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Computational Modelling Study on the Stability Li1.2Mn0.8O2 Cathode Material

: Due to the rising demand of renewable energy, lithium-ion batteries have attracted much attention with Li2MnO3 being a perfect candidate to use as the cathode material. This is due to its high energy density and specific capacity. However, Li2MnO3 suffers from poor cycling stability and voltage fade which limits its practical application. In this work the built monoclinic Li1.2Mn0.8O2 is doped with Ti and Nd to attain the fundamental understanding of the crystal cycling stability. With the application of first-principles calculations combined with the ground state search, this study will generate phases of the Ti and Nd doped Li1.2Mn0.8O2 clusters. The ground state search was able to generate 20 and 136 Li-Ti-Mn-O and Li-Nd-Mn-O new phases respectively which are thermodynamically stable with negative enthalpy of formation. The cross-validation score of the Li-Ti-Mn-O system was found to be less than 5 meV/atom which indicate accuracy of ground-state search calculations allowing the temperature profile to be implied on the different phases which showed that phase transition occurs at 1200K. Building of Li1.2Mn0.8O2 shows an improvement on the thermodynamic and electronic stability of Li2MnO3. These findings pave way for further investigations of Li1.2Mn0.8O2 as a function of temperature.

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

yes

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

Hons

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