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Computer Simulation and Phase Diagram Prediction of LiMnxNi1-xO4

Spinel LiMn2O4 is one of the most attractive material for the next generation of Li-ion batteries, due to the low cost of manganese and straightforward synthesis. In this paper, we have used the MedeA-Universal Cluster Expansion package which allows to set up, construct and automatically converge cluster expansion for LiMn2O4 spinel systems and generate the unique structures within the random mixing of LiMn2O4-LiNi2O4. A total number 46 new stable multi-component LiMn2O4-LiNi2O4 structures were generated and ranked by enthalpy of formation, of which 5 structures were thermodynamically stable. Furthermore, in order to investigate these large systems and their relative stability effectively, we calculated structural, mechanical, electronic properties and phonon spectra of the 5 stable structures. It was finally demonstrated that cluster expansion technique yielded consistent results on relative stability of LiMn0.5Ni1.5O4 (isotropic), LiNi2O4, LiMn1.4Ni0.6O4, LiMn1.5Ni0.5O4, LiMn1.75Ni0.25O4 and LiMn2O4 configurations. The elastic properties conditions are satisfied, the electronic properties indicates no pseudo gap or band gap at the fermi level and the phonon spectra show vibrational stability.

The MEDEA-UNCLE user interface is based on flowcharts. The UNCLE flowchart can be set up independently of an active system in MEDEA. The calculation ran faster at the CHPC after benchmarking it with respect to our local servers. The phonon spectra took longer locally as compared to the CHPC servers.

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