SUPPORTING INFORMATION

AlN Nanotube: Round or Faceted?

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SI 1. Validations of Basis Sets and Methods.

Validations for basis sets and methods have been carried out before systematic calculation with $Al_{12}N_{12}$ as model molecule. Optimized geometrical parameters and the corresponding strain energy (SE) values are listed in Table S1. From the data listed, we can see that the bond length of the model molecules are not so sensitive to the change of basis sets at the levels higher than 3-21G, so are the strain energy values. However, relatively large differences are observed for the bond angles between 3-21G or 6-31G basis sets and their correspondences with polarization functions. Therefore, the results at HF/6-31G* level are taken for discussion.

TABLE S1: Geometrical parameters and strain energy (SE) values of $Al_{12}N_{12}$ at various levels

Basis Set	$r_{Al\text{-}N(4\text{-}6)}$ [a]	$r_{Al\text{-}N(6\text{-}6)}$ [a]	$\theta_{N\text{-}Al\text{-}N(6)}$ [b]	$\theta_{N\text{-}Al\text{-}N(4)}$ [b]	SE
HF/STO-3G	1.787	1.74	125.3	94.1	0.595916
HF/3-21G	1.847	1.79	121.9	92.5	0.423466
HF/3-21G*	1.838	1.78	124.5	94.6	0.340846
HF/6-31G	1.862	1.79	122.0	91.9	0.531392
HF/6-31G*	1.841	1.78	125.0	94.7	0.400012
HF/6-31+G(d)	1.840	1.78	124.9	94.7	0.439689
MP2/STO-3G	1.826	1.77	128.1	94.6	0.425051
MP2/3-21G	1.885	1.82	122.5	92.7	0.193549
MP2/3-21G*	1.865	1.80	126.6	94.8	0.113738
MP2/6-31G	1.901	1.83	122.7	92.0	0.352384
MP2/6-31G*	1.868	1.80	126.2	94.6	0.236441

[a]: bond length of Al-N bonds (Å). $r_{Al\text{-}N(4\text{-}6)}$ and $r_{Al\text{-}N(6\text{-}6)}$ stand for bond length of Al-N bonds shared by square-hexagon or hexagon-hexagon, respectively.

[b]: angles between two adjacent Al-N bonds (degrees). $\theta_{N\text{-}Al\text{-}N(6)}$ and $\theta_{N\text{-}Al\text{-}N(4)}$ represent angles in hexagons and in squares, respectively.

SI 2. Optimized Geometry of All $(AlN)_n$ and $(BN)_n$ Clusters.

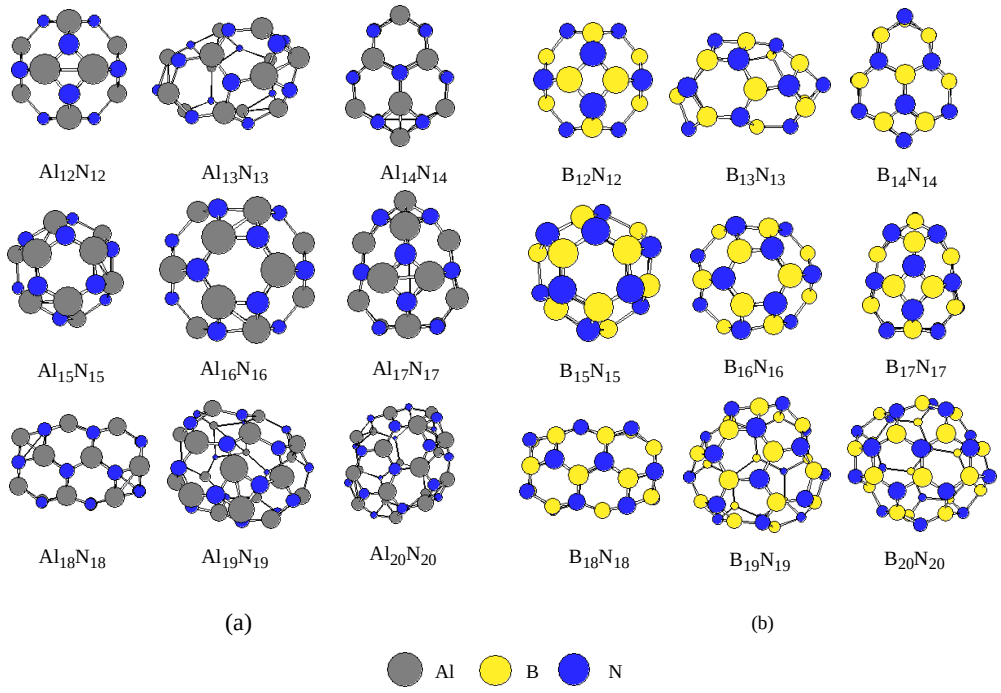


Figure S1 Optimized structures of $(AlN)_n$ and $(BN)_n$ fullerenes ($12 \leq n \leq 20$). (a) $(AlN)_n$ fullerenes; (b) $(BN)_n$ fullerenes.

SI 3. Modeling.

Model for faceted AlN nanotube is derived from the bulk crystal of wurtzite aluminum nitride. First, a four-layered AlN slab model is built (Figure S2a), which could be further modified to be AlN nanowire model (Figure S2b). Then, by removing the center atoms, the faceted AlN nanotube model is obtained with hollow interior (Figure S2c). Hydrogen atoms are finally used to saturate all the dangling bonds. Single-walled AlN nanotube model with the same number of Al and N atoms is built following the classical zig-zag (12, 0) carbon nanotube model (Figure S2d).

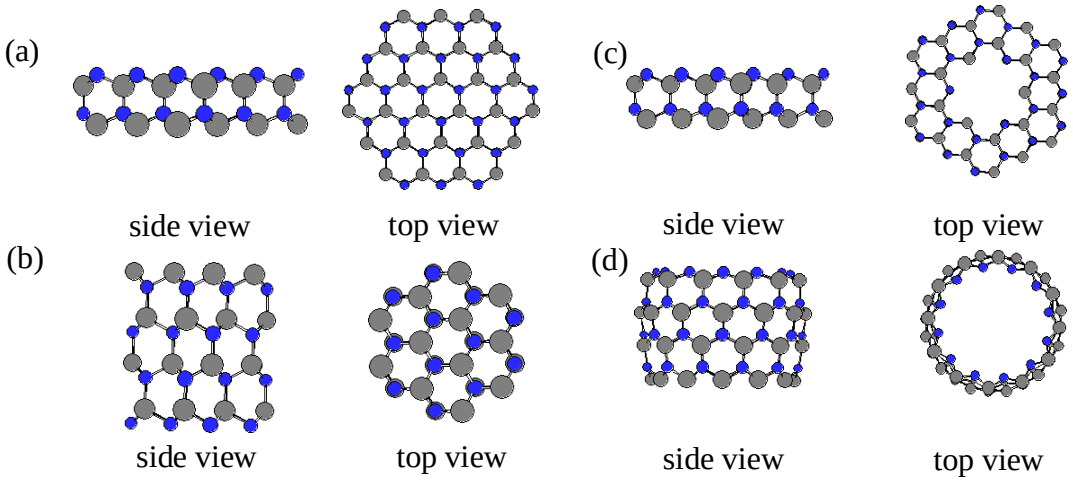


Figure S2 Models for AlN nanostructures. (a) four-layered AlN slab. (b) AlN nanowire. (c) faceted AlN nanotube. (d) single-walled AlN nanotube. Gray circles stand for Al and blue ones for N. H atoms are hidden for the sake of simplicity.

SI 4. Optimized Geometry with H Atoms Shown.

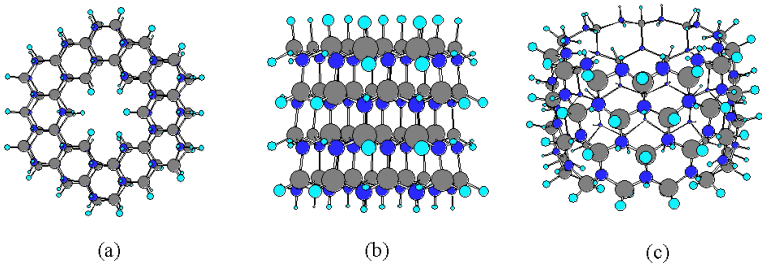
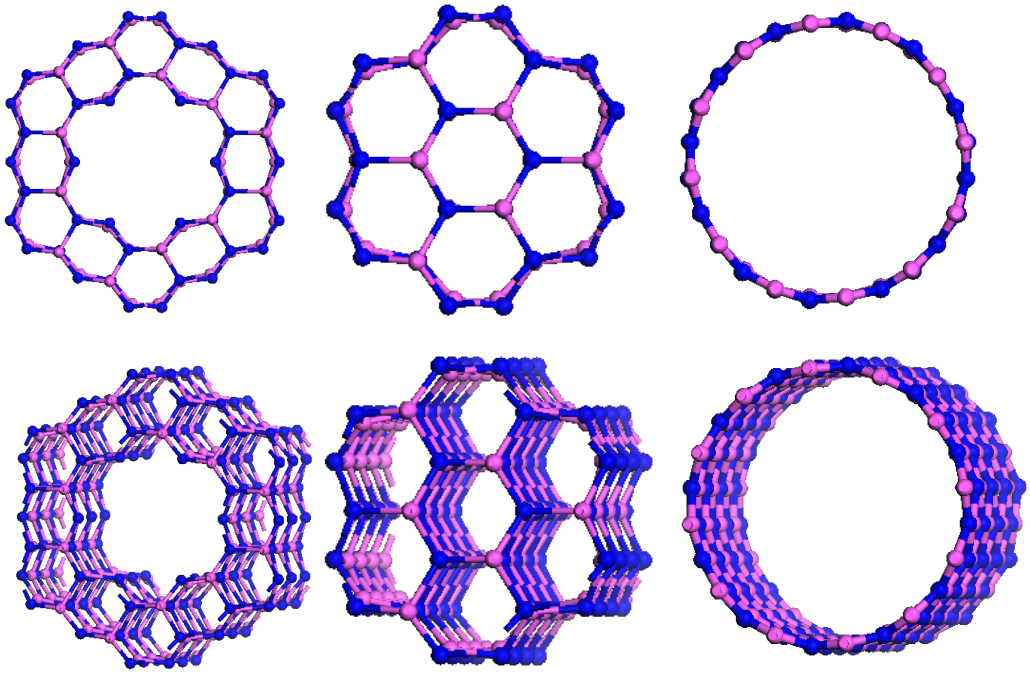


Figure S3 Optimized geometry of (a) faceted nanotube; (b) nanowire and (c) single-walled nanotube models with H atoms shown.

SI 5. AlN Nanostructures with Periodic Boundary Conditions.



$\Delta\alpha = 4.6$ $\Delta\alpha = 6.0$

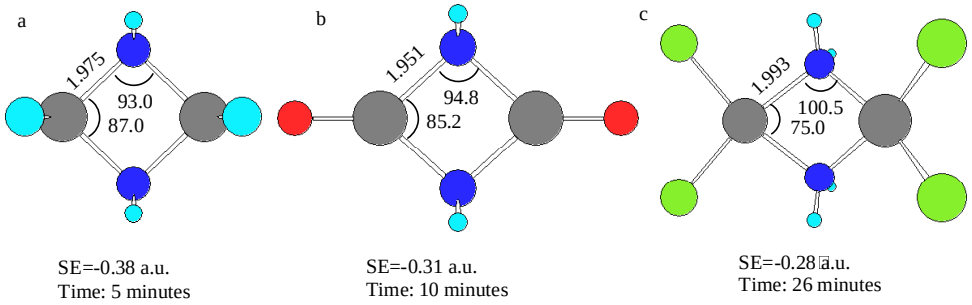
$\Delta\beta = 0.1$ $\Delta\beta = 0.3$ $\Delta\beta$ =

Figure S4. Optimized geometries of AlN nanostructures using CASTEP function in *Cerius*[2] (version 3.5). Top view (left) and tilted view (right). The bond angle variation data are list accordingly below each model.

As seen in Fig S4, not only the optimized geometries, but also the relative order of the bond angle variations is the same as that of the segment models, so the segment models in the text could be sufficient for description of the AlN nanostructures.

SI 6. Influence of Saturated Atoms.

In order to estimate the influence of various saturated atoms, we performed the strain energy (SE) calculation for square-like Al_2N_2 clusters, where dangling of Al atoms are saturated with H, Cl and O, respectively. As shown below, all clusters models are predicted to bear similar SE and geometries, but the calculation time increases dramatically from H to O atoms. So hydrogen atoms are employed to saturate all the dangling bonds in calculations of large cluster systems without much loss of generality of results.



SE=-0.38 a.u.
Time: 5 minutes

SE=-0.31 a.u.
Time: 10 minutes

SE=-0.28 a.u.
Time: 26 minutes

Figure S5. Optimized geometries of Al_2N_2 clusters passivated with (a) H, (b) O and (c) Cl. Detailed parameters are cited in corresponding clusters, all angles in degrees and bond length in angstrom (Å). SE and calculation time of each cluster are listed below the structures.

SI 7. Homodesmotic Reactions Used to Calculate the Strain Energies.

All strain energy values are calculated from following homodesmotic reactions suggested by George P. et al.[S1].

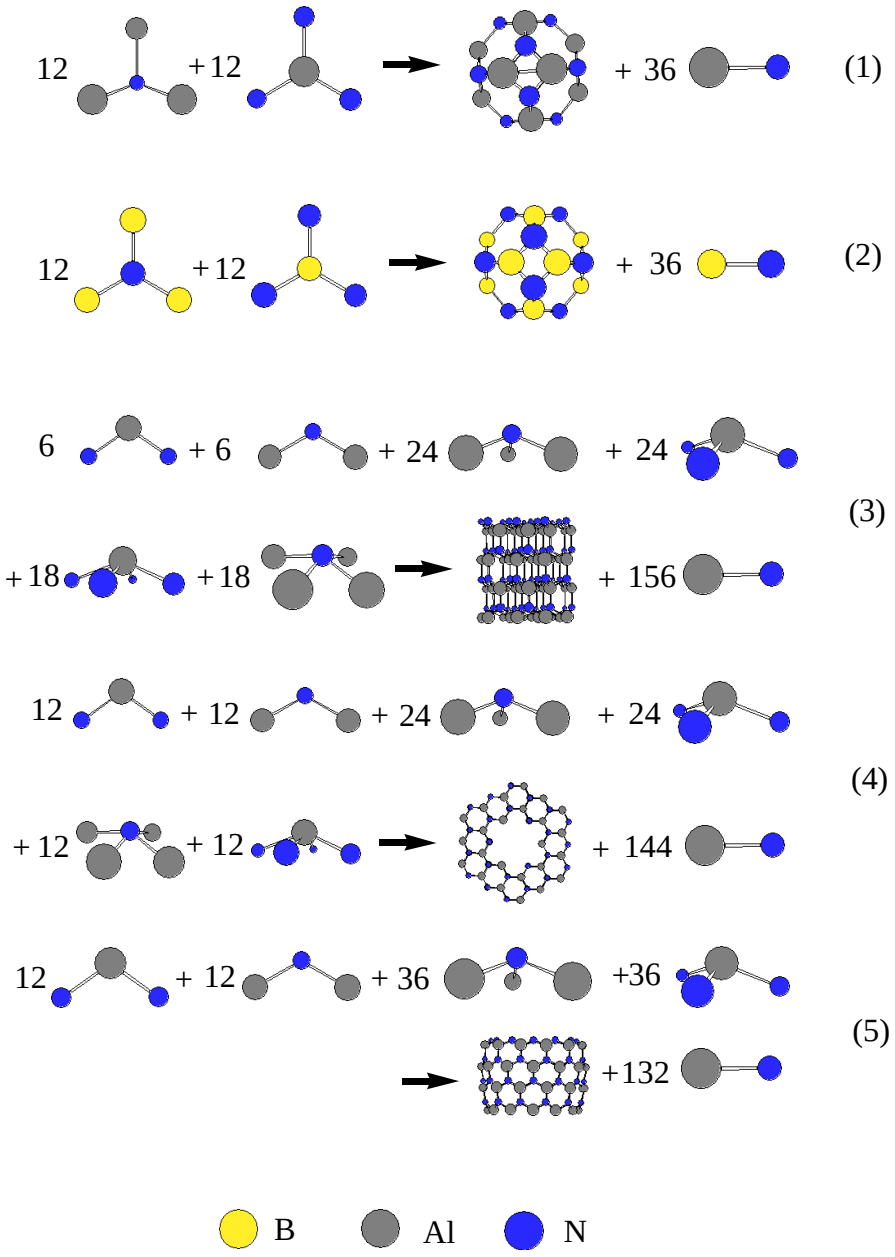


Figure S6 Homodesmotic reactions for strain energy calculations of (1) $Al_{12}N_{12}$; (2) $B_{12}N_{12}$; (3) AlN nanowire; (4) faceted AlN nanotube; (5) single-walled AlN nanotube. All H atoms are hidden for the sake of simplicity.

SI 8. Full Author List for Ref. 9 in Text.

Frisch, M. J.; Truchs, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Zakrzewski, V. G.; Millam, J. M.; Daniels, A. D.; Kudin, K. N.; Strain, M. C.; Farkas, O.; Tomasi, J.; Barone, V.; Cossi, M.; Cammi, R.; mennucci, B.; Pomelli, C.; Adamo, C.; Clifford, S.; Ochterski, J.; Petersson, G. A.; Ayala, P. Y.; Cui, Q.; Morokuma, K.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Cioslowski, J.; Ortiz, J. V.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Gomperts, R.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Gonzalez, C.; Challacombe, M.; Gill, P. M. W.; Johnson, B. G.; Chen, W.; Wong, M. W.; Andres, J. L.; Head-Gordon, M.; Replogle, E. S.; Pople, J. A. *Gaussian 98*, revision A.11; Gaussian, Inc.: Pittsburgh, PA, 1998.

Reference

[S1] George, P.; Trachtman, M.; Bock, C. W.; Brett, A. M. *Tetrahedron* **1976,** 32, 317.