Supplementary Information

A first-principles study of hydrogen storage on pristine and Li-decorated superatomic $B_{12}N_2$ monolayer

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Supplementary Contents

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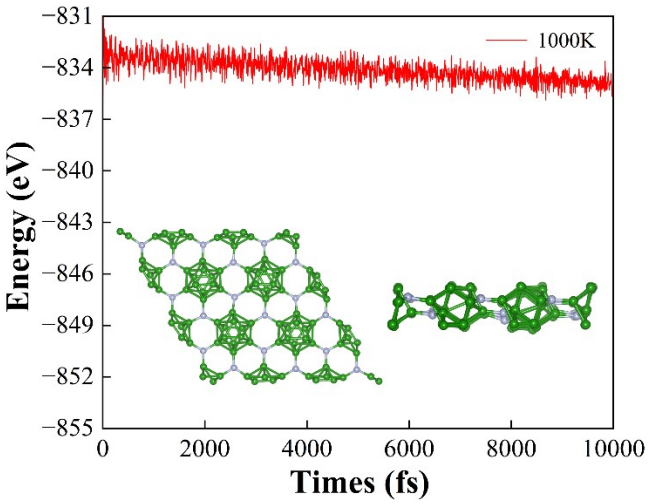

Fig. S1 Energy fluctuation depending on simulated time in molecular dynamics simulation of $B_{12}N_2$ monolayer at 1000 K after 10 ps simulation with a time step of 1 fs.

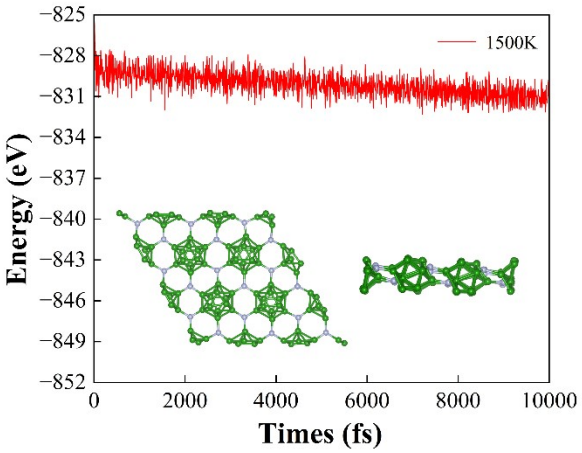

Fig. S2 Energy fluctuation depending on simulated time in molecular dynamics simulation of $B_{12}N_2$ monolayer at 1500 K after 10 ps simulation with a time step of 1 fs.

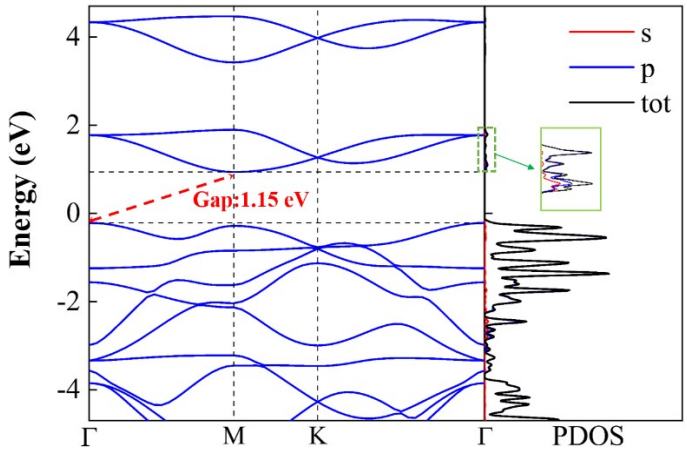

Fig. S3 Band structure and PDOS of the $B_{12}N_2$ monolayer calculated using the HSE06 functional. The Fermi level is assigned at 0 eV.

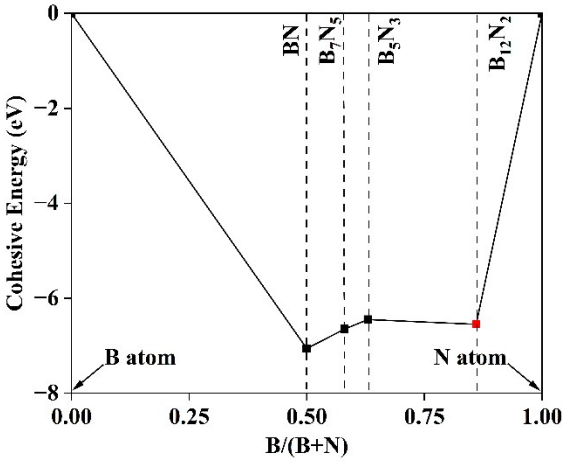

Fig. S4 Phase diagram based on cohesive energies of known B_xN_y and the $B_{12}N_2$ monolayer. The black blocks represent the cohesive energies of B_5N_3, B_7N_5, and h-BN. The red block represents the cohesive energy of $B_{12}N_2$.

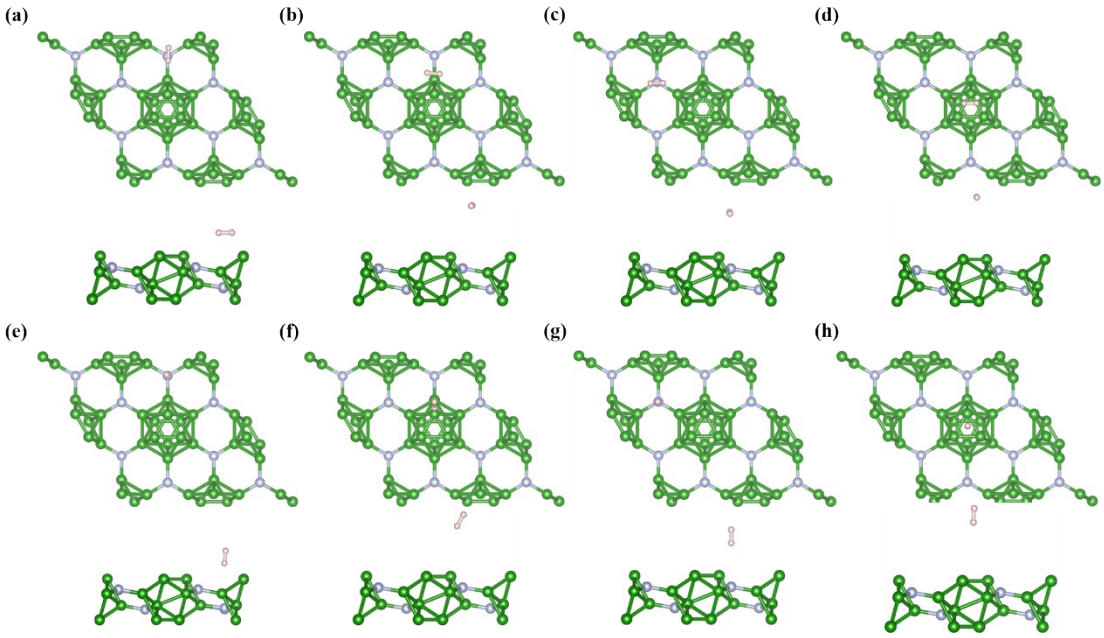

Fig. S5 Top and side views of H_2 molecule adsorption on the pristine surface in parallel (a)-(d) and perpendicular (e)-(h) orientations.

Table S1 Bader charge analysis of $B_{48}N_8Li_mH_{2n}$ (m = 0-1, and n = 1-4) compounds. (All charges are in units of e, Q_B, Q_N, Q_{Li}, Q_H represent the average net charge on B, N, Li and H atoms)

Compound	Q_B	Q_N	Q_{Li}	Q_H
$B_{48}N_8$	+0.07	−0.43	-	-
$B_{48}N_8Li$	+0.06	−0.43	+0.40	-
$B_{48}N_8LiH_2$	+0.07	−0.43	+0.33	−0.02
$B_{48}N_8LiH_4$	+0.07	−0.43	+0.39	−0.04
$B_{48}N_8LiH_6$	+0.07	−0.43	+0.43	−0.04
$B_{48}N_8LiH_8$	+0.07	−0.43	+0.42	−0.04

Table S2 Calculated Gibbs free energy (ΔG in eV) and zero-point energy (ZPE in eV) for the H_2, $B_{48}N_8$ and $B_{48}N_8H_2$ system.

		ΔG	ZPE
H_2		−6.50	0.28
$B_{48}N_8$(pristine)		−379.97	
H_2II	A_1	−386.49	0.28
	A_2	−386.51	0.29
	B_1	−386.50	0.29
	B_2	−386.53	0.29
$H_2\perp$	A_1	−386.48	0.30
	A_2	−386.50	0.33
	B_1	−386.50	0.29
	B_2	−386.51	0.30

Table S3 Calculated Gibbs free energy (ΔG in eV) and zero-point energy (ZPE in eV) for the H_2, $B_{48}N_8Li$ and $B_{48}N_8LiH_n$ system.

	ΔG	ZPE
H_2	−6.50	0.28
$B_{48}N_8Li(A_2)$	−383.44	
$B_{48}N_8LiH_2$	−390.15	0.40
$B_{48}N_8LiH_4$	−396.65	0.75
$B_{48}N_8LiH_6$	−403.17	1.08
$B_{48}N_8LiH_8$	−409.64	1.42

Table S4. Optimized coordinates of the unit cell for $(B_3CB_3)N_2$ monolayer.

$B_{12}N_2$

1.0000000000000000

5.5805169499471825 0.0000000000000000 0.0000000000000000

-2.7902584522678189 4.8328694449078444 0.0000000000000000

0.0000000000000000 0.0000000000000000 15.0000000000000000

B N

12 2

Direct

B	0.6329216324717706	0.8164682224508368	0.4762794576725682
B	0.3670783619272768	0.1835316958707978	0.5237205423274318
B	0.1835315723734894	0.8164535497570498	0.4762794576725682
B	0.8164685227352066	0.1835465699838892	0.5237205423274318
B	0.1835466397690197	0.3670782658546869	0.4762794576725682
B	0.8164534553396834	0.6329218538862520	0.5237205423274318
B	0.9046544174302511	0.0953609920563423	0.4177796036028383
B	0.0953455065095667	0.9046389262652923	0.5822203963971617
B	0.9046390769524351	0.8092934218824723	0.4177796036028383
B	0.0953609174466123	0.1907064964391694	0.5822203963971617
B	0.1907065000163612	0.0953455043828271	0.4177796036028383
B	0.8092933960086341	0.9046544956171729	0.5822203963971617
N	0.6666667554258652	0.3333334403867454	0.5399037548845058
N	0.3333333396828380	0.6666666793541935	0.4600962451154942