Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Boron-substituted graphyne as a versatile material with high Storage capacities of Li and H_2: A multiscale theoretical study

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S1. Computational details

The original force field (FF) parameters can not completely describe the interactions between the atoms in this work, so the Dreiding FF which is selected to perform the GCMC simulations should be appropriately modified. We calculated the potential energy relationships between H_2 and host materials and fitted the data by using the Morse equation[1] as

$$U_{ij}(r_{ij}) = D\left\{\exp\left[\alpha\left(1-\frac{r_{ij}}{r_o}\right)\right] - 2\cdot\exp\left[\frac{\alpha}{2}\left(1-\frac{r_{ij}}{r_o}\right)\right]\right\}$$

with the well depth D, the force constant α, and the equilibrium bond distance r_0.

Fig. S1 shows the calculated results from DFT methods with the Grimme correction and the fitted results. It is clear that the fitted line is in good agreement with the calculated data. All FF parameters used in this work are listed in Table S1.

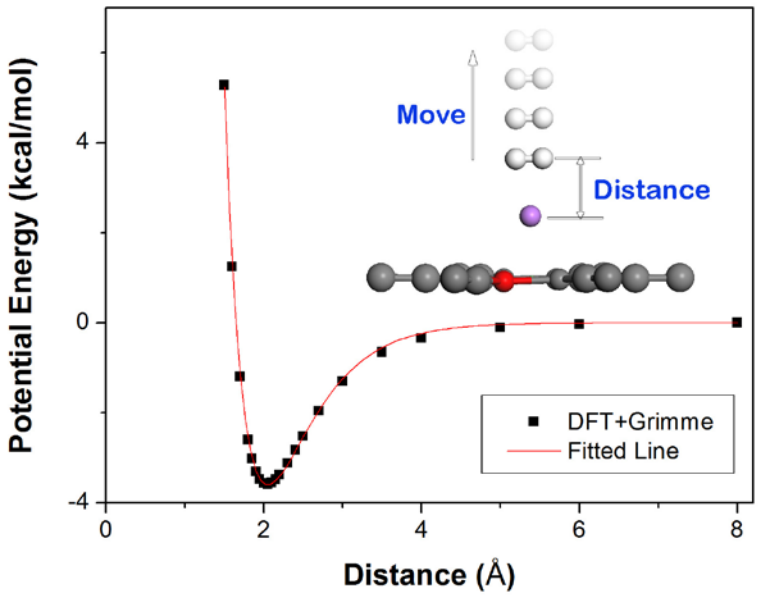

Fig. S1. The interaction energy between H_2 and Li-BG.

Table S1. FF parameters (Li_1 is the Li atoms at P-I and Li_2 at P-II).

Terms	*D* (kcal/mol)	*α*	r_0 (Å)
H__A---H__A	0.01850	10.70940	3.56980
B---H__A	0.02801	12.78312	3.40987
C---H__A	0.10041	10.39184	3.14283
Li_1---H__A	1.80100	7.32310	2.08068
Li_2---H__A	1.12918	7.68084	2.18644

S2. Complementary data

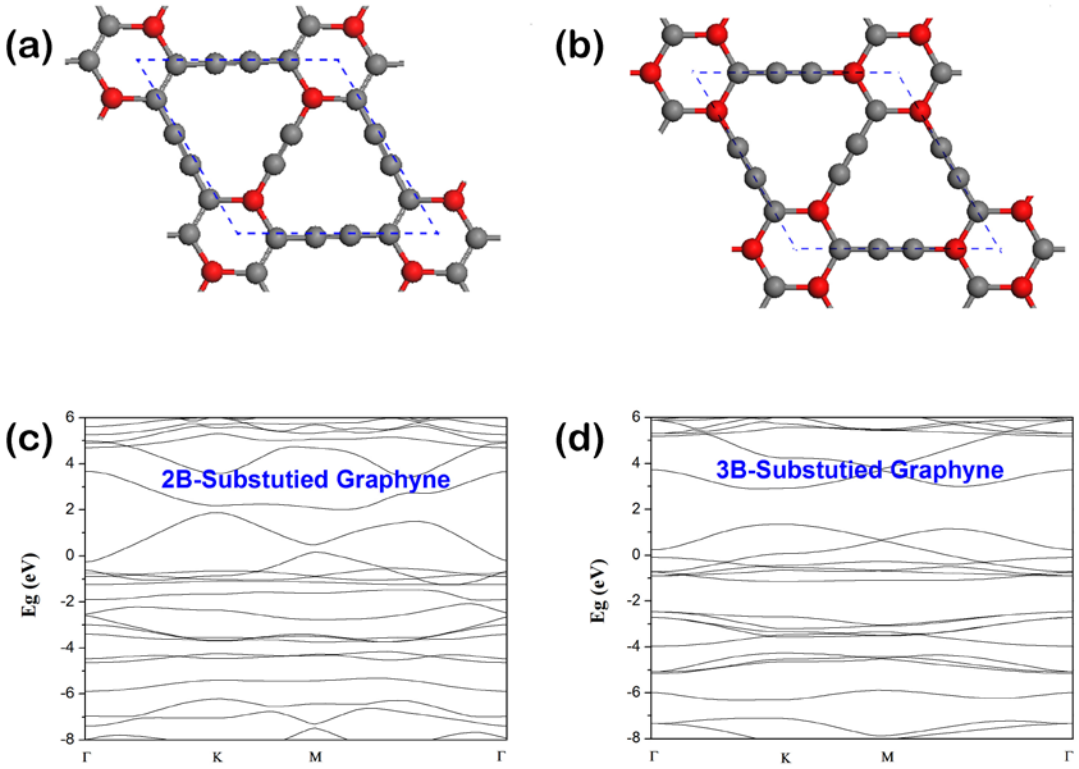

Fig. S2. The geometric and band structures of 2BG and 3BG.

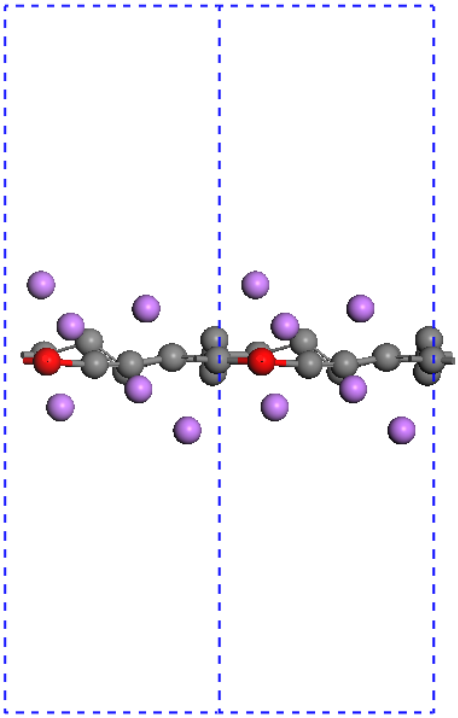

Fig. S3. The structure of fully Li loaded on 1BG at 500 K after 2 ps MD simulation.

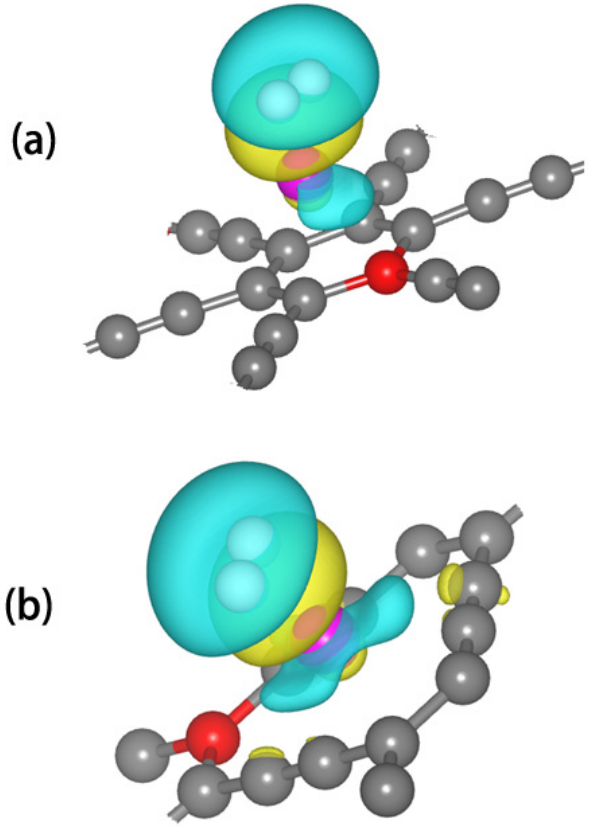

Fig. S4. Charge density differences of H_2 adsorbed around Li atoms: (a) at P-I and (b) at P-II.

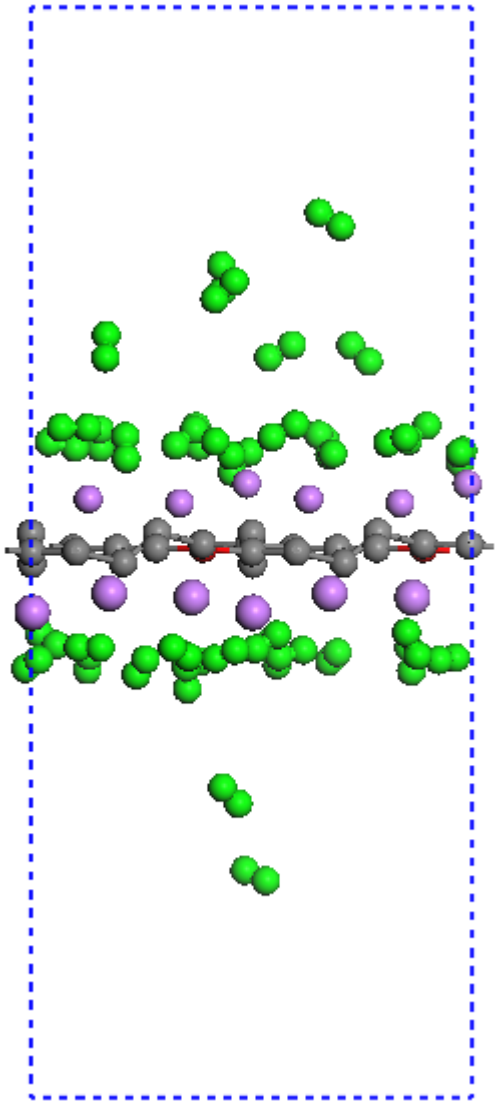

Fig. S5. The snapshot of H_2 stored in 6Li@1BG at 298 K and 100 bar simulated by GCMC method.

Reference

1. P. M. Morse, *Phys. Rev.*, 1929, **34**, 57-64.