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## Borophene: A Promising Anode Material Offering High Specific Capacity and High Rate Capability for Lithium-Ion Batteries

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### Abstract

In this work, we adopt first-principles calculations and *ab-initio* molecular dynamics simulations to investigate the potential of borophene as an anode material for lithium-ion batteries. It is found that borophene has an adsorption energy to lithium atom of -1.12 eV, which is large enough to ensure a good lithium-borophene stability during the lithiation process. The fully lithiated phase of borophene is  $\text{Li}_{0.75}\text{B}$ , corresponding to a theoretical specific capacity of  $1860 \text{ mAh g}^{-1}$ , which is about 4 times larger than that of the commercial graphite anode ( $372 \text{ mAh g}^{-1}$ ). More excitingly, it is found that the energy barrier along the furrow of corrugated borophene is only 2.6 meV, which is much lower than those of other widely investigated anode materials such as phosphorene (80 meV) and  $\text{Ti}_3\text{C}_2$  (70 meV). The finding suggests that lithium diffusion on borophene can be extremely fast. In the meantime, a strong directional anisotropy is observed for lithium diffusion, with a 325.1 meV barrier perpendicular to the furrow of borophene. This phenomenon is further proved by

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<sup>1</sup> These authors contributed equally to this work.

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