

Supporting Information

Reversible hydrogen storage in pristine and Li decorated 2D boron hydride

Long Chen^a, Xianfei Chen^{a*}, Chao Duan^a, Yi Huang^{b,c†}, Qian Zhang^a, Beibei Xiao^d

^a College of Materials and Chemistry & Chemical Engineering, Chengdu University of Technology, Chengdu 610059, China

^b State Environmental Protection Key Laboratory of Synergetic Control and Joint Remediation for Soil & Water Pollution, Chengdu University of Technology, Chengdu 610059, China

^c College of Environment and Ecology, Chengdu University of Technology, Chengdu 610059, China

^d School of Energy and Power Engineering, Jiangsu University of Science and Technology, Zhenjiang 212003, China

* Corresponding author. Email: chenxianfei2014@cdut.edu.cn;

† Corresponding author. Email: huangyi@cdut.cn

Fig. S1 The most favorable atomic configuration of single H₂ adsorption on 2×3 BH, E_{ad} and h indicate the adsorption energy of H₂ molecule and the distance from H₂ molecule to BH layer.

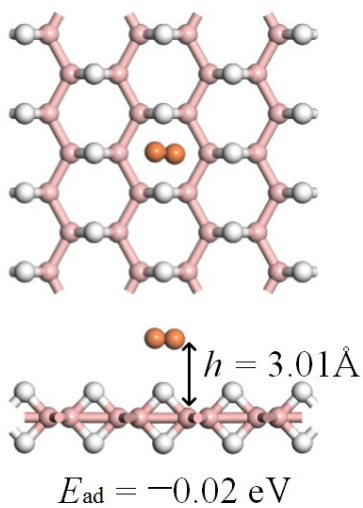


Fig. S2 The atomic configuration of 2×3 (BH) with Na, K, Al, Ca and Mg doped on BH, respectively, h indicates the distance from the metal atom to the BH layer.

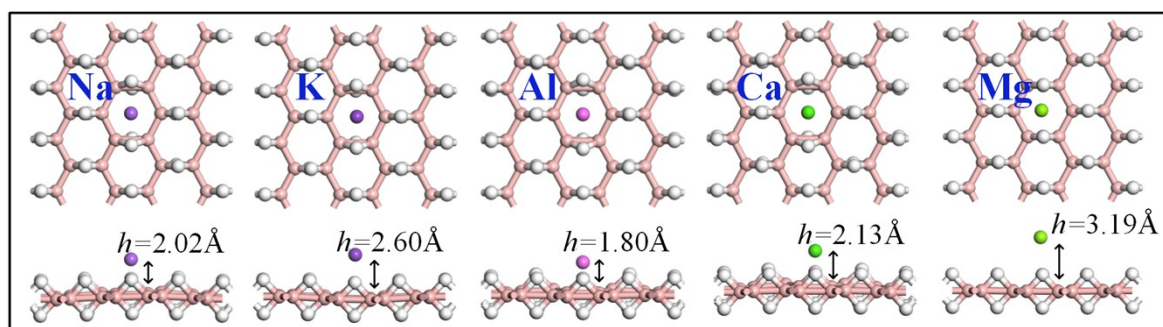


Fig. S3 The optimized structures of Li-BH system with (a) one H₂, (b) two H₂, (c) three H₂ and (d) four H₂. The l indicates the nearest distance of H₂ to the Li. The red balls refer to the adsorbed H₂ molecules for clarity.

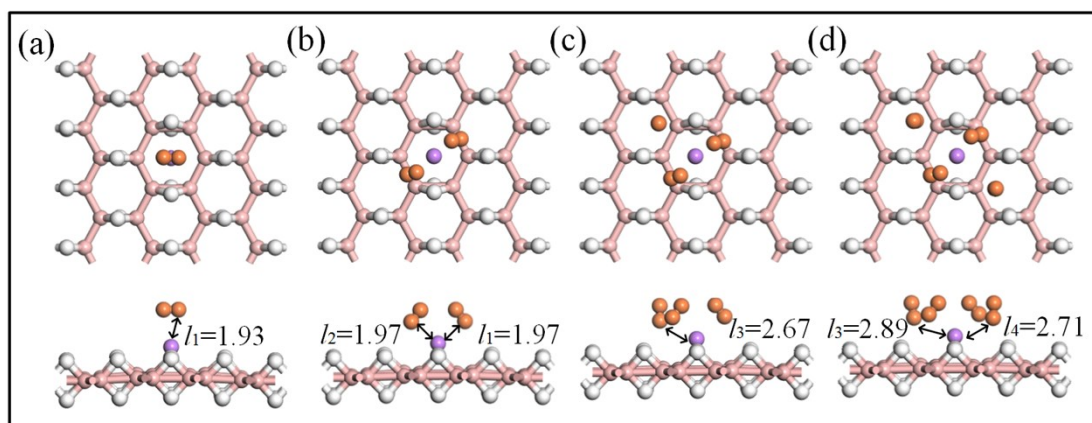


Fig. S4 The most favorable atomic configurations of 4, 6 and 8 Li atoms adsorption on 2×2 BH, E_b indicates the average binding energy of Li atom.

