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A search for stable structures of doped Li2MnO3 using cluster expansion and Monte Carlo simulations.

Li2MnO3 has been considered a potential cathode material due to its high theoretical capacity, nontoxicity and natural abundance of Mn. However, it has not been commercialized due to poor structural stability during cycling that results in capacity fade. Doping Li2MnO3 with transition metals is one of the ways that are extensively explored to optimize its properties and stability. To study large systems and effect of temperature effectively, the cluster expansion technique and Monte Carlo simulations within UNCLE code were used. All calculations were carried out on the CHPC cluster, using 48 cores .The cluster expansion formalism was used to investigate the nickel and cobalt doped Li2MnO3 phase stabilities. The method determines stable multi-component crystal structures and ranks metastable structures by the enthalpy of formation while maintaining the predictive power and accuracy of first-principles density functional methods. The ground-state phase diagram generated various structures of Li2MnNiO3 and Li2MnCoO3 with different concentrations and symmetries. The findings predict that all Li2MnNiO3 and Li2MnCoO3 structures on the ground state line are the most stable. Cross-validation scores of 3.7 meV/atomic position and 1.6 meV/atomic position were obtained, which is a statistical way of describing how good the cluster expansion is at predicting the energy of each stable structure. Monte Carlo simulation produced thermodynamic properties of Li2MnNiO3 and Li2MnCoO3 for entire range of Ni and Co concentrations. It further showed that Li2MnNiO3 and Li2MnCoO3 remain phase separating at 0 K, but the systems mix at 850 K and 700 K respectively.

Student?

Yes

Supervisor name

Dr Raesibe Sylvia Ledwba

Supervisor email

raesibe.ledwaba@ul.ac.za

Primary author: Ms MPHAHLELE, Mamonamane (University of Limpopo)

Co-authors: Dr MASEDI, Cliffton (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo); Dr LEDWABA, Raesibe (University of Limpopo)

Presenter: Ms MPHAHLELE, Mamonamane (University of Limpopo)

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