Contribution ID: **89** Type: **Student Micro-talk**

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 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 doped Li1.2Mn0.8O2 clusters. The ground state search was able to generate 20 new phases which are thermodynamically stable with negative enthalpy of formation. The cross-validation score 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. The analysis paves the way for further research on the crystal's stability as a function of temperature.

Keywords: Li-ion batteries, Cathode, First-principles, Cluster Expansion, Cross-Validation Score, Monte-Carlo.

Student?

Yes

Supervisor name

Dr Kemeridge Tumelo Malatji. Dr Cliffton Masedi

Supervisor email

kemeridge.malatji@ul.ac.za cliffton.masedi@ul.ac.za

Primary author: Ms MIKOSI, vusani (student)

Co-authors: Ms MAPHOTO, refiloe (supervisor); Dr MALATJI, kemeridge (supervisor); Dr MASEDI, cliffton (supervisor)

Presenter: Ms MIKOSI, vusani (student)

Session Classification: Micro-talks

Track Classification: Materials Science