Supplementary Material (ESI) for *PCCP*

Supporting Information for

The role of interstitial H_2 in hydrogen diffusion in light metal borohydrides

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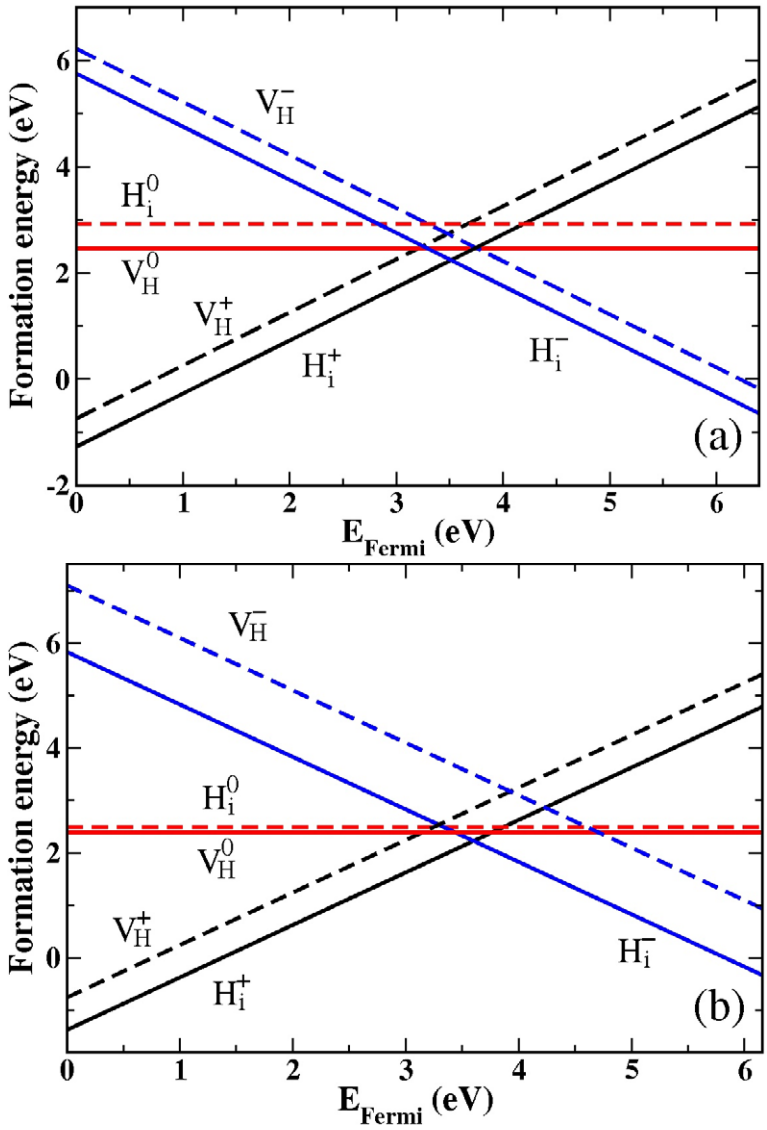

FIG. S1 Calculated formation energy for V_H and H_i with different charge states in (a) $NaBH_4$ and (b) KBH_4.

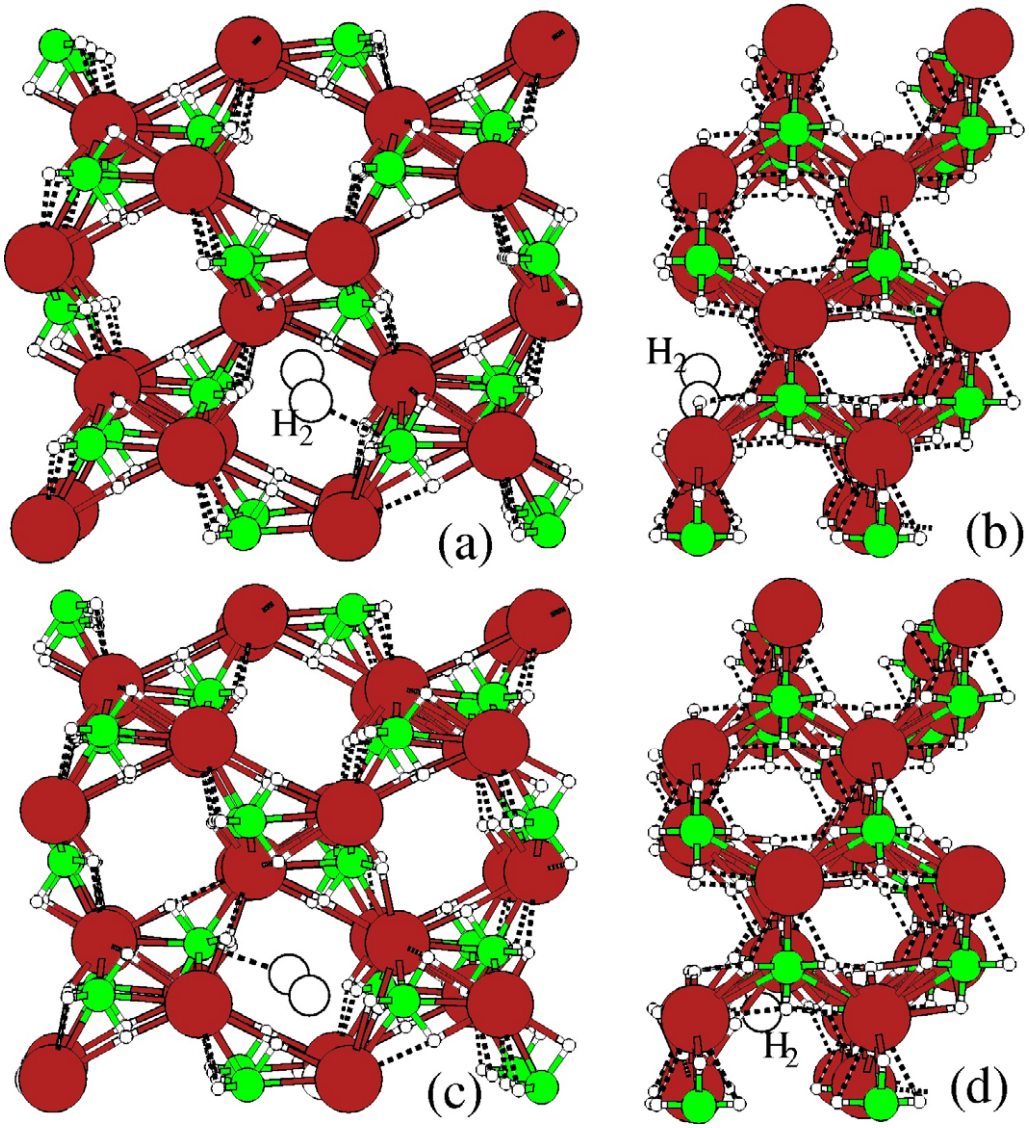

FIG. S2: H_2 diffusion pathway in $LiBH_4$. (a) initial state of H_2 viewed from [010] direction; (b) initial state of H_2 viewed from [100] direction; (c) transition state of H_2 viewed from [010] direction; (d) transition state of H_2 viewed from [100] direction. For the initial state, the distance of the center of mass of H_2 to the nearby Li atoms is 3.12 Å; for the transition state, the distance of center of mass of H_2 to the nearby Li (B) atoms is 2.8 Å (2.9 Å).

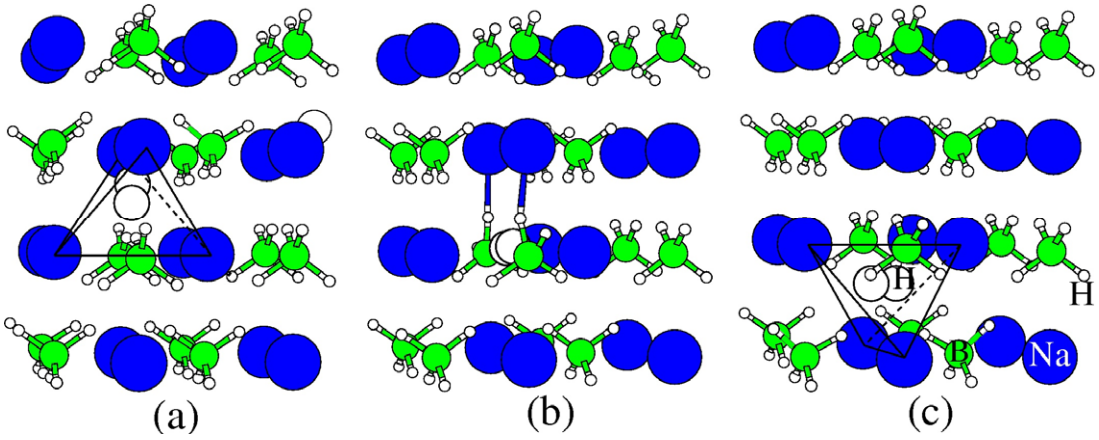

FIG. S3: H_2 diffusion pathway in $NaBH_4$. (a) initial state of H_2 ; (b) transition state of H_2 ; (c) final state of H_2. For the initial and final state of H_2, the distance of center of mass of H_2 to the nearby corner of the tetrahedron shown in the figure is 2.62 Å. For the transition state of H_2, the distance between the center of mass of H_2 and corners of the cube defined by the nearby NA atoms is 2.32 Å.