Short Communication

Structural and Electronic Properties of Cation Doping on the Spinel LiMn$_2$O$_4$: a First-Principles Theory

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The structural and electronic properties of cation doping on the spinel LiMn$_2$O$_4$ were investigated by the first-principles theory. The calculated results indicate that due to the formation energy of LiAl$_{0.5}$Mn$_{1.5}$O$_4$ is the smallest, the structure of LiAl$_{0.5}$Mn$_{1.5}$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 LiAl$_{0.5}$Mn$_{1.5}$O$_4$ and LiCo$_{0.5}$Mn$_{1.5}$O$_4$ may be better. For LiCr$_{0.5}$Mn$_{1.5}$O$_4$ and LiSr$_{0.5}$Mn$_{1.5}$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 LiCr$_{0.5}$Mn$_{1.5}$O$_4$ and LiSr$_{0.5}$Mn$_{1.5}$O$_4$ is improved. For LiAl$_{0.5}$Mn$_{1.5}$O$_4$ and LiCo$_{0.5}$Mn$_{1.5}$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 LiAl$_{0.5}$Mn$_{1.5}$O$_4$ and LiCo$_{0.5}$Mn$_{1.5}$O$_4$ structural stability is dramatically increased and may behave better electronic properties and more capacity.

Keywords: spinel LiMn$_2$O$_4$, first-principles, formation energy, charge density

FULL TEXT

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