Short Communication

Structural and Electronic Properties of Cation Doping on the Spinel LiMn_2O_4 : a First-Principles Theory

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The structural and electronic properties of cation doping on the spinel LiMn_2O_4 were investigated by the first-principles theory. The calculated results indicate that due to the formation energy of $\text{LiAl}_{0.5}\text{Mn}_{1.5}\text{O}_4$ is the smallest, the structure of $\text{LiAl}_{0.5}\text{Mn}_{1.5}\text{O}_4$ may be the most stable material, so the cycle performance may be the best. Both Cr-O and Sr-O bonds are longer than Co-O and Al-O bonds, thereby the cycle performance of $\text{LiAl}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ may be better. For $\text{LiCr}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{LiSr}_{0.5}\text{Mn}_{1.5}\text{O}_4$, the charge density among Sr, Cr, Mn and O atoms decreases, so the partial charge from Sr, Cr, Mn and O atoms is centralized near Li-site atoms, which is beneficial to the transition of lithium. Therefore the electronic conductivity of $\text{LiCr}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{LiSr}_{0.5}\text{Mn}_{1.5}\text{O}_4$ is improved. For $\text{LiAl}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$, the charge overlap around Mn, Ni and O atoms significantly increased, the charge of Co, Al, Mn and O atoms formed Co-O, Al-O and Mn-O stable bonds, therefore $\text{LiAl}_{0.5}\text{Mn}_{1.5}\text{O}_4$ and $\text{LiCo}_{0.5}\text{Mn}_{1.5}\text{O}_4$ structural stability is dramatically increased and may behave better electronic properties and more capacity.

Keywords: spinel LiMn_2O_4 , first-principles, formation energy, charge density

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