

Supporting material (ESI) for PCCP

First-Principles Study of the Formation and Migration of Native Defects in LiNH_2BH_3

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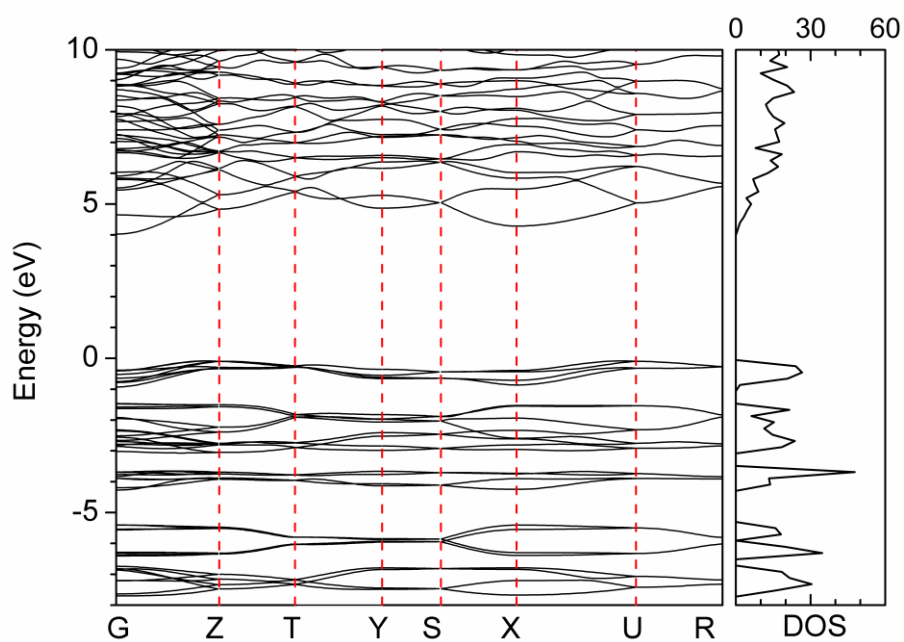


Figure S1. The left panel contains the calculated band structure of the ground state of LiNH_2BH_3 . The right panel is the complete electron density of states, in arbitrary units.

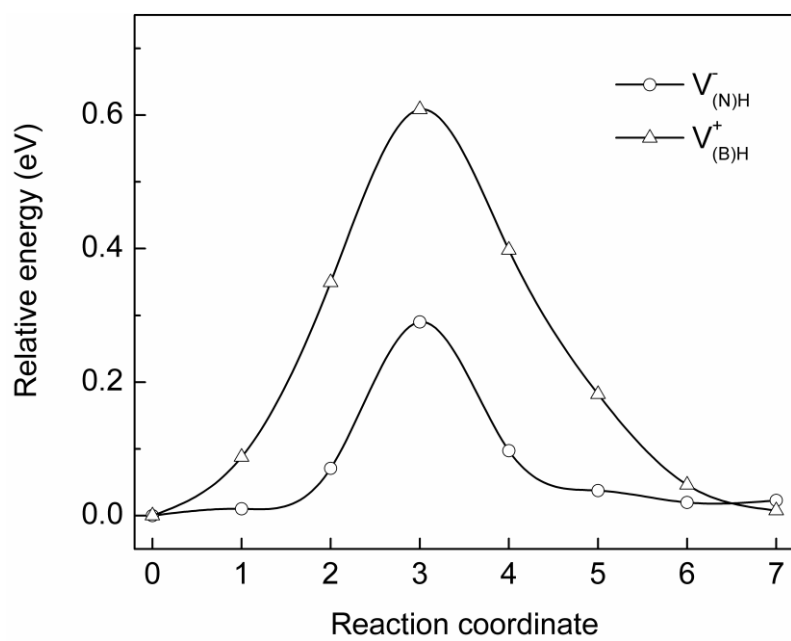


Figure S2. The energy profiles for the migration of $V_{(B)H}^+$ and $V_{(N)H}^-$.

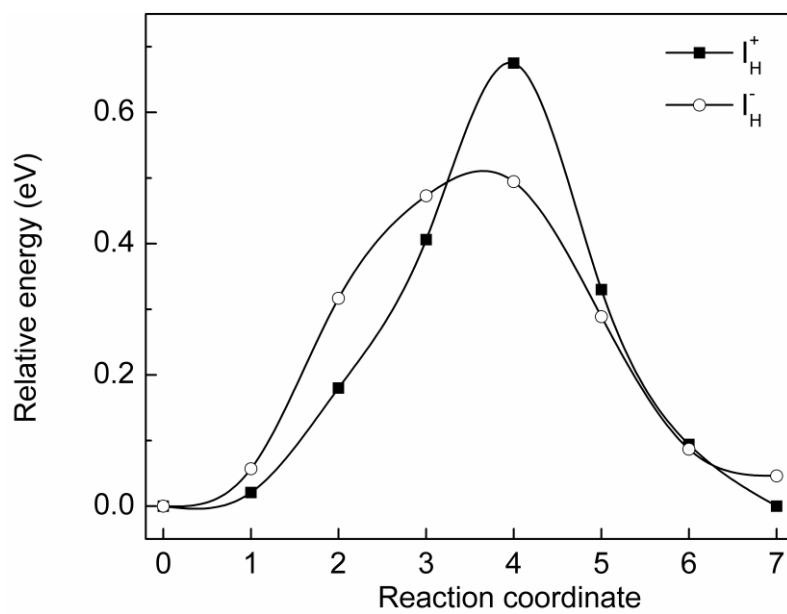


Figure S3. The energy profiles for the migration of I_H^+ and I_H^- .

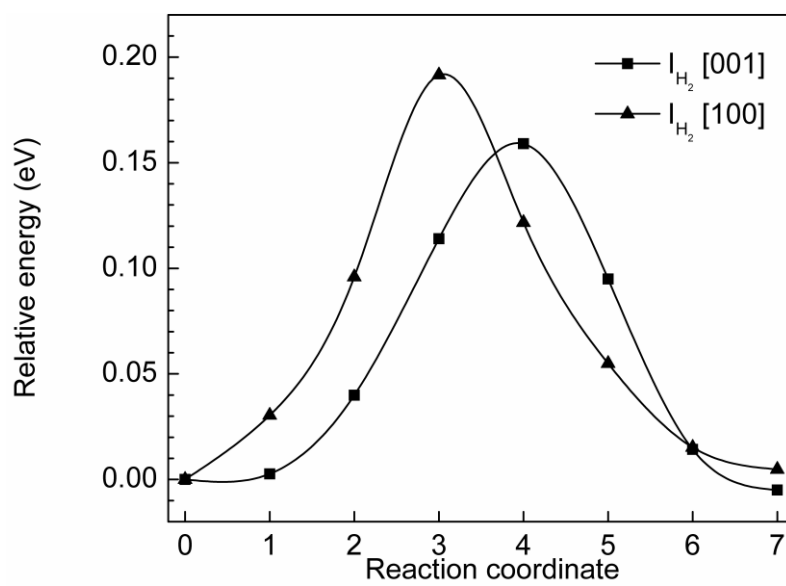


Figure S4. The energy profiles for the migration of neutral H₂ interstitial along [100] and [001] direction.

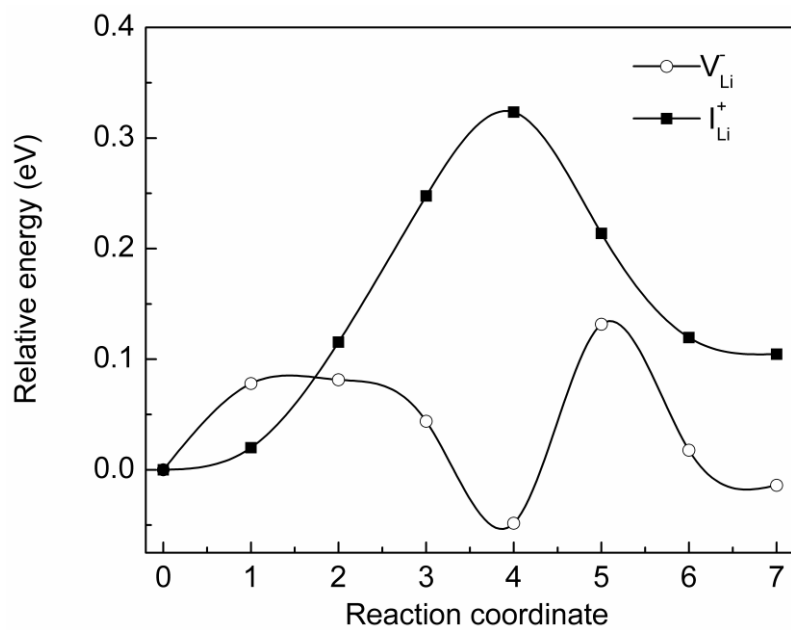


Figure S5. The energy profiles for the migration of I_{Li}^+ and V_{Li}^- .