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Structure and Phase Stability Study of Nickel Doped Spinel LiMn₂ O₄ using Cluster Expansion Method

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The demand for lithium-ion batteries with higher specific energy and higher power capacity for application in electric vehicles and portable electronics has led to a search for electrode materials with much higher electrochemical performance than conventional materials. Spinel LiMn₂ O₄ is a low-cost, environmentally friendly, and highly abundant material and is used as a cathode material in Li-ion batteries. However, lithium manganese oxide (LMO) suffers from limited cycle life that is triggered by manganese dissolution into the electrolyte during electrochemical cycling. Doping in battery materials tends to improve the efficiency in maintaining electrochemical capacity over a large number of cycles without sacrificing initial reversible capacity at room temperature. In this paper, Universal Cluster Expansion (UNCLE) code implemented in cluster expansion formalism is used to investigate nickel doped LMO phase stabilities. The method determines stable multi-component crystal structures and rank metastable structures by enthalpy of formation, while maintaining the predictive power and accuracy of first-principles density functional methods. Complex configurations of nickel doped LMO systems with various concentrations are determined at different temperatures by means of Monte Carlo random sampling. The ground state phase diagram generated various structures with different concentrations and symmetries. The findings predict that nickel doped LMO with 50:50 concentration of manganese and nickel is the most stable phase.

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