Supplementary Information

A new 3D metallic, ductile, and porous boron nitride as a promising anode material for sodium-ion battery

Wei Sun [a], Qian Wang [a, *], and Puru Jena [b]

[a] School of Materials Science and Engineering, CAPT, Peking University, Beijing 100871, China. * Corresponding author. E-mail: qianwang2@pku.edu.cn

[b] Department of Physics, Institute for Sustainable Energy and Environment, Virginia Commonwealth University, Richmond, VA 23284, USA

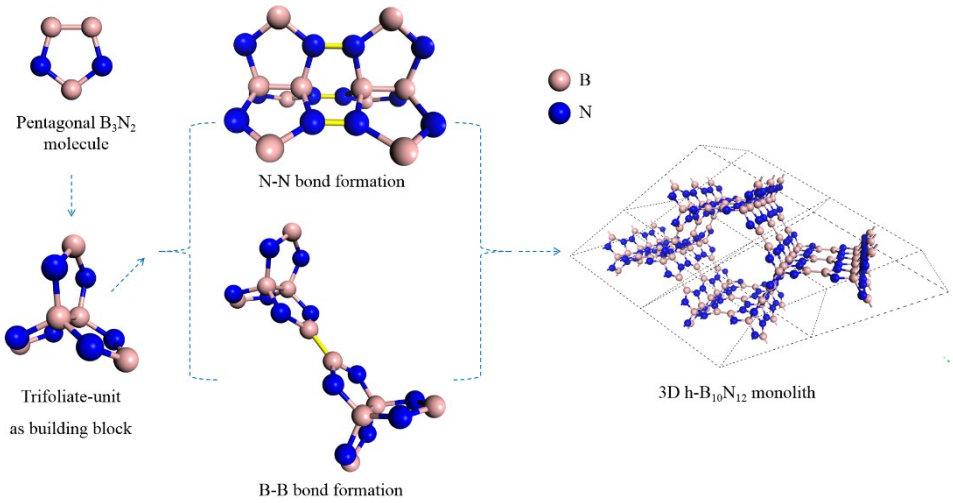

Figure S1. Proposed synthesis pathway of using the bottom-up assembly from pentagonal B_3N_2 molecule to the 3D h-$B_{10}N_{12}$ monolith.

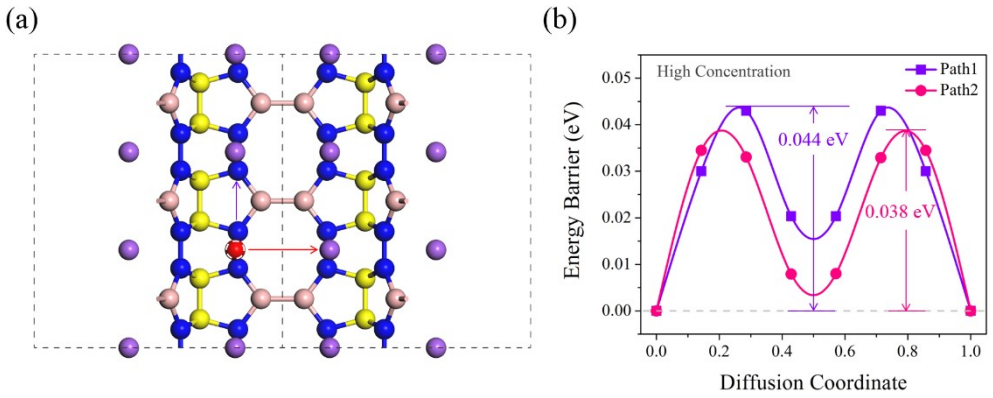

Figure S2. (a) Diffusion paths of Na-ions in high concentration, and (b) corresponding diffusion energy barrier profiles of h-$B_{10}N_{12}$.

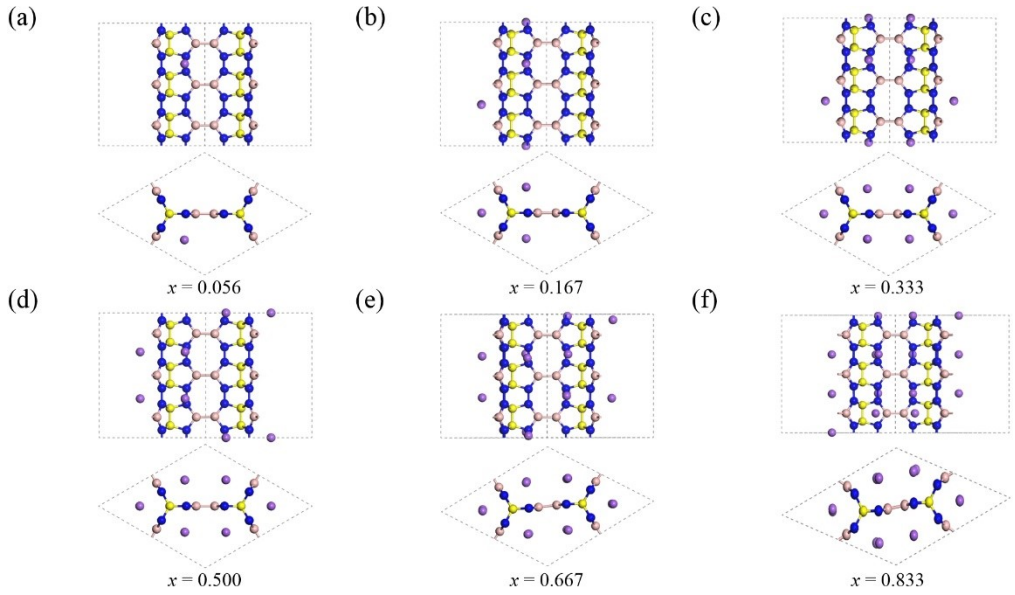

Figure S3. Selected energetically most favorable adsorption configurations of h-$B_{10}N_{12}$ with Na-ion concentrations of (a) $x = 0.056$, (b) $x = 0.167$, (c) $x = 0.333$, (d) $x = 0.500$, (e) $x = 0.667$, and (f) $x = 0.833$.

Table S1. Comparison h-$B_{10}N_{12}$ with some previously reported boron nitrides in terms of metallicity, porosity, ductility, and their application as SIB anode materials.

Structure	Metallic	Porous	Ductile	SIB anode
h-$B_{10}N_{12}$ [This work]	√	√	√	√
HCBN-1/2 [22]	√	√	√	×
3D-B_2N_2 [27]	×	√	√	√
(P-6M2)-BN [21]	√	√	√	×
(IMM2)-BN [21]	√	√	×	×
penta-B_4N_7 [25]	√	√	×	×
lz1-BN [27,54]	×	√	×	√
T-B_3N_3 [20]	√	×	×	×
M-BN [23]	√	×	×	×
t-BN_2 [24]	√	×	×	×
*t*P-BN [72]	√	×	×	×
oA-B_3N_5 [73]	√	×	×	×
$B_{28}N_{32}$ [74]	√	×	×	×

Reference

[72] M. Xiong, Z. Gao, K. Luo, F. Ling, Y. Gao, C. Chen, D. Yu, Z. Zhao, S. Wei, Three metallic BN polymorphs: 1D multi-threaded conduction in a 3D network, Phys. Chem. Chem. Phys. 22 (2020) 489-496.

[73] M. Xiong, Q. Zhang, M. Gao, Y. Zhou, D. Jin, M. Ma, F. Mao, C. Zhang, Z. Yuan, S. Wei, Prediction of three-dimensional B_3N_5 with one-dimensional metallicity, Chem. Phys. Lett. 760 (2020) 138002.

[74] M. Xiong, Z. Yuan, F. Mao, X. Wang, D. Jin, Q. Zhang, D. Yu, C. Wang, S. Wei, Superhard $B_{28}N_{32}$ with three-dimensional metallicity: First-principles prediction, Comput. Mater. Sci. 188 (2021) 110121.