Supplementary Material for

Enhanced Ions Diffusion Induced by Structural

Transition for Li-Modified Borophosphene

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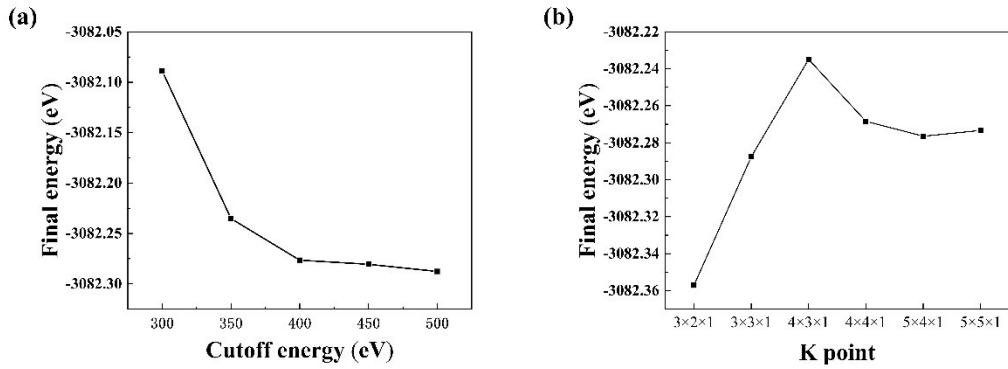
Figure S1. (a) The total energy of $B_{12}P_{12}$ at different cutoff energy when Monkhorst-Pack K-point mesh is set as 5×4×1. **(b)** The total energy of $B_{12}P_{12}$ at different Monkhorst-Pack K-point mesh.
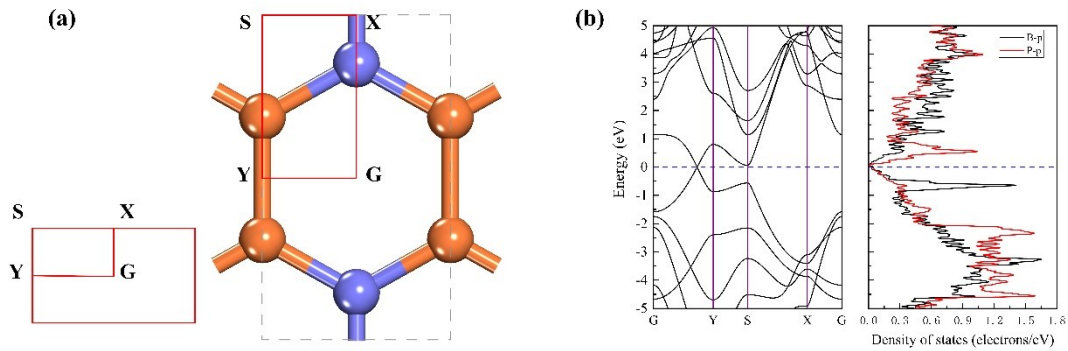

Figure S2. (a) the integration path in the Brillouin zone for the unit cell of monolayer borophosphene. **(b)** The band structure and partial density of states of monolayer borophosphene.
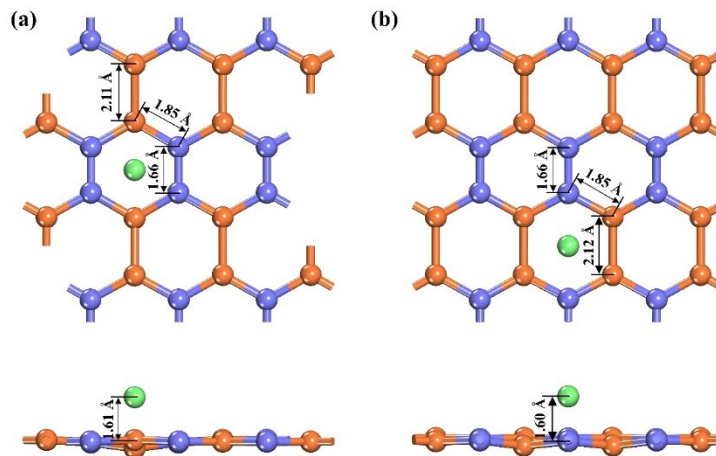

Figure S3. The structural information for Li adsorption in $B_{12}P_{12}$ at binding sites of **(a)** B_4P_2-ring and **(b)** B_2P_4-ring centers, respectively.
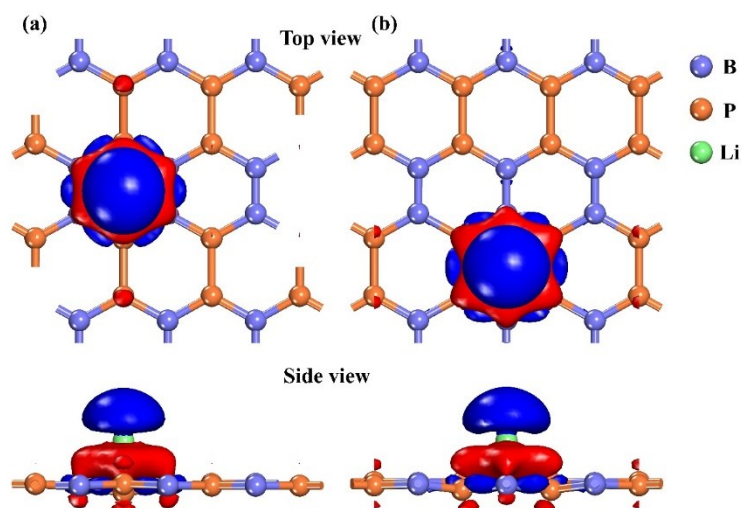
Figure S4. The differential charge density distribution of $LiB_{12}P_{12}$ at (a) α site and (b) β site, with red and blue areas illustrating charge sufficient and charge deficient regions respectively at isosurface of 0.01 $e/Å^3$. The green ball represents lithium atom.
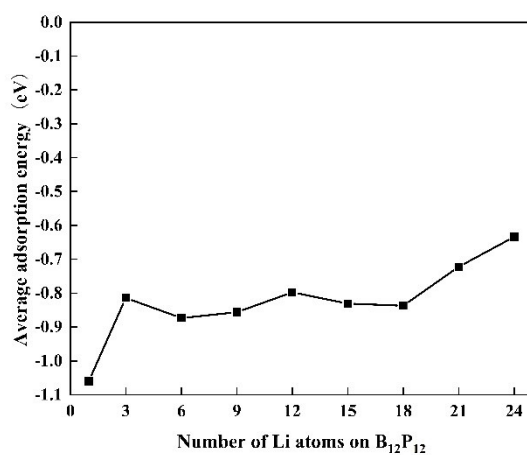
Figure S5. The average adsorption energy of $Li_xB_{12}P_{12}$ at Li concentration x of 1, 3, 6, 9, ... , and 24, respectively.
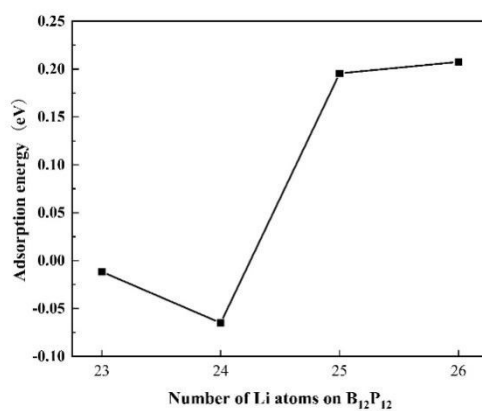
Figure S6. Adsorption energy of the *x*-th Li atom in $Li_xB_{12}P_{12}$ (*x* = 23, 24, 25, 26).
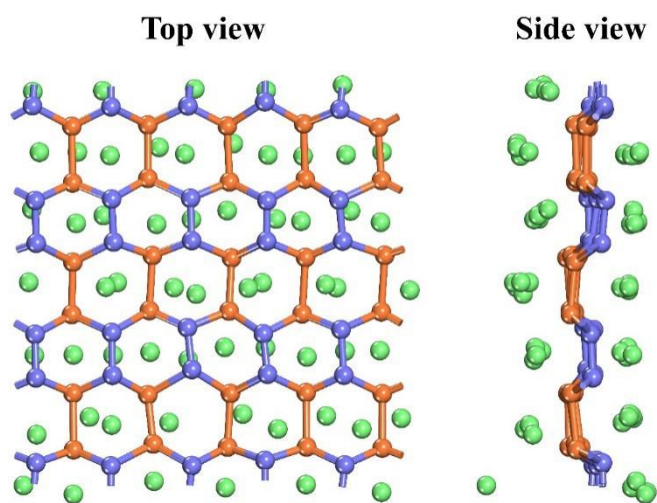
Figure S7. Top and side views of AIMD simulations for $Li_{60}B_{30}P_{30}$ supercell at 500K after 5 ps.