Materials Today: Proceedings

https://doi.org/10.1016/j.matpr.2020.02.285

Theoretical analysis of borophene for lithium ion electrode

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ABSTRACT

Borophene, a 2-dimensional material with efficacious properties (electrical, thermal and mechanical), is a very promising material that is expected to contribute, significantly, in the revolutionization of electrochemical energy storage, for improved energy and power density. In order to prove the potency of borophene as a potential anode electrode in lithium-ion batteries, density function theory simulation is performed. The study considered the interaction of stable striped, (β12), and honeycomb (Hb) borophene, with lithium ions. The main interest is to investigate the adsorption energy of the materials, and their specific capacities. The calculated average adsorption energies for the two promising electrodes are: −1.710 eV, and −0.517 eV. Moreover, the estimated specific capacities of the batteries, are: 929 mAh/g and 584 mAh/g; these results evidently proved that borophene may deliver the total energy demand of the globe, if more attention is paid into it, through dedicated research and development.