

# Metallic B<sub>2</sub>C<sub>3</sub>P Monolayer As Li-Ion Battery Materials: A First-Principles Study

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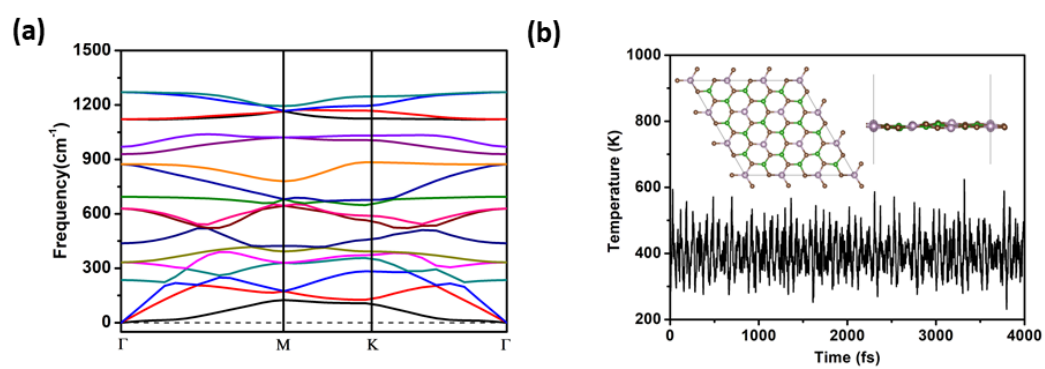
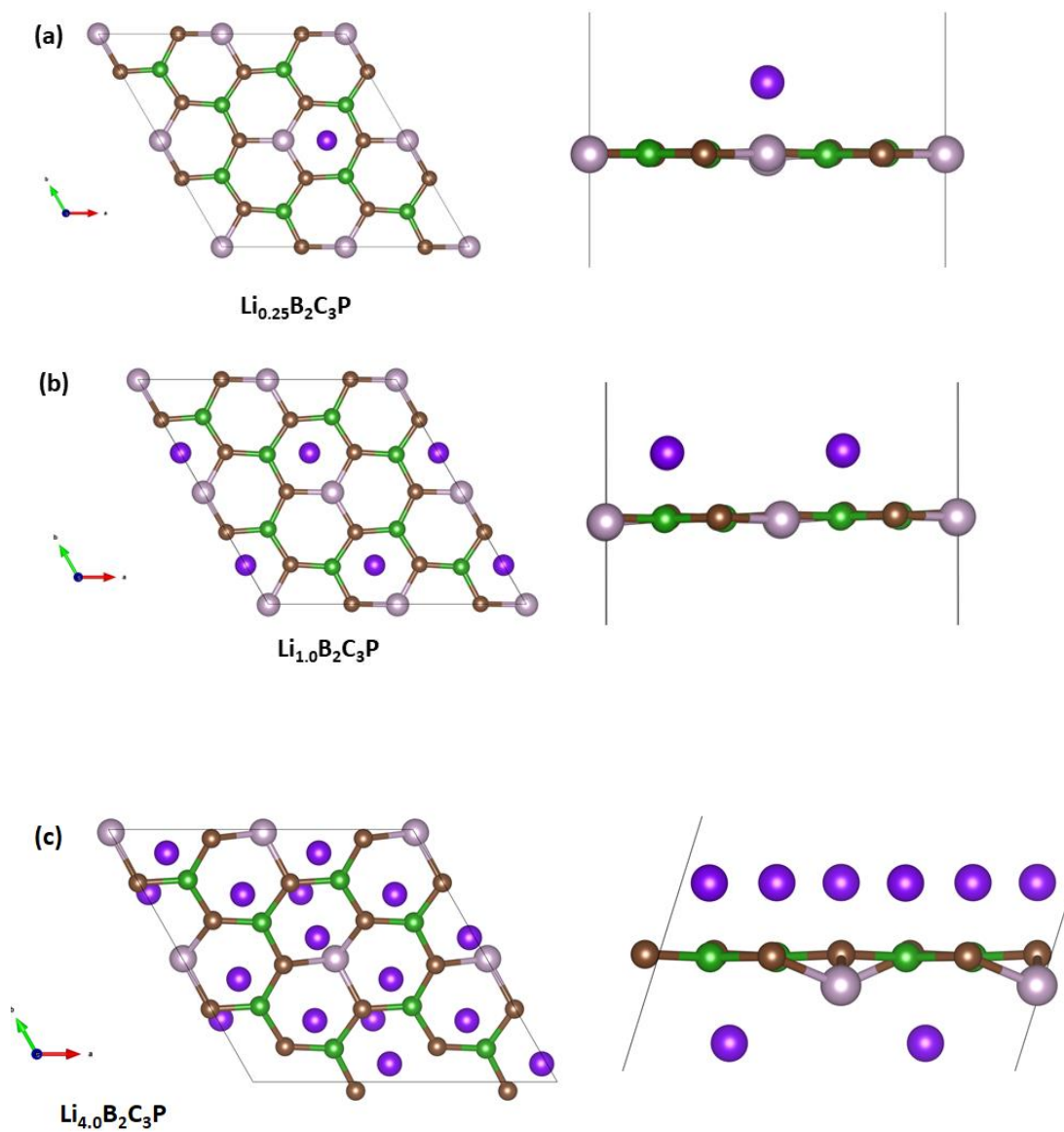


Figure S1 (a) Phonon spectra curve of  $B_2C_3P$ . (b) Variations of temperature in the AIMD simulations of the  $B_2C_3P$  at 400 K. The insets is the structure of  $B_2C_3P$  at the end of the AIMD simulation.



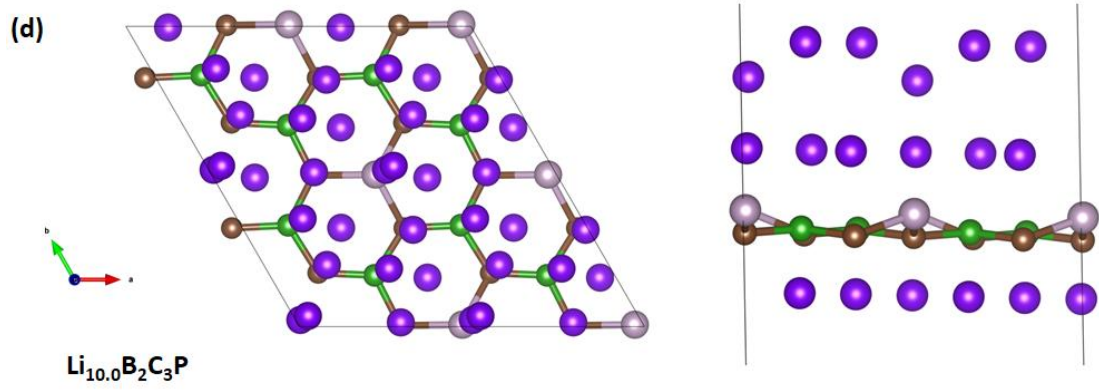


Figure S2 Top and side views of the lithiated structures of (a)  $\text{Li}_{0.25}\text{B}_2\text{C}_3\text{P}$ , (b)  $\text{Li}_{1.0}\text{B}_2\text{C}_3\text{P}$ , (c)  $\text{Li}_{4.0}\text{B}_2\text{C}_3\text{P}$ . (d)  $\text{Li}_{10.0}\text{B}_2\text{C}_3\text{P}$ . The B, C, P, and Li atoms are denoted by green, brown, gray, and purple balls, respectively. When all the lithiated structures are illustrated, a  $2\times 2\times 1$  supercell is used.

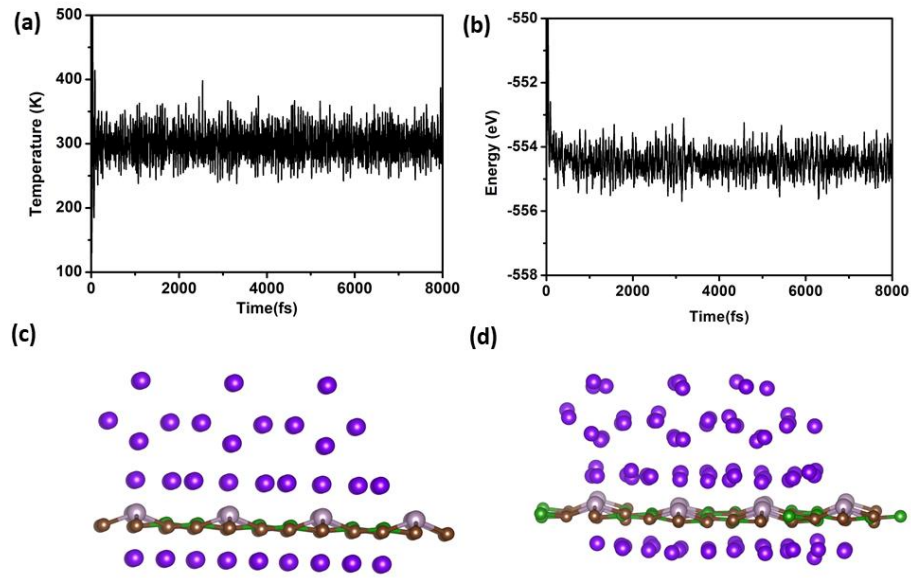


Figure S3. Variations of temperature (a) and energy (b) in the AIMD simulations of the  $\text{Li}_{10.0}\text{B}_2\text{C}_3\text{P}$  at 300 K.  $\text{Li}_{10.0}\text{B}_2\text{C}_3\text{P}$  with Li ions adsorbed on the surface of 2D  $\text{B}_2\text{C}_3\text{P}$  monolayer before the AIMD simulation (c) and the structure of  $\text{Li}_{10.0}\text{B}_2\text{C}_3\text{P}$  at the end of the AIMD simulation (d).