Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Supplementary information

Lithium decorated 2D orthorhombic (o)-B_2X_2 monolayers for hydrogen storage: first principles calculations†

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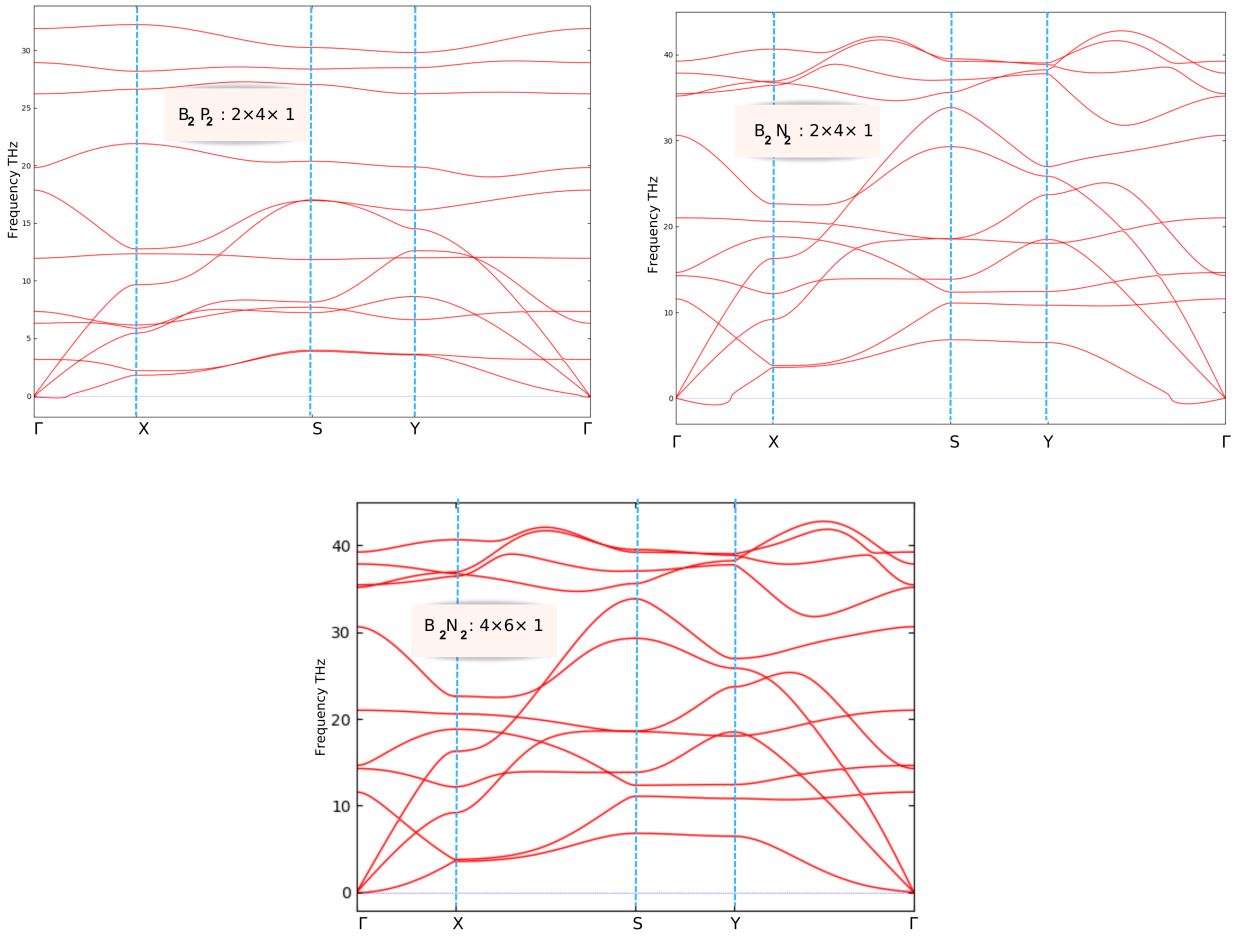

Fig. S1 Phonon dispersions of the 2D orthorhombic (o)-B_2P_2 and (o)-B_2N_2 materials, following a Brillouin zone path of Γ–X–S–Y–Γ.

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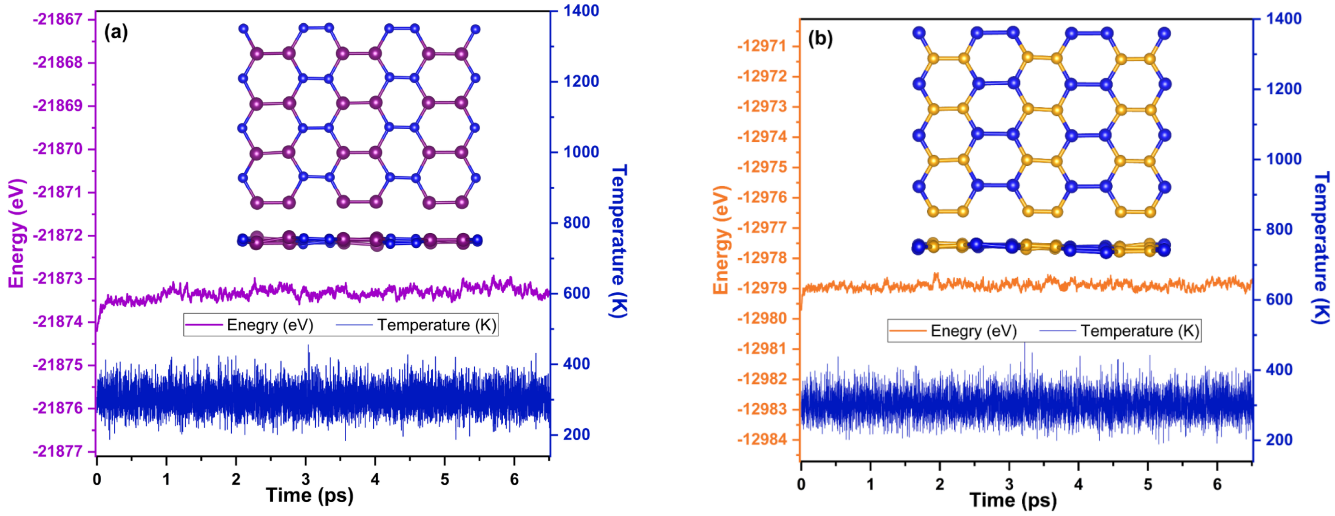

Fig. S2 AIMD results of 2D (a) (o)-B_2P_2 and (b) (o)-B_2N_2 monolayers at 300 K. The total energy and temperature fluctuations with respect to time are shown by orange and blue lines, respectively. The insert structures are the snap shots after 6.5 ps

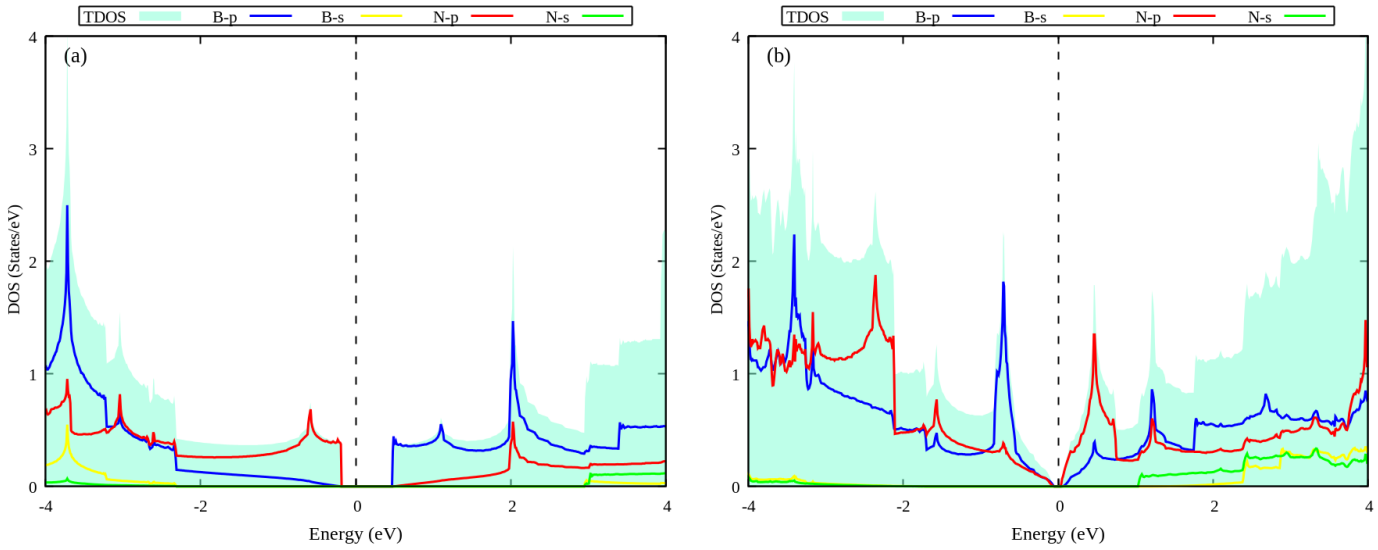

Fig. S3 (a) and (b) Projected density of states (PDOS) of (o)-B_2N_2 and (o)-B_2P_2, respectively, calculated using GGA-PBE method.

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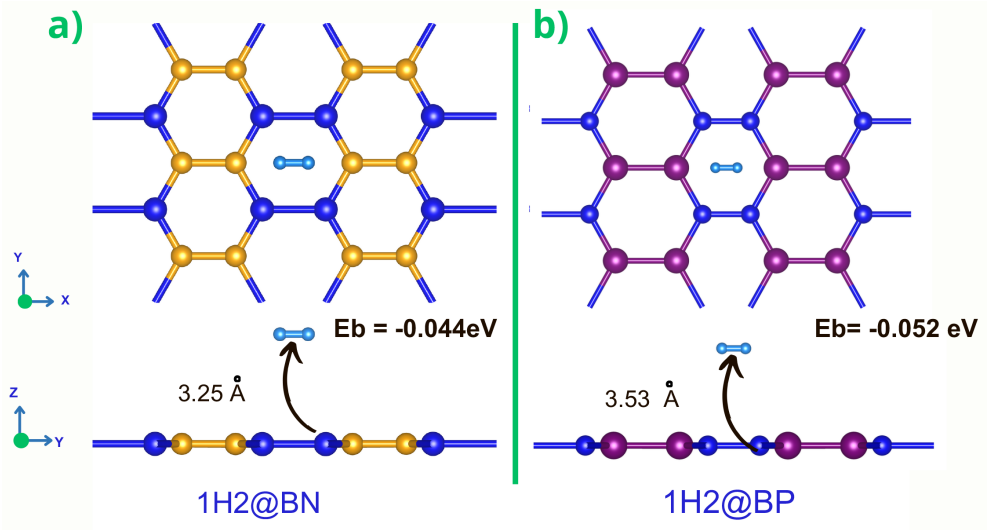

Fig. S4 Optimized atomic structure of o-B_2N_2 and o-B_2P_2 with single H_2 molecule adsorbed on each monolayer at the most stable site, H1-site. The corresponding binding energy and distance between the molecule and the monolayer are also illustrated.

Table. S1 Binding energy of adsorbed single lithium atom in the seven possible sites of B_2N_2 and B_2P_2 monolayers

B_2N_2 sites							
	hollow 1	hollow 2	top of B	top of N	bridge B-B	bridge B-N	bridge N-N
Binding energy (eV)	-1.98	-1.70	-1.43	-1.58	-1.58	-1.98	-1.40
Stability	stable	stable	stable	not stable	stable	not stable	stable
Description	—	—	—	goes to N-N bridge	—	goes to hollow 1	—
B_2P_2 sites							
	hollow 1	hollow 2	top of B	top of P	bridge B-B	bridge B-P	bridge P-P
Binding energy (eV)	-3.09	-2.82	-2.61	-3.08	-2.61	-3.08	-2.82
Stability	stable	stable	not stable	not stable	stable	not stable	not stable
Description	—	—	goes to B-B bridge	goes to hollow 1	—	goes to hollow 1	goes to hollow 2

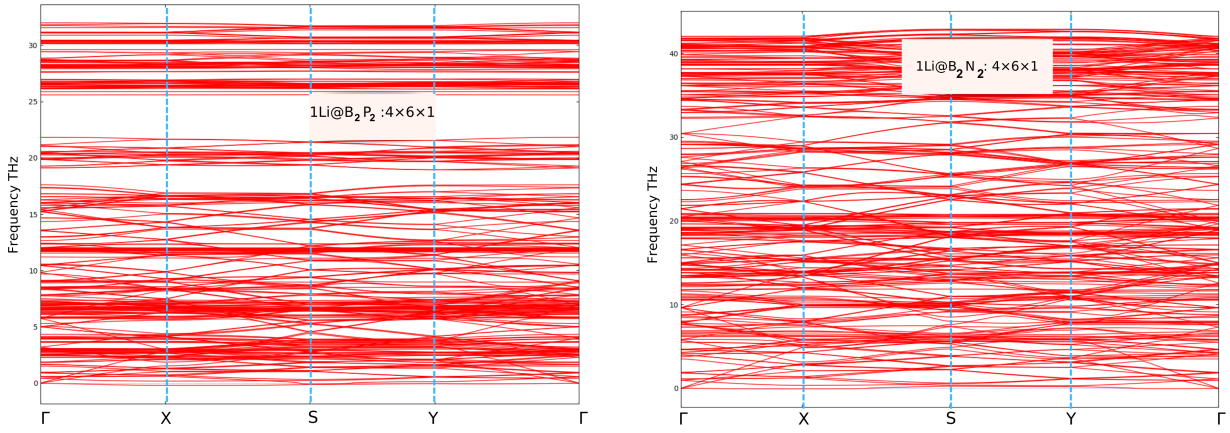

Fig. S5 Phonon dispersions of Li@B_2P_2 and Li@B_2N_2 systems , following a Brillouin zone path of Γ–X–S–Y–Γ.

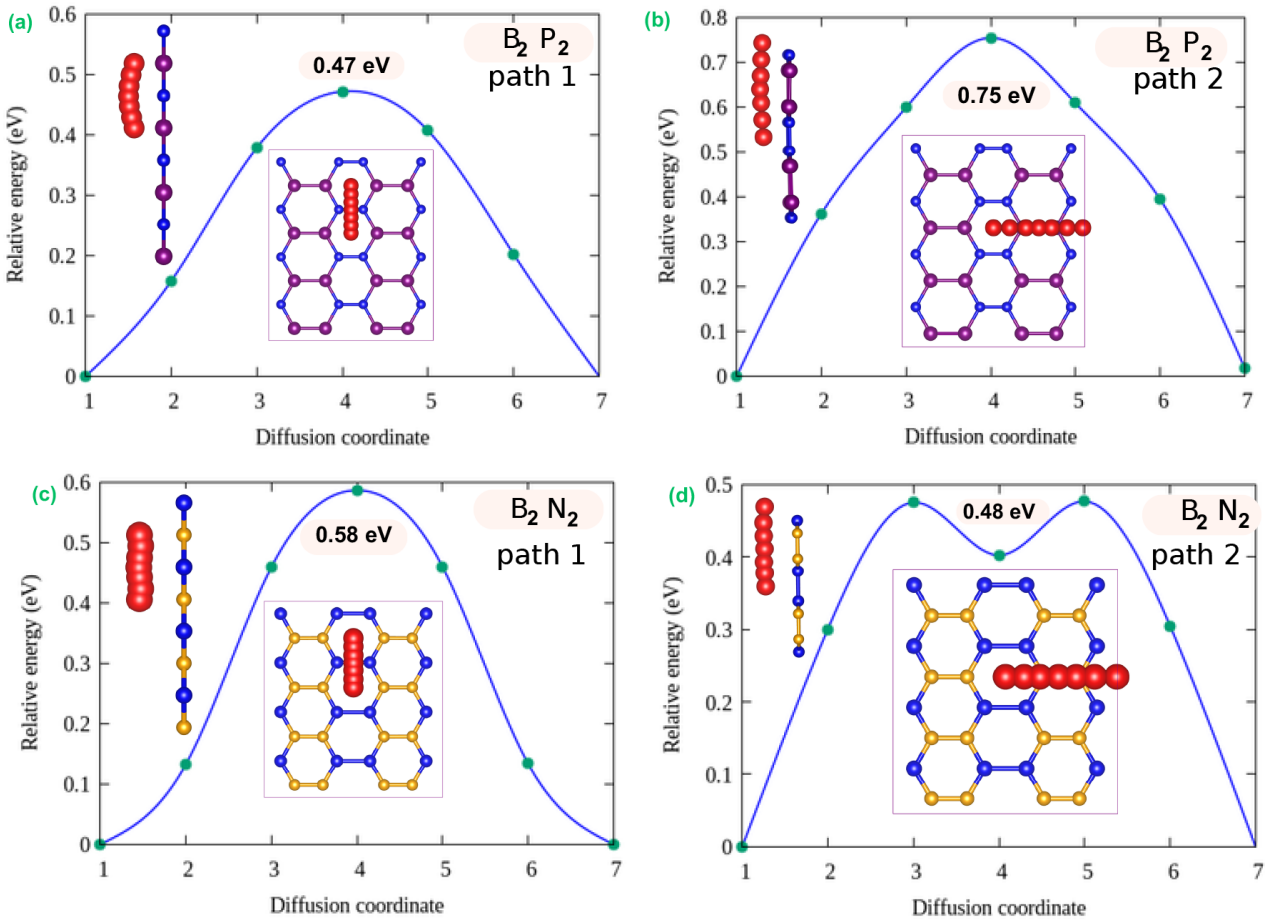

Fig. S6 (a), (b), (c) and (d), Lithium atom displacement following two paths from one stable configuration to the other on B_2P_2 and B_2N_2 monolayers. The energy profiles are shown by the blue curves.

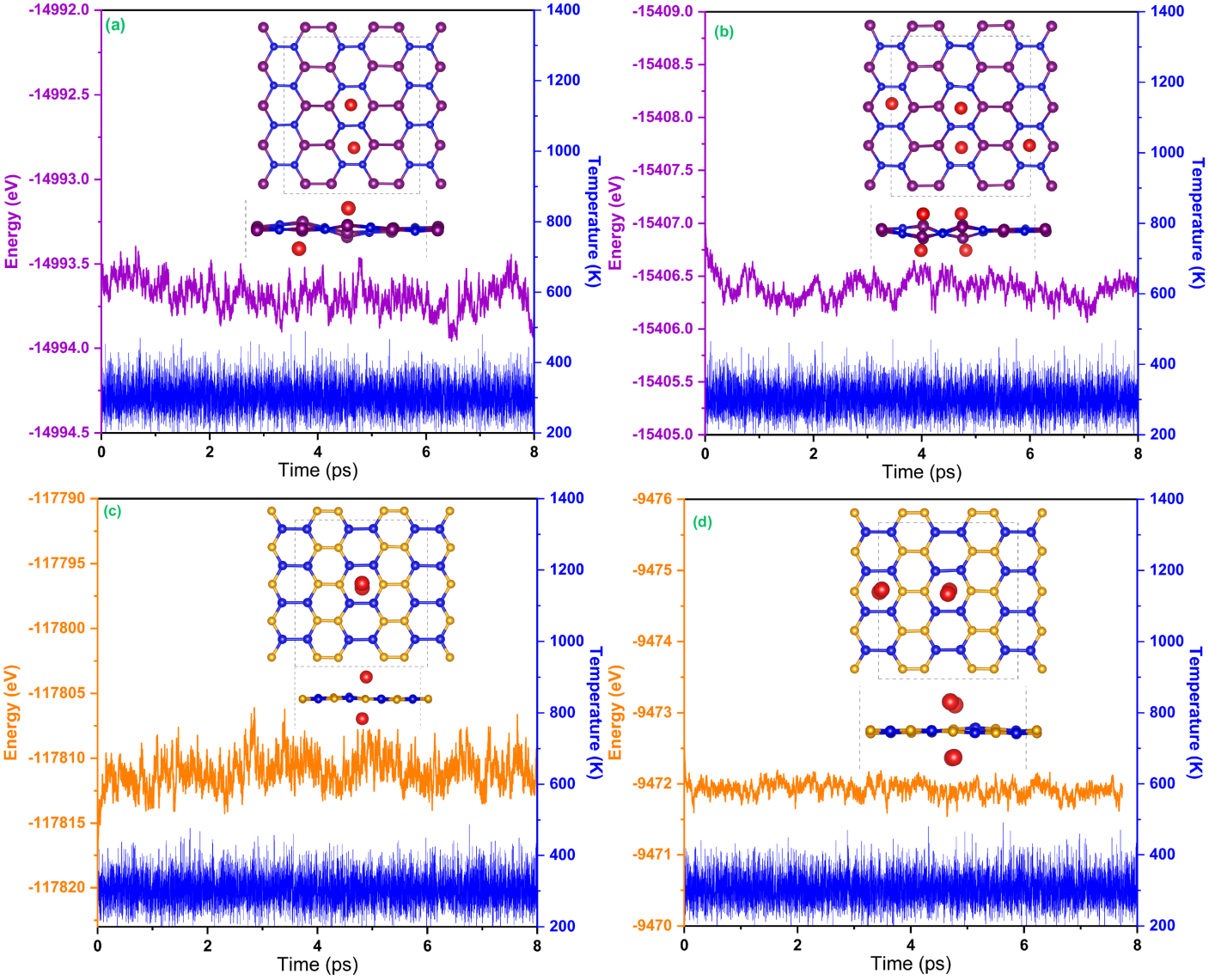

Fig. S7 (a), (b), (c) and (d) AIMD results of $2Li@B_2P_2$, $4Li@B_2P_2$, $2Li@B_2N_2$ and $4Li@B_2N_2$ systems, receptively, at 300 K. The total energy and temperature fluctuations with respect to time are shown by orange, purple and blue lines, respectively. The insert structures are the snap shots after 8 ps.

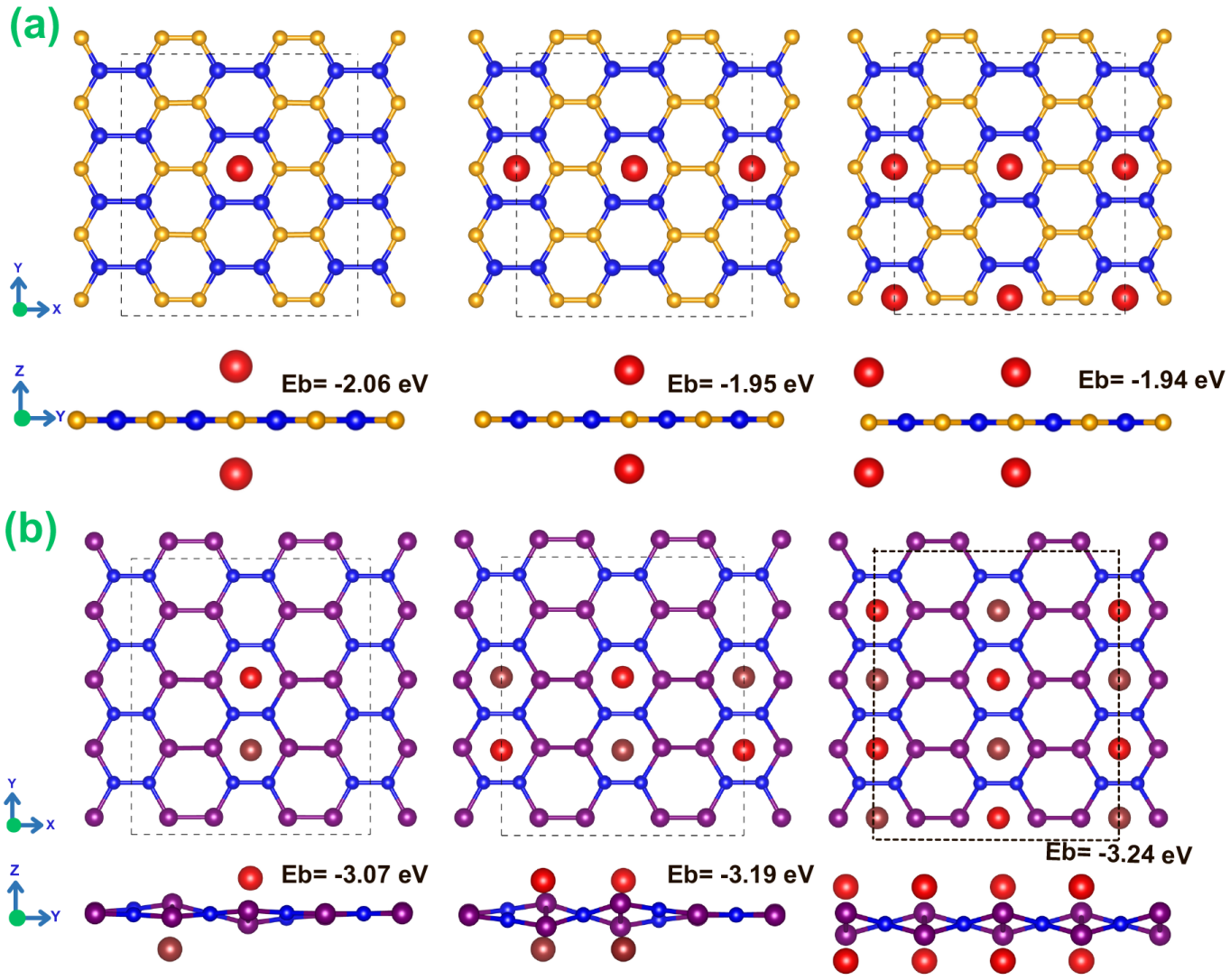

Fig. S8 (a) and (b) The most favorable atomic configurations of 2, 4, and 8 double-sided lithium atoms adsorbed in the most stable site (hollow 1) for 2×4×1 o-B_2N_2 and o-B_2P_2 supercells respectively, as well as the corresponding binding energies.