Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

The effect of electric field on hydrogen storage for B/N-codoped graphyne

Lihong Zhang[a], Ning Wang[a], Shengli Zhang[b], Shiping Huang*[a]

[a]State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing 100029, China

[b]School of Materials Science and Engineering, Nanjing University of Science and Technology, Nanjing, Jiangsu, 210094, China

* Corresponding author: Fax: +86-10-64427616 E-mail: huangsp@mail.buct.edu.cn (S. Huang)

Table S1 The total energy of H_2 absorbed B/C/N sheet without dispersion correction (E_0), dispersion correction (E_{disp}), BSSE correction (E_{BSSE}), and the total energy of H_2 absorbed B/C/N sheet with dispersion and BSSE corrections (E_{total})for single H_2 adsorption on different site of N_bB_f doped graphyne.

Adsorption sites	**E_0(eV)**	**E_{disp}(eV)**	**E_{BSSE}(eV)**	**E_{total}(eV)**
bighollow	-49449.32	-2.71	-0.0077	-49452.03
smallhollow	-49449.26	-2.60	-0.0019	-49451.87
top1	-49449.26	-2.62	-0.0078	-49451.89
top2	-49449.26	-2.63	-0.0064	-49451.90
top3	-49449.26	-2.64	-0.0090	-49451.91
top4	-49449.27	-2.64	-0.0076	-49451.91
top5	-49449.28	-2.63	-0.0066	-49451.92
bridge1	-49449.27	-2.64	-0.0058	-49451.92
bridge2	-49449.26	-2.63	-0.0074	-49451.90
bridge3	-49449.26	-2.63	-0.0061	-49451.90
bridge4	-49449.26	-2.64	-0.0054	-49451.91
bridge5	-49449.26	-2.61	-0.0057	-49451.88

Table S2 The total energy of H_2 absorbed B/C/N sheet without dispersion correction (E_0), dispersion correction (E_{disp}),BSSE correction (E_{BSSE}), and the total energy of H_2 absorbed B/C/N sheet with dispersion and BSSE corrections (E_{total}) for single H_2 adsorption on N_bB_f doped graphyne with different electric field.

E-field(a.u.)	**E_0(eV)**	**E_{disp}(eV)**	**E_{BSSE}(eV)**	**E_{total}(eV)**
0	-49449.32	-2.71	-0.0077	-49452.03
0.005	-49449.37	-2.71	-0.0094	-49452.08
0.01	-49449.52	-2.70	-0.0090	-49452.23
0.015	-49449.77	-2.71	-0.0091	-49452.48
0.02	-49450.12	-2.70	-0.0089	-49452.83
0.025	-49450.57	-2.66	-0.0074	-49453.23
0.03	-49451.15	-2.64	-0.0065	-49453.79
0.035	-49451.87	-2.62	-0.0064	-49454.50