Short Communication

Structural and Properties of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_{4-\delta}$ and $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$ Spinels: A first-Principles Investigation

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The structural and properties of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$ and $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$ spinels as the high-voltage cathode materials were investigated by the first-principles theory. The calculated results indicate that the crystal structure of the $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$ is beneficial to the transition of lithium compared with $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$. Due to the charge overlap of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$ around Mn, Ni and O atoms significantly increased compared with $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$, which form a stable bond, therefore their structure is significantly increased. The lengths of the bonds of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$ are shorter than that of the $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$, indicating that the energy of the bond is smaller, thus the structure of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$ is more stable, but the Mn-Mn bonds hinder the shuttle movement of lithium ions, so the cycle performance of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$ may be better than that of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$. The calculated results exhibit the band gap of $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$ and $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}P4_332$ are 0.487 eV and 0.718 eV, respectively, which indicate that the eletro-conductive performance $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4\text{-}Fd\text{-}3m$ is better.

Keywords: first-principles, electrochemical performance, structure, spinel $\text{LiNi}_{0.5}\text{Mn}_{1.5}\text{O}_4$

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