Vibrational and Thermodynamic Properties of Layered $\text{LiM}_{0.5}\text{Ni}_{0.5}\text{O}_2$ (M=Mn, Co) Cathode Materials for Li Ion Batteries

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As the potential electrode materials, the layered lithium mixed transition metal oxides have received wide attention in the lithium ion battery (LIB) research field. In this work, the vibrational and related thermodynamic properties of $\text{LiM}_{0.5}\text{Ni}_{0.5}\text{O}_2$ (M= Mn, Co) are systematically studied by using density functional perturbation theory (DFPT) and quasi-harmonic approximation (QHA). The phonon dispersion and the thermodynamic functions of $\text{LiM}_{0.5}\text{Ni}_{0.5}\text{O}_2$ (M= Mn, Co) yield similar results for the local density approximation with the Hubbard model correction (LDA+*U*) and generalized gradient approximation with the Hubbard model correction (GGA+*U*), except for a slight difference for the $\text{LiMn}_{0.5}\text{Ni}_{0.5}\text{O}_2$ system. No imaginary frequency is observed in the phonon spectra of $\text{LiM}_{0.5}\text{Ni}_{0.5}\text{O}_2$ (M= Mn, Co), indicating that the compounds are dynamically stable. Furthermore, the thermodynamic quantities as a function of temperature of $\text{LiMn}_{0.5}\text{Ni}_{0.5}\text{O}_2$ have almost the same trend with that of $\text{LiCo}_{0.5}\text{Ni}_{0.5}\text{O}_2$, suggesting the insensitivity of the thermodynamic properties of $\text{LiM}_{0.5}\text{Ni}_{0.5}\text{O}_2$ (M= Mn, Co) compounds to the types of the transition metal elements. Our results are helpful to understand the finite-temperature thermodynamic properties of the lithium mixed transition metal oxides as electrode materials, in turn to accurately describe the performance of LIB.

Keywords: Lithium ion battery; Lattice vibrational property, Thermodynamic property; Density functional perturbation theory

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