Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Borophene's Tryst with Stability: Exploring 2D Hydrogen Boride as Electrode for Rechargeable Batteries

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(a) (b)

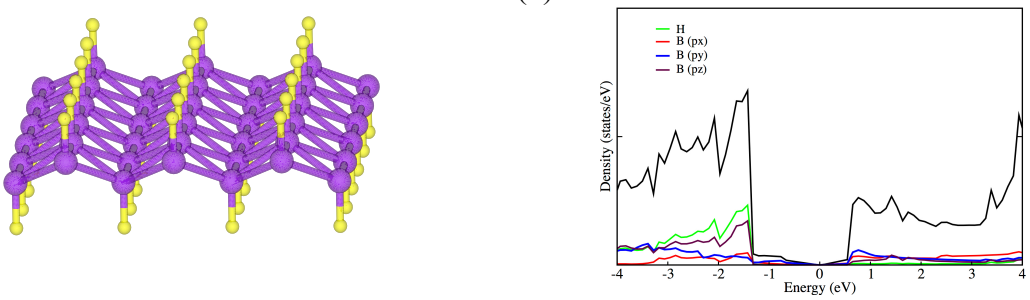

Figure S1: Structure (a) and (b) Projected density of states for computaionally predicted hydrogen boride (c-HB)

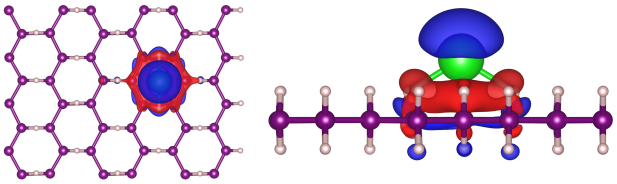

Figure S2. Charge density difference plots for Na-atom adsorption on HB (top and side views; Isosurface value is 0.002 a.u.; isosurface colors: red for electron sufficient and blue for electron deficient regions).

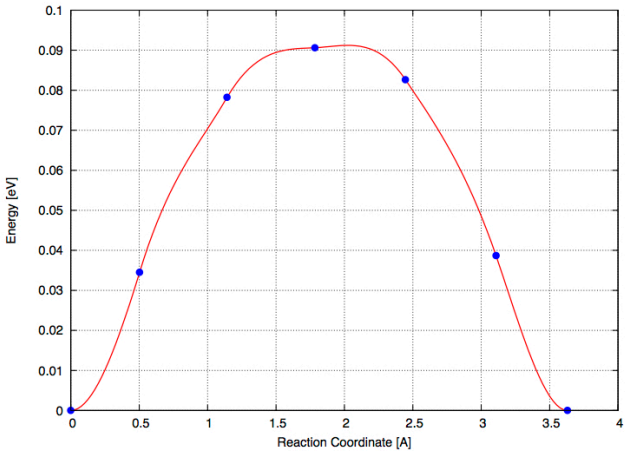

Figure S3. Minimum energy path for Na diffusion on 2D HB