Short Communication

Study on the $\text{Li}_{1-x}\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ for Lithium Ion Batteries: a First-Principles Theory

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doi: 10.20964/2017.12.59

Received: 17 February 2017 / Accepted: 4 October 2017 / Published: 12 November 2017

The crystal structure, voltage and capacity of $\text{Li}_{1-x}\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ were studied by using the first principle theory. The results show that the structure of $\text{Li}_{1-x}\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ has changed, and the lattice parameter decreased from 8.342 Å to 8.247 Å with the decrease of Li content. But the change in each direction is the same, so the octahedral structure is unchanged in the process of de-lithium. The length of Ni-O and Mn-O bonds decreases with the increase of de-lithium. The Mn-O bond decreases from 2.101 Å to 1.911 Å, while the Ni-O bond decreases from 2.065 Å To 1.965 Å. The total energy decrease from -28731.220 eV to -27178.422 eV, and the voltage decreased from 4.7 V to 4.3 V with the reduction of Li amount. All the formation energy of $\text{Li}_{1-x}\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (P4₃32) is negative, which display that the structure of crystal is stable with no phase separation. The theoretical capacity reduced from 146 mAhg⁻¹ to 0 with the increase of delithiated amount or Li/Mn molar ratio.

Keywords: $\text{Li}_{1-x}\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$, first-principles, formation energy, delithiated

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