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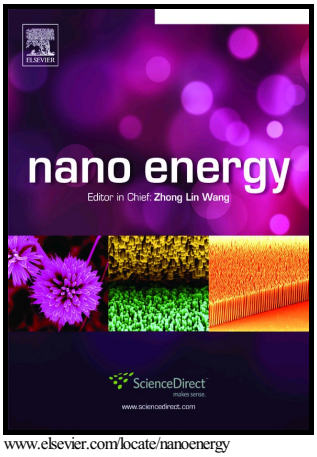

www.elsevier.com/locate/nanoenergy

PII: S2211-2855(16)30022-2
DOI: http://dx.doi.org/10.1016/j.nanoen.2016.03.013
Reference: NANOEN1191

To appear in: *Nano Energy*

Received date: 31 January 2016
Revised date: 13 March 2016
Accepted date: 15 March 2016

Cite this article as: H.R. Jiang, Ziheng Lu, M.C. Wu, Francesco Ciucci and T.S Zhao, Borophene: A promising anode material offering high specific capacity anc high rate capability for lithium-ion batteries, *Nano Energy* http://dx.doi.org/10.1016/j.nanoen.2016.03.013

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 $Li_{0.75}B$, corresponding to a theoretical specific capacity of 1860 mAh g^{-1}, which is about 4 times larger than that of the commercial graphite anode (372 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 Ti_3C_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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