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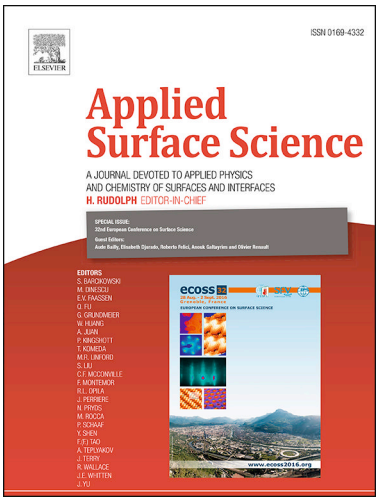

Full Length Article

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How to boost the sluggish lithium-ion hopping dynamic in borophene?

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Abstract

In light of low atomic mass, three types of experimentally synthetized borophene including β_{12}, χ_3 and striped t-sheet have been predicted to be promising anode materials for lithium-ion batteries (LIBs) with extremely high capacity. However, the rate performances of β_{12} and χ_3 are quite poor with high diffusion barrier of 0.66 ~ 0.81 eV on β_{12} and 0.60 ~ 0.85 eV on χ_3 in contrast with that in t-sheet (typically < 0.1 eV). Isolation of t-sheet from their blend remains a fundamental challenge in the field of nanotechnology and a mechanistic understanding and control over the hopping dynamic of Li^+ therein are thus of extremely important to facilitate the development of borophene-based anode material, but still lacking. In this work, we performed a comprehensive theoretical investigation on the adsorptions and migrations of Li^+ on perfect and defective β_{12} and χ_3 based on density functional theory. We determined a new kind of vacancy in β_{12} that modulates the adsorption and boosts the diffusion of Li^+ nearby remarkably. With the aid of charge doping, we uncover a general mechanism (charge-concentration mechanism) involved with the celebrated bonding theory of borophene, where the hopping barrier of Li^+ on β_{12} could be reduced to be 0.06 eV, rationalizing the boosting Li^+ hopping as a result of electron deficiency in vacant borophene. By extending our calculations to H functionalized borophene and Ag supported borophene, we further confirm the validity of the "charge-concentration mechanism" under more realistic experimental conditions. The proposed mechanism could be used as a guiding principle to improve or develop new borophene-based electrode materials with high rate performance for LIBs.

Key words: borophene, Li ion hopping dynamic, vacancy defect, Li ion battery, anode material, density functional theory