

Supporting Information

Two-Dimensional Penta-BN₂ with High Specific Capacity for Li-Ion Batteries

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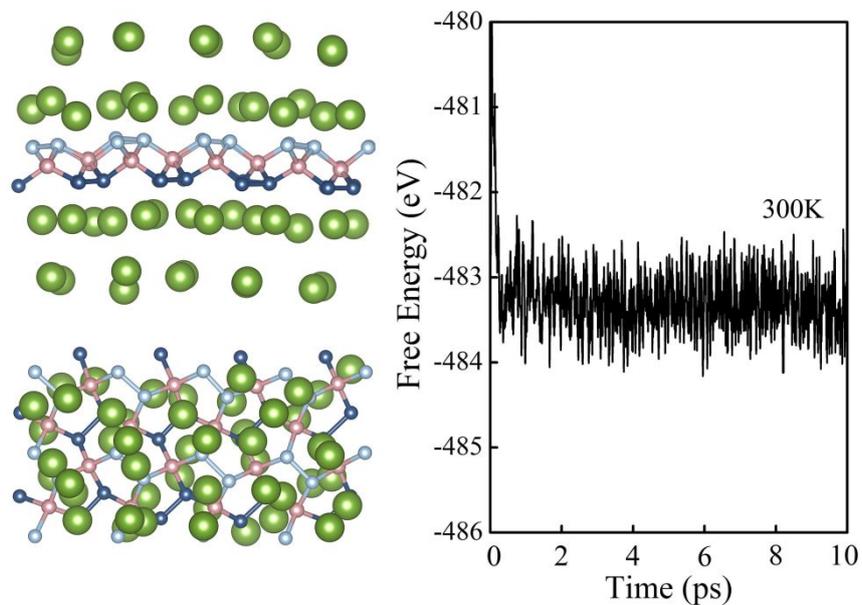


Figure S1. Time evolution of free energy during the 10 ps AIMD simulations and the snapshot of 300 K for Li_3BN_2 .

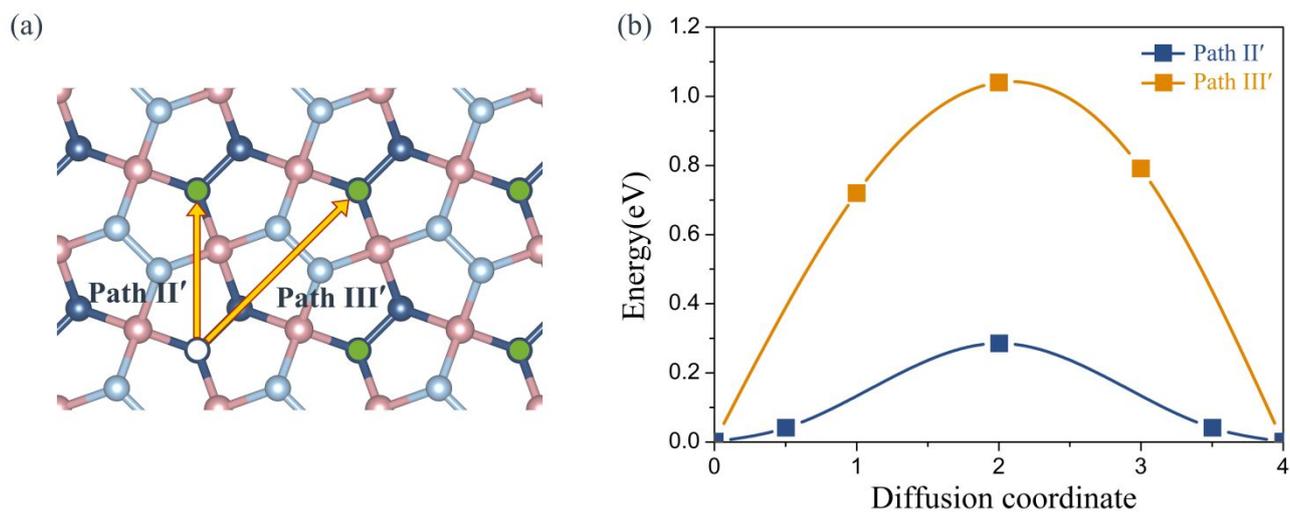


Figure S2. (a) Top view of single Li vacancy diffusion along the Path II' and Path III'. (b) The corresponding energy barriers of the Path II' and Path III'.