Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Isomers of $C_{12}N_{12}$ as Potential Hydrogen Storage Materials and the Effect of Electric Field Therein

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Table S1: Binding energies (E, kcal/mol) of $nH_2@C_{12}N_{12}$-A, $nH_2@C_{12}N_{12}$-B, and $nH_2@C_{12}N_{12}$-C with increasing values of n

No. of H_2 Molecules (n)	$nH_2@C_{12}N_{12}$-A	$nH_2@C_{12}N_{12}$-B	$nH_2@C_{12}N_{12}$-C
	Average Binding Energy (E, kcal/mol)	Average Binding Energy (E, kcal/mol)	Average Binding Energy (E, kcal/mol)
1	1.43	0.89	1.34
2	1.24	1.30	1.18
3	1.19	1.60	1.18
4	1.21	1.41	1.19
5	1.21	1.31	1.24
6	1.18	1.24	1.21
7	1.18	1.18	1.21
8	1.20	1.17	1.19
9	1.19	1.13	1.18
10	1.16	1.11	1.16
11	1.16	1.06	1.11
12	1.17	1.03	1.05

Method = DFT-D-B3LYP/6-31G(d)

Table S2: Hardness (η, eV) of $C_{12}N_{12}$ isomers and H_2 loaded $C_{12}N_{12}$ isomers

No. of H_2 Molecules (n)	Hardness (η, eV)		
	$nH_2@C_{12}N_{12}$-A	$nH_2@C_{12}N_{12}$-B	$nH_2@C_{12}N_{12}$-C
0	3.879	2.519	1.724
1	3.881	2.515	1.721
2	3.879	2.520	1.705
3	3.878	2.525	1.708
4	3.886	2.524	1.711
5	3.882	2.527	1.719
6	3.878	2.526	1.716
7	3.882	2.528	1.714
8	3.884	2.525	1.757
9	3.889	2.525	1.713
10	3.894	2.524	1.725
11	3.898	2.524	1.713
12	3.903	2.527	1.725