Electronic Supplementary Information

Theoretical Investigation of the Ability of Borazine-Melamine Polymer as Novel Candidate for Hydrogen Storage Applications

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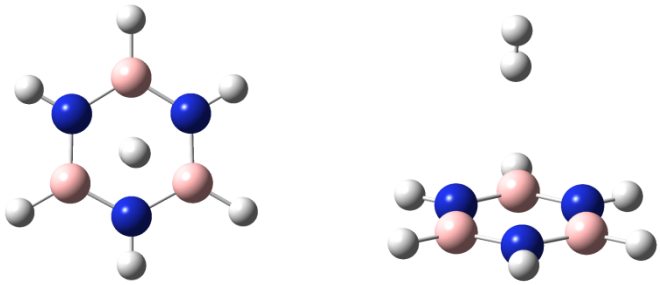


Fig. S1. The optimized structure of borazine with one adsorbed H_2 molecule calculated at CCSD(T) /6-311+G(d,p) level of theory. Top and side views are given on the left and right panel, respectively. Nitrogen, boron, and hydrogen atoms are shown in blue, pink and white colors, respectively.

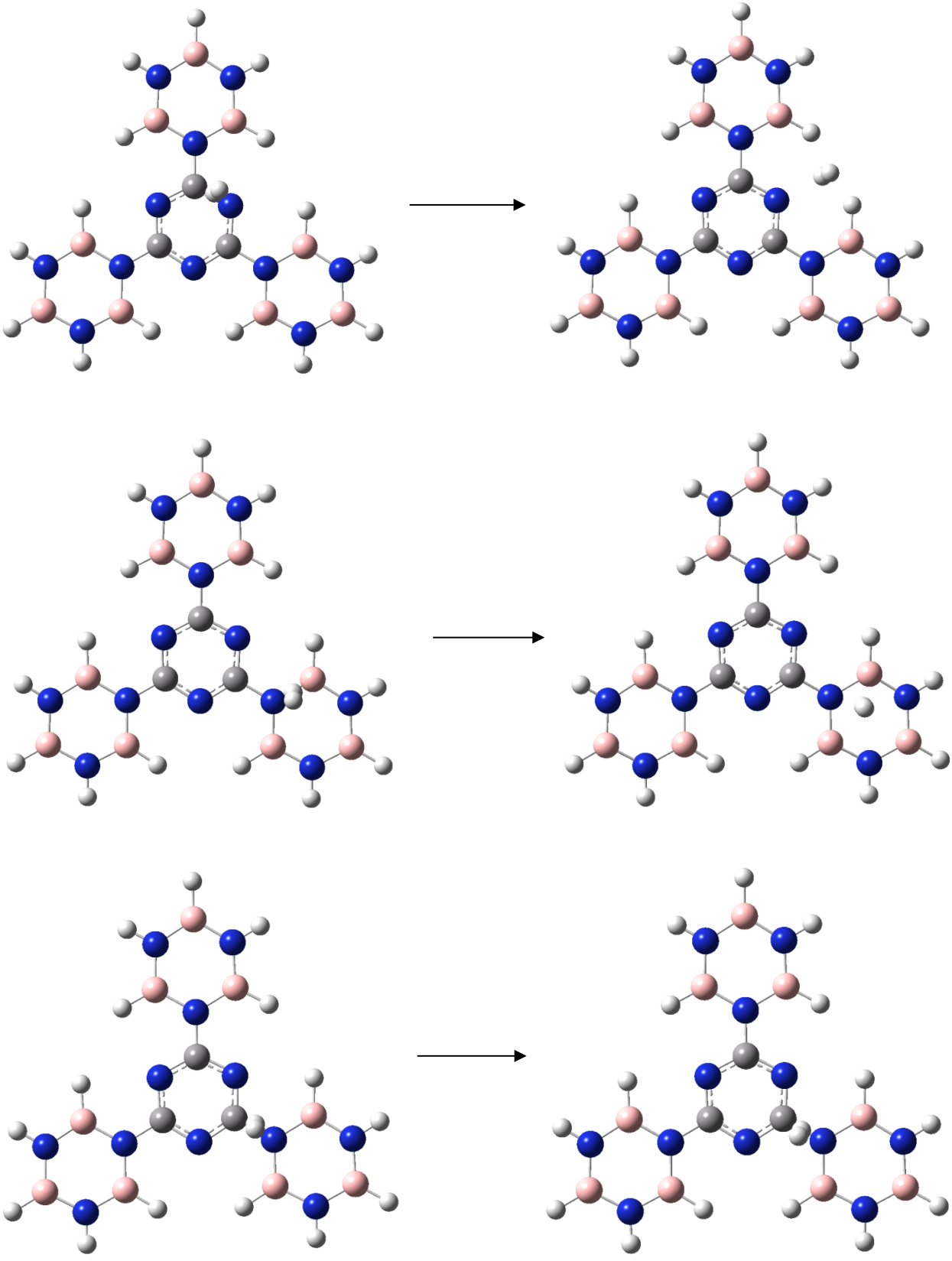


Fig. S2. Different bridge positions of H_2 molecules on BMP-H calculated at CAM-B3LYP/6-311+G(d,p) model. Initial and optimized structures are given on the left and right panel, respectively. Carbon, nitrogen, boron, and hydrogen atoms are shown in grey, blue, pink and white colors, respectively.

Table S1. Interaction potential parameters for adsorbent and adsorbate atoms used in this work.

Atoms of BMP-H (adsorbent)	ε/k_B (K)	σ (Å)
C	52.87	3.43
H	22.16	2.57
N	34.75	3.26
B	47.76	3.453

H_2 (adsorbate)	ε/k_B (K)	σ (Å)
H_2	34.20	2.96

Table S2. Calculated average adsorption energies (kcal/mol)a and addition adsorption energies (kcal/mol)a of BMP-H adsorbed with different numbers of hydrogen molecules using CAM-B3LYP/6-311+G(d,p) level of theory.

	Ea (kcal/mol)	Eadd (kcal/mol)
$3H_2$	-0.169	-0.169
$4H_2$	-0.279	-0.644
$5H_2$	-0.231	-0.057

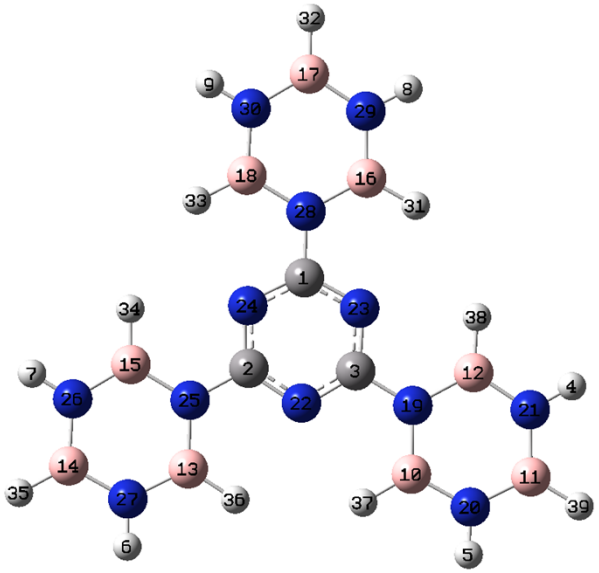
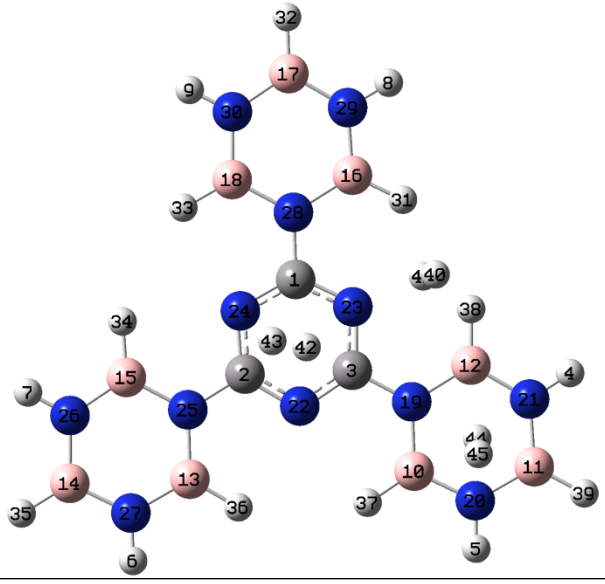
$6H_2$	-0.195	0.018
$7H_2$	-0.182	-0.136
$8H_2$	-0.201	-0.433
$9H_2$	-0.222	-0.458
$10H_2$	-0.235	-0.415
$11H_2$	-0.217	-0.032
$12H_2$	-0.199	-0.001

[a] All energy values have been BSSE corrected

Table S3. Calculated BSSE values (kcal/mol) of BMP-H adsorbed with different numbers of hydrogen molecules using CAM-B3LYP/6-311+G(d,p) and MP2/6-311+G(d,p) levels of theory.

	BSSE values of CAM-B3LYP(kcal/mol)	BSSE values of MP2(kcal/mol)
$3H_2$	-0.0892	0.7494
$4H_2$	-0.0588	0.6361
$5H_2$	-0.0429	0.5557
$6H_2$	-0.0416	0.511
$7H_2$	-0.0312	0.4957
$8H_2$	-0.0145	0.52
$9H_2$	-0.0051	0.5113
$10H_2$	0.0011	0.517
$11H_2$	0.0012	0.4939
$12H_2$	0.0006	0.4827

Table S4. Mulliken charge analysis of BMP-H before and after hydrogen adsorption.

Mulliken atomic charges before H-adsorption to BMP-H	Mulliken atomic charges after H-adsorption to BMP-H with three H_2
	
1 C 0.079346	1 C 0.036905
2 C 0.079614	2 C -0.018941
3 C 0.078396	3 C 0.145900
4 H 0.287886	4 H 0.288486
5 H 0.287893	5 H 0.289180
6 H 0.287896	6 H 0.288420
7 H 0.287876	7 H 0.288378
8 H 0.287897	8 H 0.287929
9 H 0.287879	9 H 0.288359
10 B 0.380676	10 B 0.408193
11 B 0.248916	11 B 0.249344
12 B 0.380450	12 B 0.405869
13 B 0.380466	13 B 0.387723
14 B 0.248927	14 B 0.258672
15 B 0.380304	15 B 0.378139
16 B 0.380349	16 B 0.386068
17 B 0.248878	17 B 0.258587
18 B 0.380347	18 B 0.381740
19 N -0.665691	19 N -0.676427
20 N -0.457860	20 N -0.470219
21 N -0.457832	21 N -0.468648
22 N -0.051842	22 N -0.034683
23 N -0.051920	23 N -0.052141
24 N -0.052241	24 N -0.002600
25 N -0.666309	25 N -0.672874
26 N -0.457876	26 N -0.466644
27 N -0.457678	27 N -0.464775
28 N -0.666215	28 N -0.663799
29 N -0.457673	29 N -0.464624

30 N -0.457846	30 N -0.466225
31 H -0.001325	31 H 0.000754
32 H -0.028358	32 H -0.026815
33 H -0.001265	33 H 0.000476
34 H -0.001279	34 H 0.000529
35 H -0.028360	35 H -0.026729
36 H -0.001306	36 H 0.000755
37 H -0.001373	37 H 0.001378
38 H -0.001379	38 H 0.003477
39 H -0.028368	39 H -0.026816
	40 H 0.006284
	41 H -0.021691
	42 H 0.002188
	43 H -0.010734
	44 H -0.021849
	45 H 0.013501