"Supporting Information"

Lithium-Decorated Porous BC_2P Monolayer: A Novel High-Capacity Material for Efficient and Reversible Hydrogen Molecule Storage

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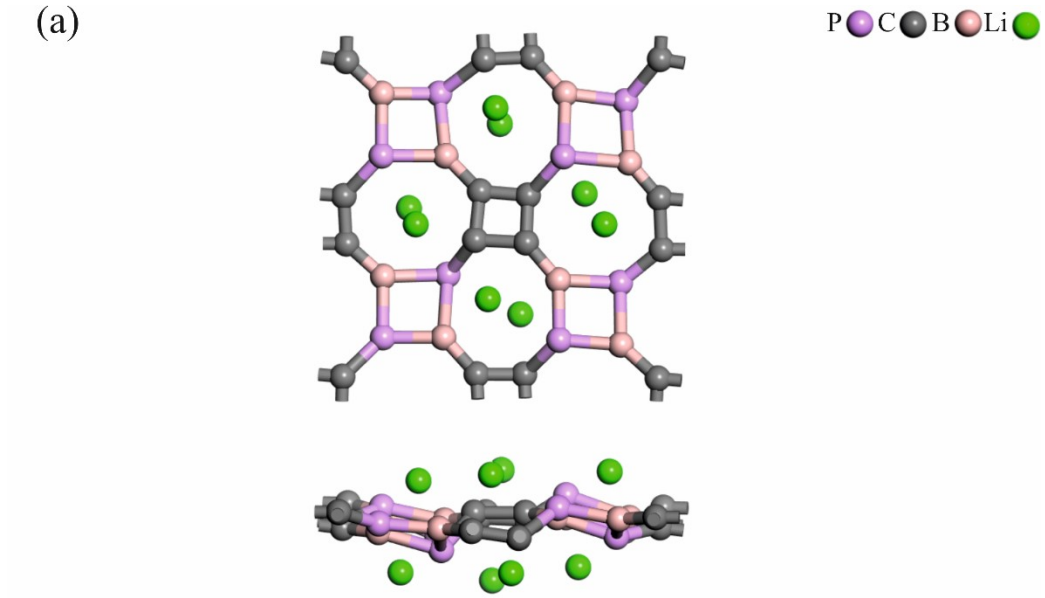
Figure S1. (a) Final structure of AIMD simulated Li@BC_2P monolayer (at T=500 K, time step=1 fs) from top and side views, and (b) corresponding potential energy diagram versus simulations time



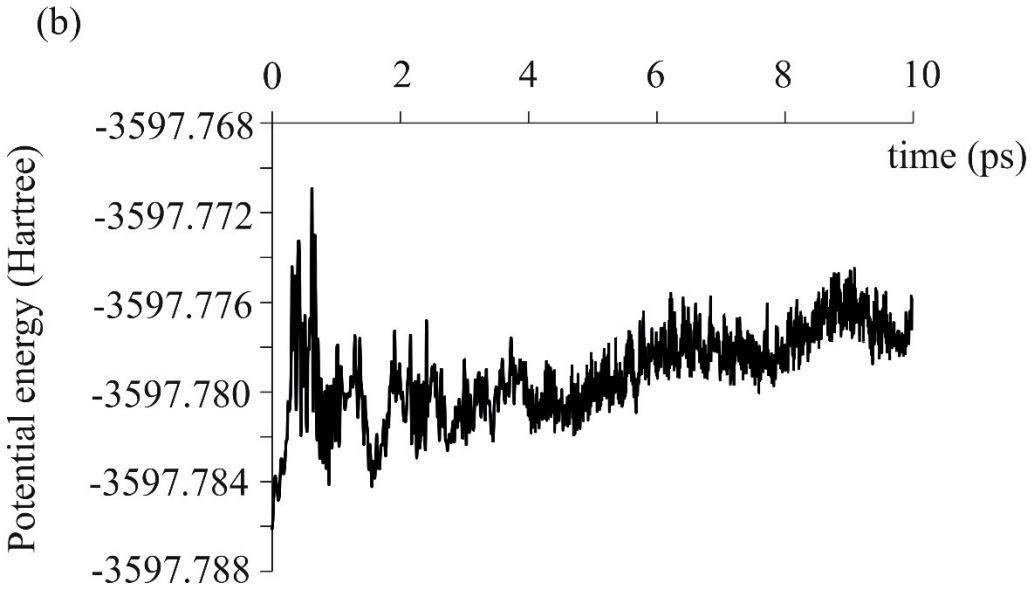


Figure S2. AIMD simulations and snapshots of $24H_2/Li@BC_2P$ at T=300 K (with a time step of 1 fs)