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Electronic structure of lithium borocarbide as a cathode material for a rechargeable Li-ion battery: First-principles calculation QIANG XU, CHUNMEI BAN, ANNE DILLON, SUHUAI WEI, YUFENG ZHAO, National Renewable Energy Laboratory — Traditional cathode materials, such as transition-metal oxides, are heavy, expensive, and often not benign. Therefore, alternative materials without transition metal elements are highly desirable in order to design high-capacity Li-ion batteries of light weight and low price. Here we report on potential application of the LiBC compound as cathode materials, in which graphene-like BC sheets are intercalated by Li ions. The crystal structure and properties of LiBC were firstly reported by Wörle et al. in 1995. Importantly, it was found that the 75% Li ions can be retrieved out of the compound without changing the layered structure. We have performed first-principles calculations based on density functional theory, as implemented in the Vienna Ab-initio Simulation Package. According to our calculation, the layered Li_xBC structure can be well preserved at $x > 0.5$. The reversible electrochemical reaction, $LiBC \leftrightarrow Li_{0.5}BC + 0.5Li$, gives an energy capacity of 609mAh/g and an open-circuit voltage of 2.42V. The volume change is only about 5% during the charging and discharging process. All these results point to a potentially promising application of LiBC as a novel cathode material for high-capacity Li-ion batteries in replacement of the transition metal oxides.

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