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Computational and Experimental Studies on Mn-rich LiMn1.5Ni0.5O2 Cathode Material

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Abstract

Lithium-ion rechargeable batteries, in particular the cathode materials, are now more essential than ever before as improved, reliable, and effective energy storage systems. Lithium cobalt oxide (LCO), the cathode material now in use, has a reputation for being toxic, expensive, and cobalt-scarce. Due to their accessibility, affordability, and non-toxicity, Nickel Manganese Cobalt (NMC) has been suggested as an alternative cathode material for lithium-ion batteries. In addition, due to their high capacity and improved structural stability, lithium, and manganese-rich composites LiMnNiO2 have gained a lot of interest as potential cathode materials for Li-ion batteries.

In this study, we employed experimental and computational modelling techniques to investigate the stability of manganese nickel oxide LiMn1.5Ni0.5O2 system. The heats of formations indicated that the structure is thermodynamically stable. The results of the lattice parameters, elastic properties and x-ray diffraction agreed with computational and experimental data. A cluster expansion technique generated new thermodynamically stable phases of LiMn1.5Ni0.5O2 system doped with Co and F which could be used for future battery developments.

Keywords: Computational, Doping, Experimental, Structural Properties, Stability.

Apply to be considered for a student ; award (Yes / No)?

yes

Level for award;(Hons, MSc, PhD, N/A)?

Hons

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