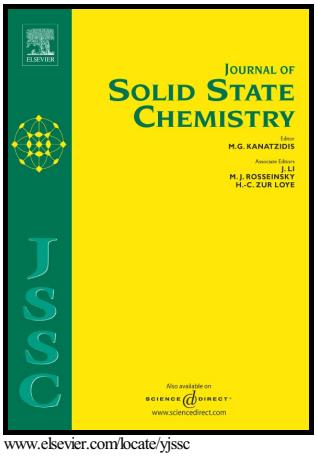

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Influence of electric charge on the stability of graphite-like BC_2

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Abstract

Graphite-like BC_2 has yet to be synthesized; however, it stably exists in the $Sc_2B_{1.1}C_{3.2}$ compound, where the boron atoms are arranged as far apart from each other as possible. Recently, a theoretical study on monolayer BC_2 reported that in the most stable structure, B atoms are positioned adjacent to each other. We anticipated that graphite-like BC_2 might take a different structure based on the electric charge. Therefore, we carried out first principles calculations to investigate whether this is true or not. The most stable structure among the six possible structures changed with the increase in the negative electric charge, which well explained both the previous results without contradiction. The most stable structure was also dependent on the pressure. The Li intercalation potential for BC_2 was calculated to investigate its applicability as an anode for lithium-ion batteries. Our results revealed that Li atoms can be intercalated into BC_2 to yield $Li_{1.5}BC_2$, whose gravimetric capacity is approximately 3.1 times higher than that of LiC_6. However, the most stable structure with intercalated Li atoms became unstable when all the Li atoms were extracted. This feature may hinder the repetitive charge–discharge cycle of the anode and hence needs to be carefully considered.

Li intercalation potentials for graphite-like BC_2. Li atoms can be intercalated into BC_2 to yield $Li_{1.5}BC_2$.

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