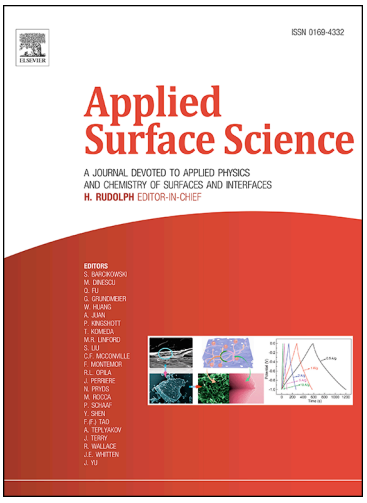

Full Length Article

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The adsorption, diffusion and capacity of lithium on novel boron-doped graphene nanoribbon: A density functional theory study

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Abstract

Inspired by the experimental synthesis of novel boron-doped graphene nanoribbon (BGNR), we have performed density functional theory (DFT) calculations to reveal the adsorption behaviors of lithium (Li) atoms on BGNR. We systematically studied the adsorption, diffusion and capacity of Li on BGNR with 7 carbon atoms in width. It is found that due to the doping effects of boron (B) atoms, BGNR exhibits a narrower band gap than graphene nanoribbon (GNR) with the same width. Individual Li atom exhibits much stronger binding on BGNR than that on GNR, attributing to the stronger Li-C interaction caused by doping of B atoms. A zigzag diffusion path along the growth direction of BGNR is confirmed for diffusion of Li. The maximum theoretical storage capacity of Li on BGNR is determined as 783 mAh/g, which is 15 times than that on GNR with same width (52 mAh/g). Our results demonstrated that doping of B atoms greatly enhances the adsorption and storage performance of Li, which provides a theoretical foundation of researches on the novel BGNR and other similar structures for adsorption and storage of Li.

Keywords: Graphene nanoribbon; Boron doping; Lithium adsorption and diffusion; Density functional calculations