Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Multidimensional B_4N as novel anode materials for lithium ion batteries

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Table S1. Cell parameters, bond length and properties of band structure of unit cell of B_4N.

	a (Å)	b (Å)	B-N (Å)	B-B (Å)	Band Structure
Our work	2.98	10.74	1.33	1.67/1.81	nonmagnetic metal
Ref. [20]	2.97	10.70	1.33	1.65/1.81	nonmagnetic metal

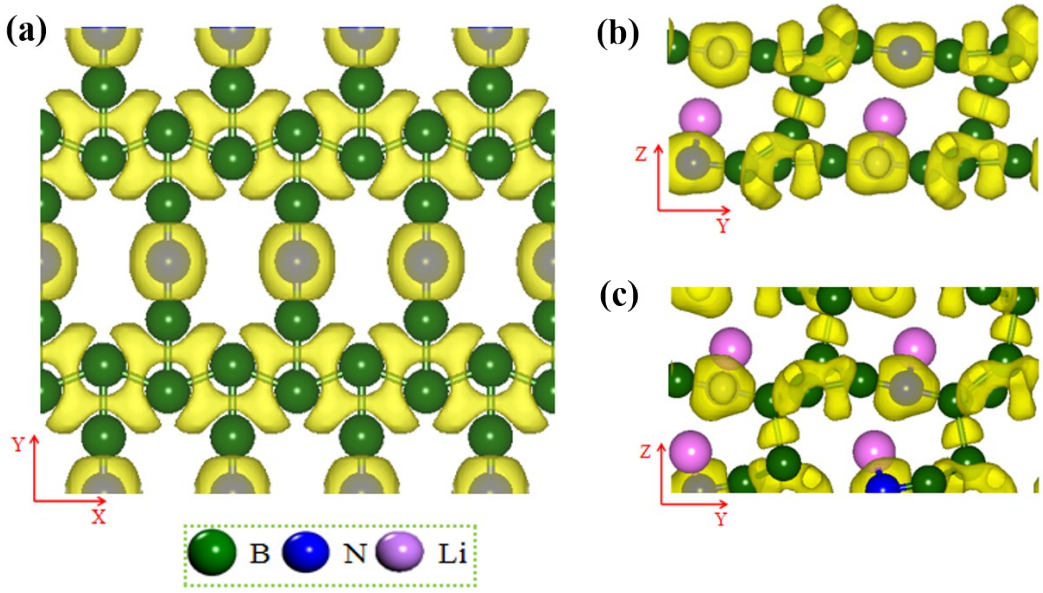

Fig. S1 Electron localization function of pristine monolayer B_4N (a), lithiation of bilayer (b) and bulk B_4N (c). Yellows are the local electrons with the isosurface of 0.72 e/Å^3.

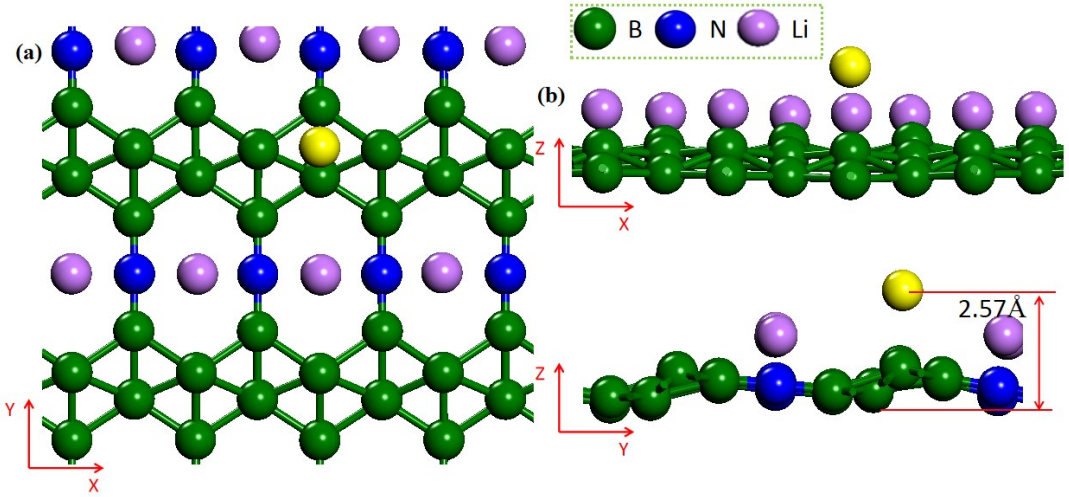

Fig. S2 Deposition of the ninth Li atom (yellow sphere) would result in a seed for the second layer. (a) Top view and (b) side view.

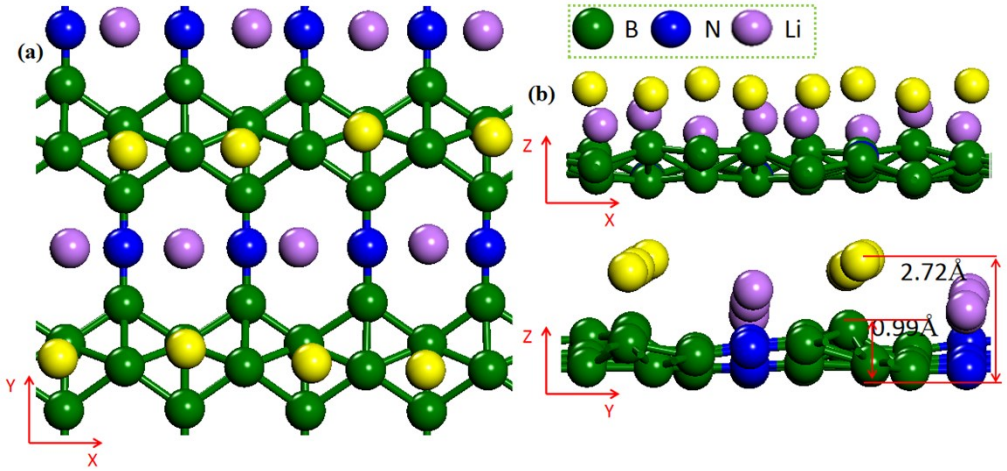

Fig. S3 After the complete second Li layer is formed, there are sixteen Li atoms on the substrate.(a) Top view and (b) side view.

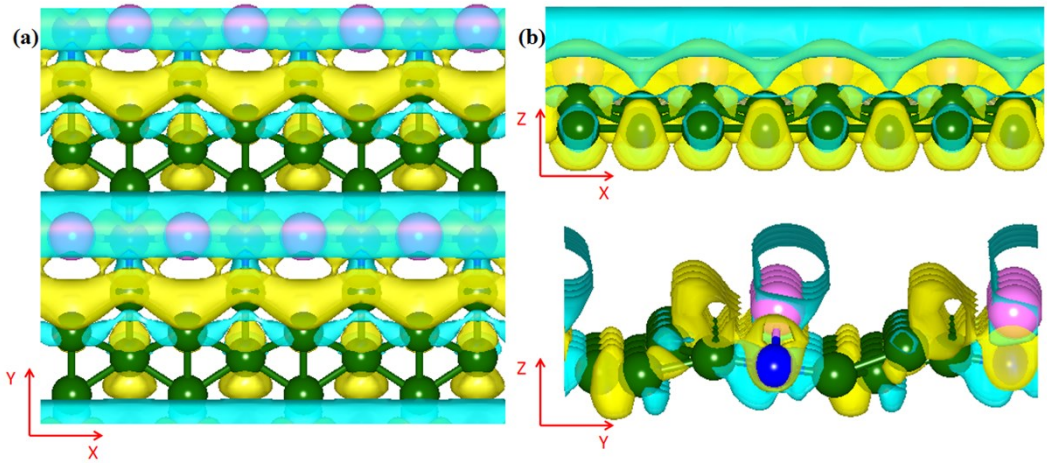

Fig. S4 Charge density difference plots of eight Li atom adsorbed on B_4N monolayer. The yellow and cyan areas denote electron accumulation and depletion with the isosurface level of 1.5×10^{-3} e/Å^3.(a) Top view and (b) side view.

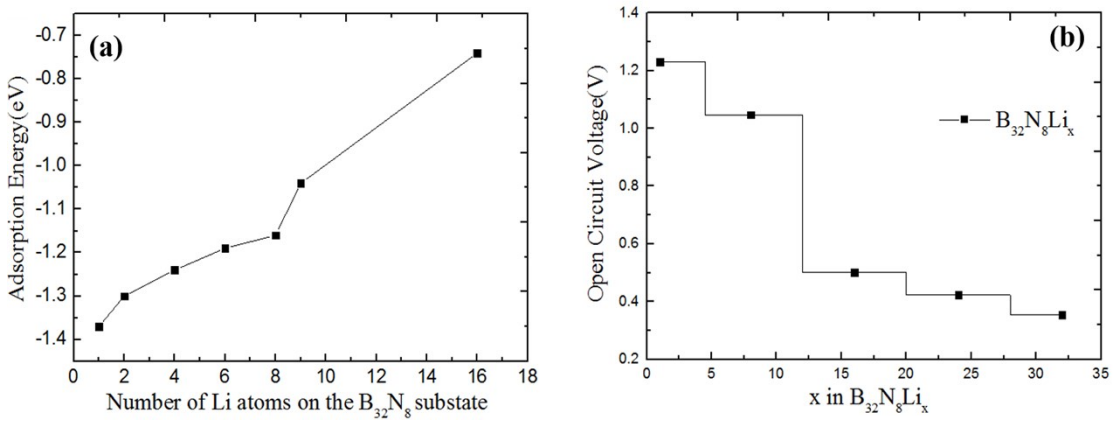

Fig. S5 (a) Adsorption energy and (b) open circuit voltage profiles of $B_{32}N_8Li_x$ as a function of Li concentration (x).

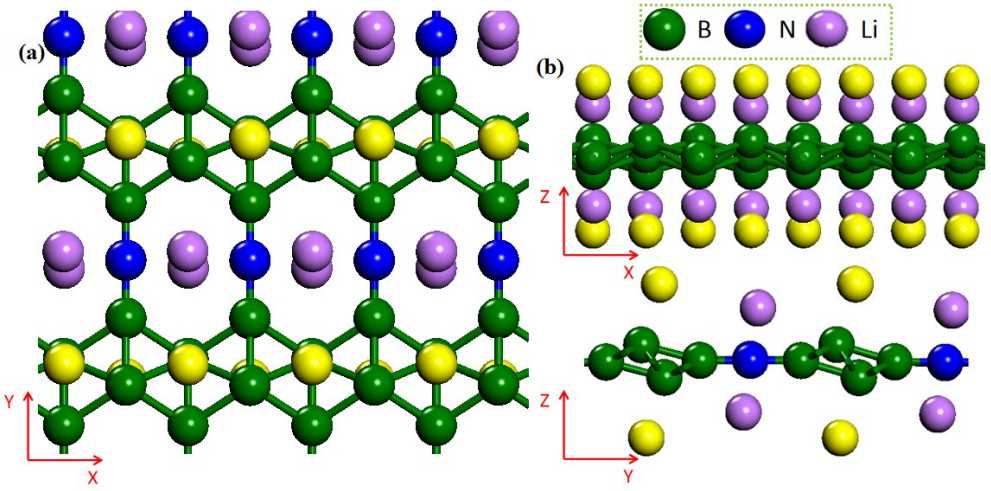

Fig. S6 Two layers of Li atoms were adsorbed on each side of the monolayer B_4N substrate. (a) Top view and (b) side view. Yellow spheres are denoted as the second layer of Li atoms.

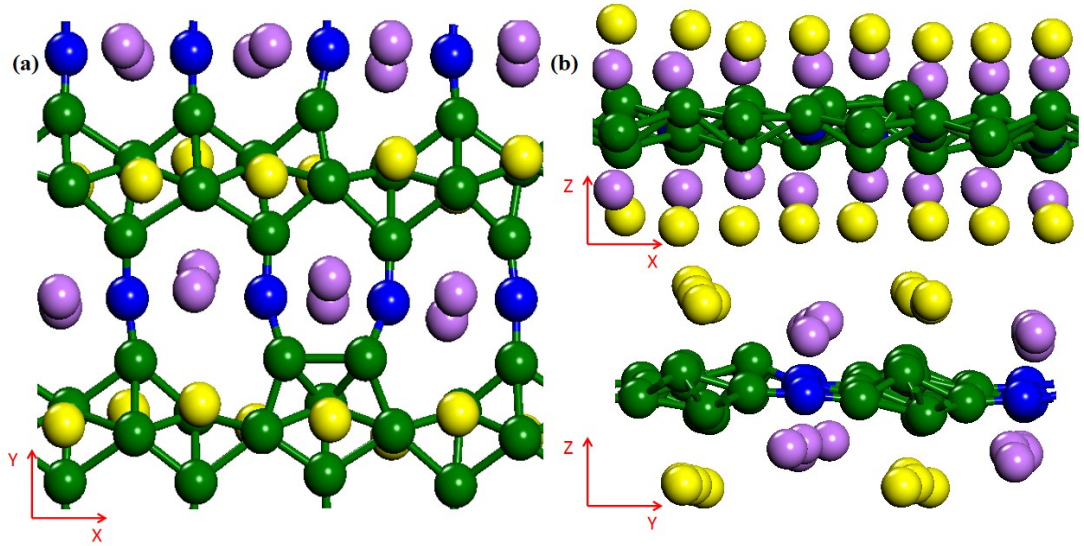

Fig. S7 AIMD simulation structures including the two layers of Li adsorption on each side at temperature of 350 K after 5 ps. (a) Top view and (b) side view. Yellow spheres are denoted as the second layer of Li atoms.

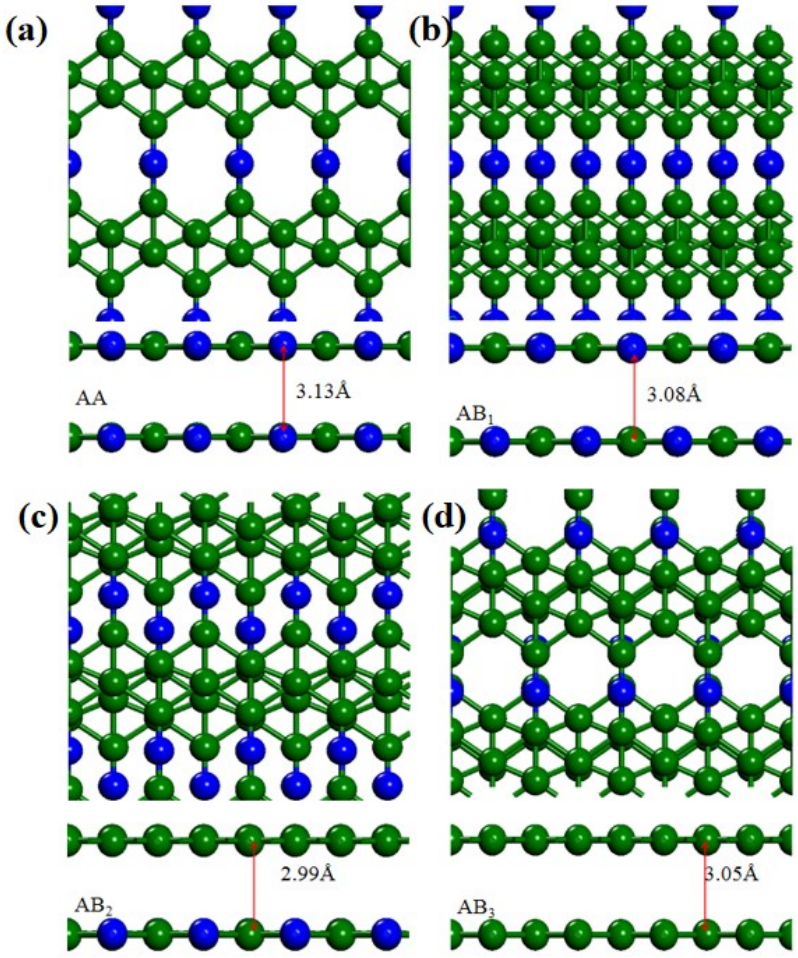

Fig. S8 Top and side views of optimized structure for bilayer B_4N with different stacking configuration.

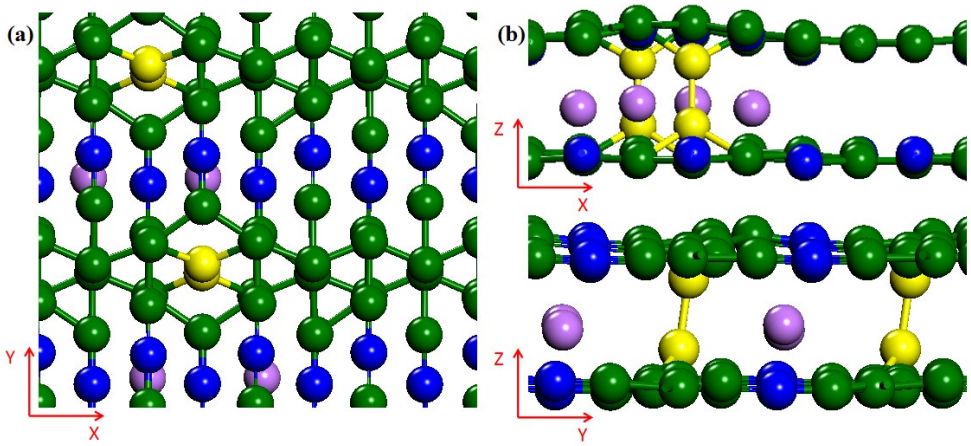

Fig. S9 The optimized structure for bilayer B_4N with four Li atoms adsorption. (a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

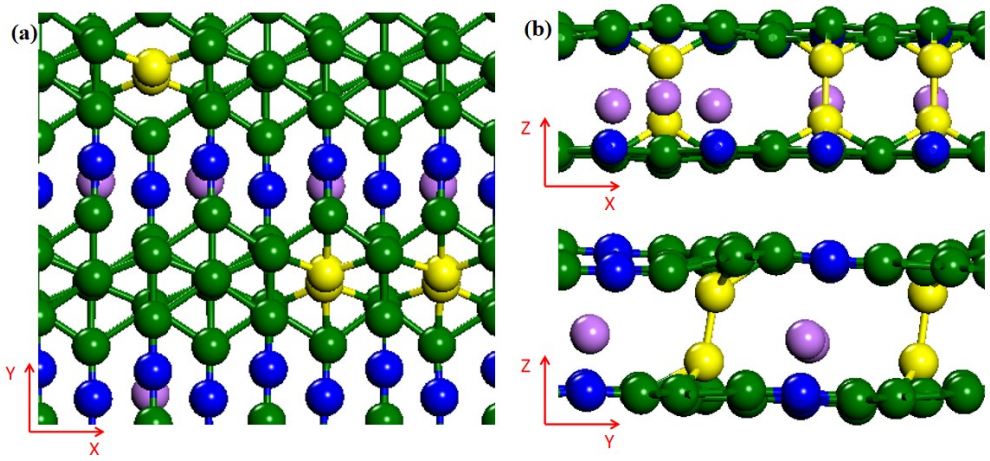

Fig. S10 The optimized structure for bilayer B_4N with five Li atoms adsorption. (a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

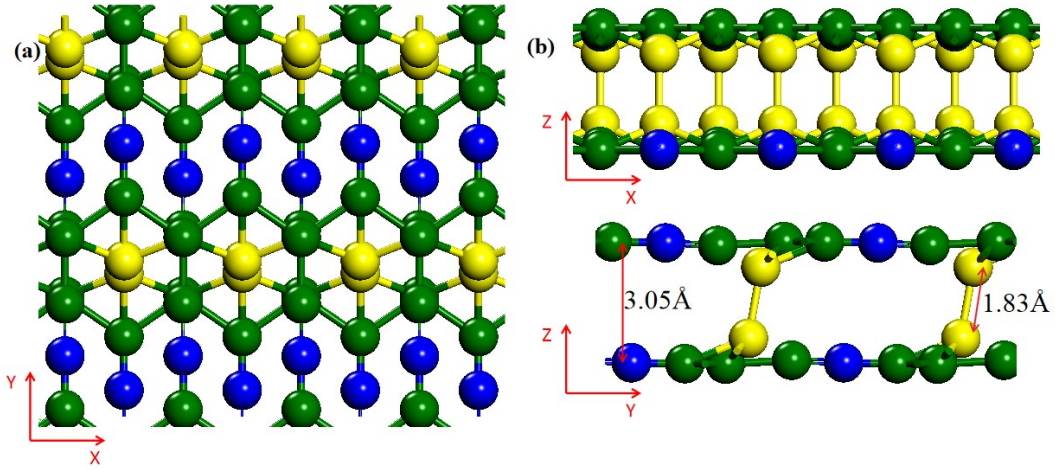

Fig. S11 Optimized bilayer B_4N after removing all the adsorbed Li atoms.(a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

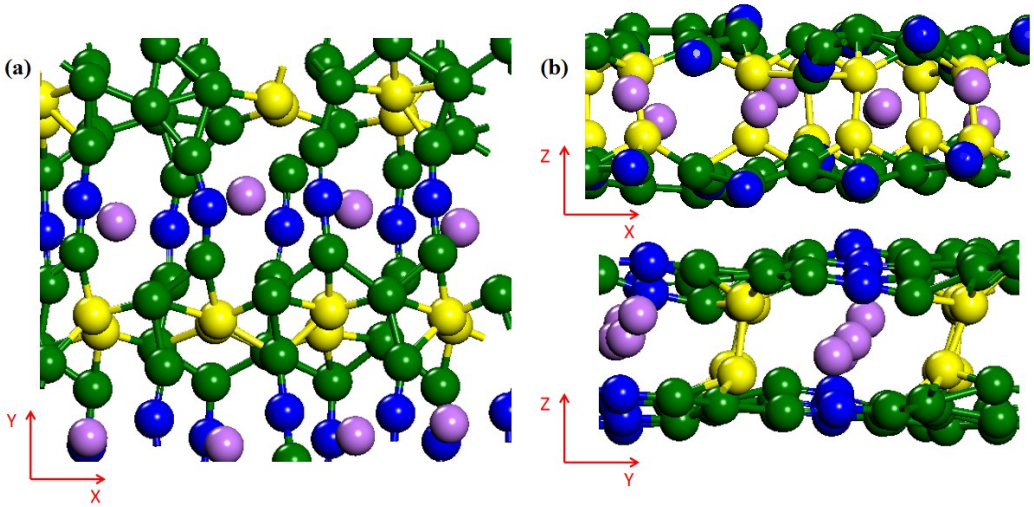

Fig. S12 AIMD simulation structures including the bilayer B_4N with saturation Li adsorption at temperature of 350 K after 5 ps. (a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

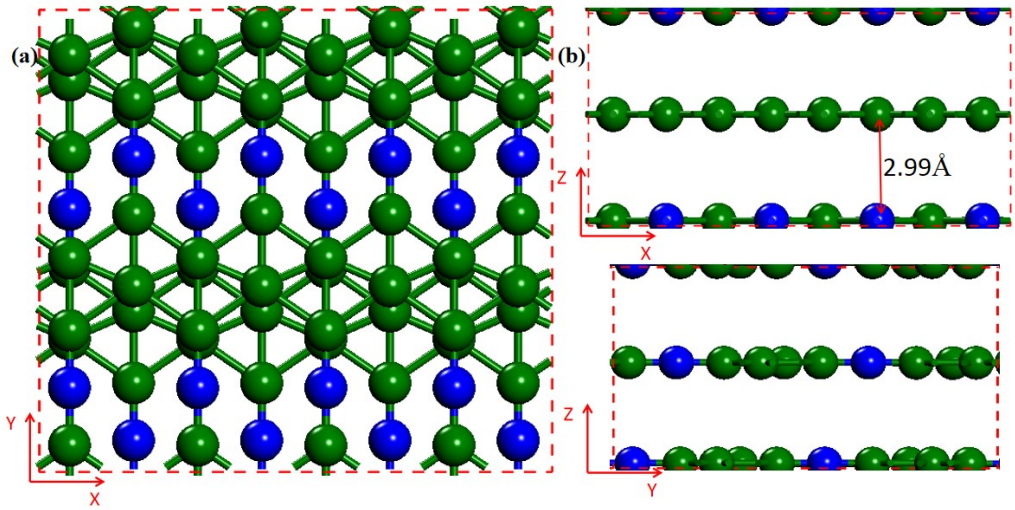

Fig. S13 The optimized layered bulk B_4N structures.(a) Top view and (b) side view.

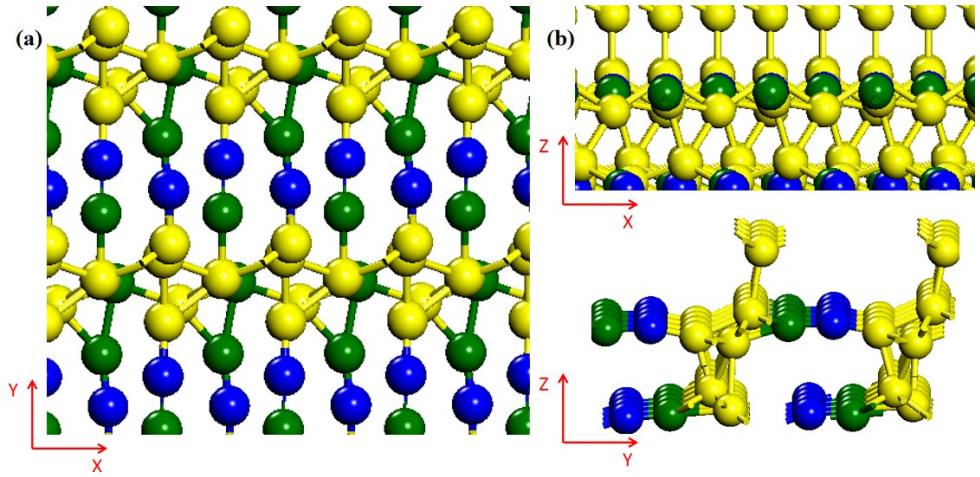

Fig. S14 Optimized bulk B_4N after removing all the adsorbed Li atoms. (a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

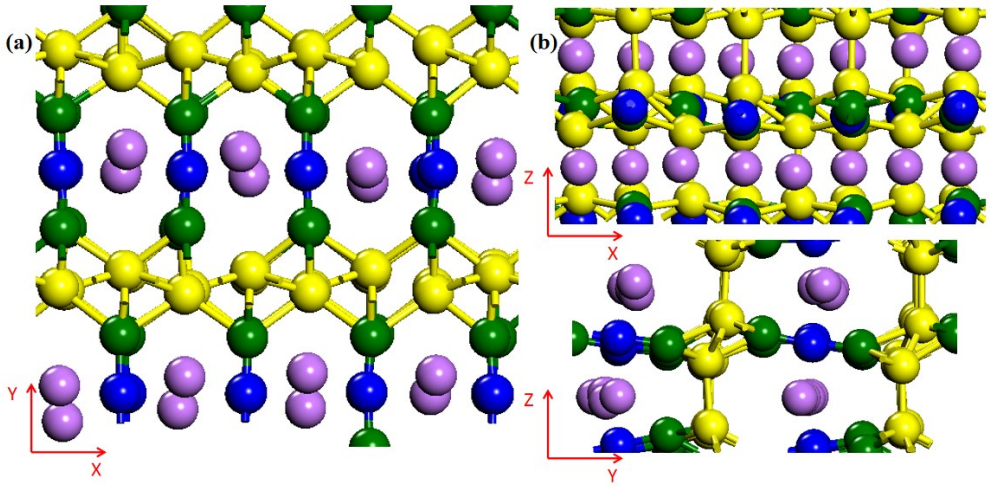

Fig. S15 AIMD simulation structures for the bulk B_4N with saturation Li adsorption at temperature of 350 K after 5 ps. (a) Top view and (b) side view. Yellow spheres are the connected B atoms between up and down.

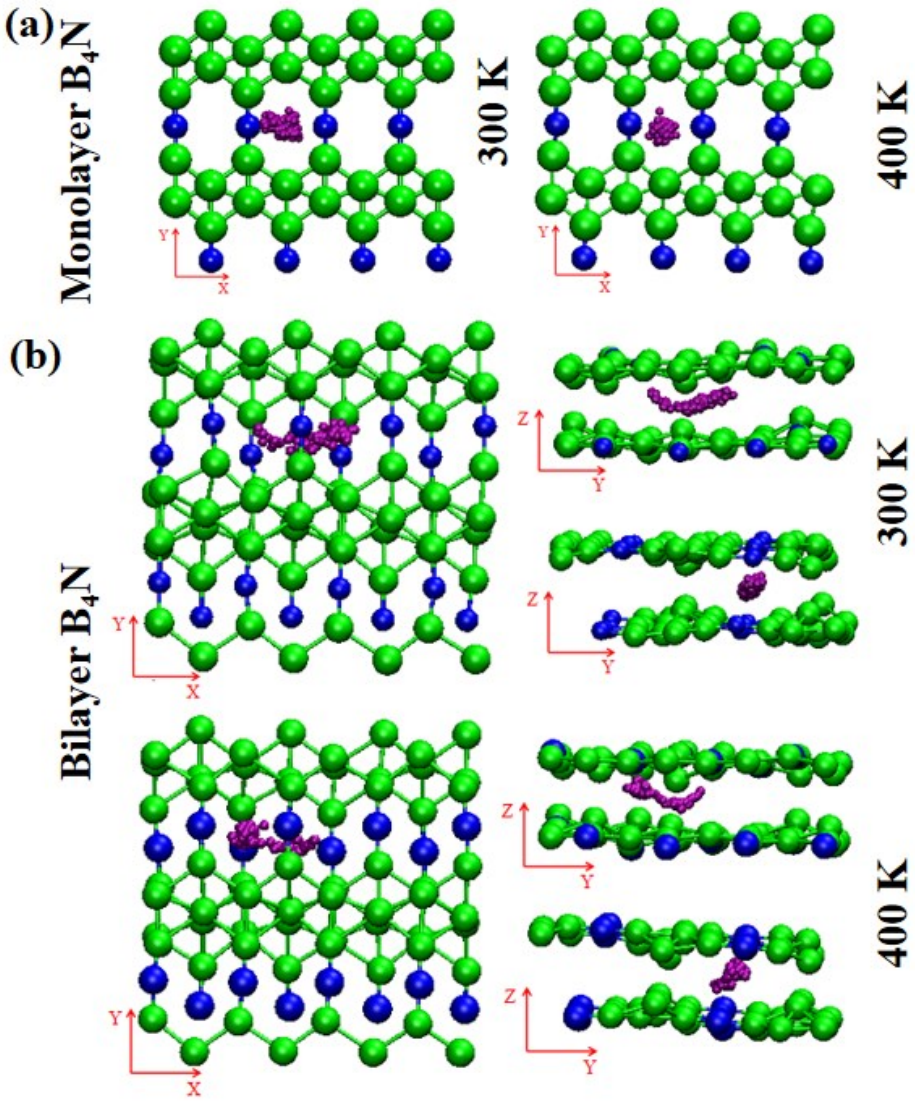

Fig. S16 Views of single Li atom movement on the monolayer (a) and bilayer B_4N (b) during the AIMD calculations of 300 K and 400 K. The purple messy point trajectories show the movement of the Li atom for 5000 fs. The green and blue spheres are the B and N atoms and they are shown as a solid background.