

عنوان مقاله:

encapsulated and hydrogenated B₂₄N₂₄ nanocluster as an anode for Li-ion batteries: A DFT study

محل انتشار:

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خلاصه مقاله:

We investigated the performance of a BN nanocluster, and its structurally manipulated forms as anode materials for Li-ion batteries (LIBs) by means of density functional theory calculations. The pristine cluster shows a low performance with the electrochemical cell voltage (V_{cell}) of about 1.07 V. Thus, we introduced two strategies to improve the performance of the cluster, including the hydrogenation of B atoms of the B₂₄N₂₄ or encapsulation an anion inside the cage. The first strategy failed by demonstrating a negative V_{cell} because of the stronger interaction of atomic Li with the hydrogenated cluster compared to the cationic Li. While, encapsulating a fluoride inside the B₂₄N₂₄ nanocage significantly increases the V_{cell} from 1.07 to 2.90 V which is larger in comparison to the V_{cell} which has been predicted for carbon nanotubes, C₂₄ fullerene, and functionalized BN nanosheets.

کلمات کلیدی:

nanocluster, batteries, B₂₄N₂₄

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