Short Communication

First-principle Study on Sr-doped $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$

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doi: 10.20964/2019.07.73

Received: 15 March 2019 / Accepted: 15 May 2019 / Published: 10 June 2019

Applying supersoft pseudopotential plane wave method of the first principle based on functional theory to investigate the band and density of states of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and Sr^{2+} doped $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$. Theoretical calculations demonstrated that $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ is a conductor material as well as the site of Mn doping Sr^{2+} will increase the bands number of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$. Furthermore, after $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ doping Sr^{2+} , it will help to shorten bond length between Mn-O and Ni-O bond, making the crystal structure more stable. The distance of Li-O bond is elongated, which will benefit the diffusion in the 3D channel thereby increasing the electronic conductivity and the rate performance of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$. According to electronic density analysis, the hybridization of Mn 3d and O 2p states is more obvious, which indicating that the covalent bond formed by the two atoms is stronger and the crystal structure is not easily collapsed, thereby improving the cycle stability of the material.

Keywords: $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$; lithium-ion batteries; first-principles

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