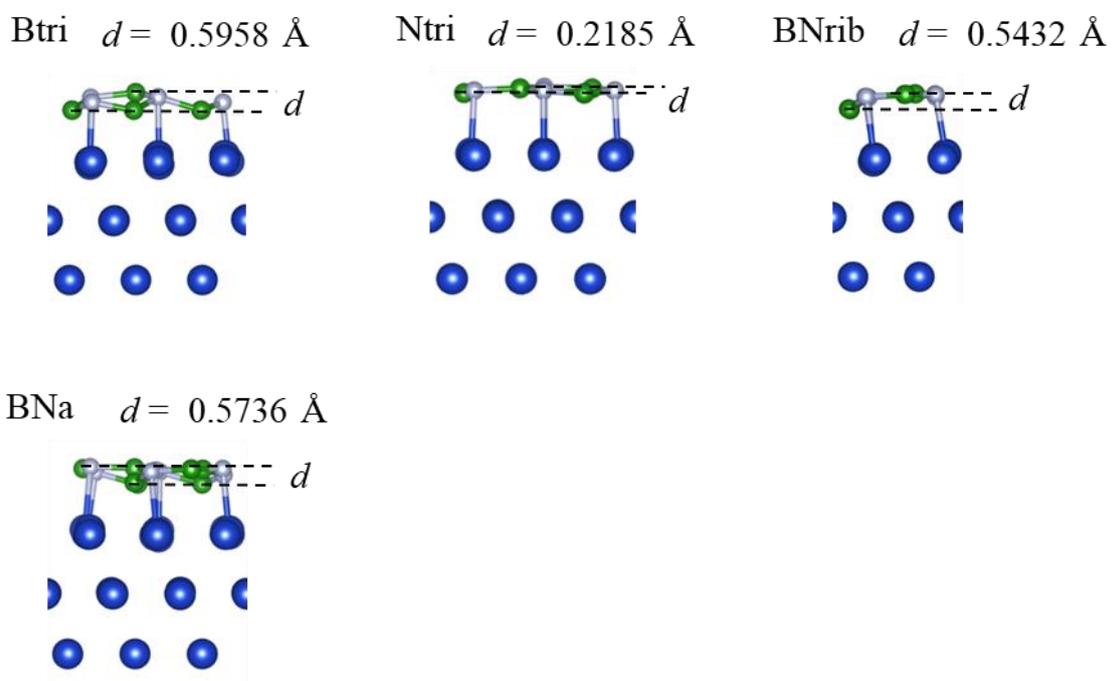


Figure S13. Side views of optimized hBN islands with 3 six-membered rings, calculated with B86r. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.

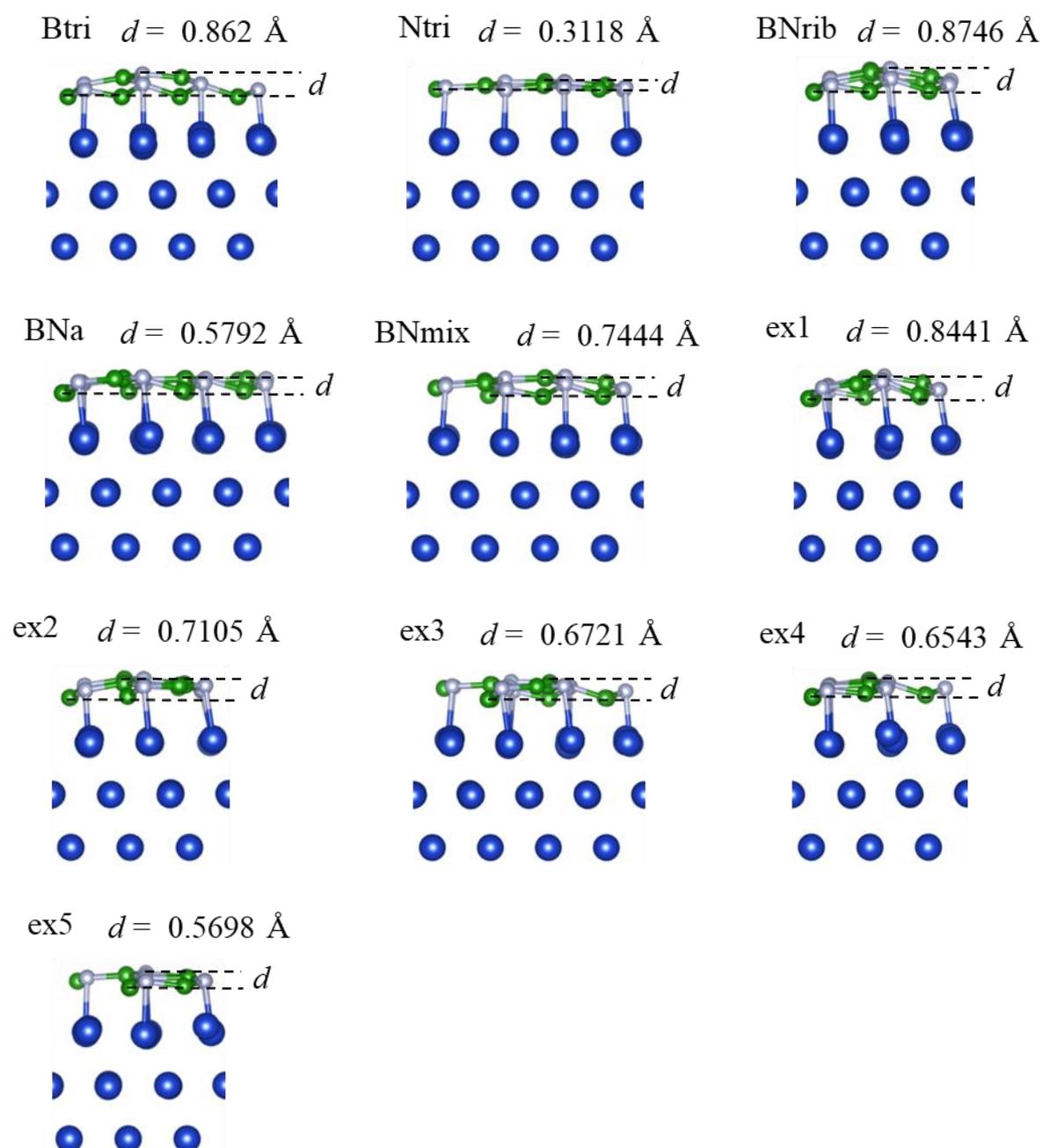


Figure S14. Side views optimized hBN islands with 6 six-membered rings, calculated with B86r. Blue, green, and silver balls represent Cu, B, and N atoms, respectively.