Contribution ID: **37** Type: **Oral Presentation**

Fluorination of Li1.2Mn0.8O2 Cathode Material: A Computational Study

Wednesday, 5 July 2023 09:40 (20 minutes)

Anion doping is considered an effective way to enhance the stability of Li-rich Mn-based cathode materials as it mitigates oxygen loss and enlarge the inter-slab spacing of these materials. In this study we investigate the effects of fluorine doping on Li1.2Mn0.8O2 cathode material which was constructed from Li2MnO3 that is well known for its high energy density and high specific capacity. We use the genetic algorithm within the cluster expansion to generate phases of F-doped Li1.2Mn0.8O2, and consequently determine the most stable phases. The genetic algorithm generated 78 new phases of the F-doped Li1.2Mn0.8O2 with negative enthalpies of formation indicating that the constituents are miscible. Eleven (11) of these phases are at a specific x-concentration on the ground state line of the binary diagram and are predicted to be thermodynamically stable. The most stable phase is Li1.2Mn0.8OF which lies at the position x=0.5 on the binary diagram since it has the lowest energy of formation. In addition, First-principle calculations were performed to study the structural, mechanical, and electronic properties of the most stable structure. The obtained elastic constants showed that the material is mechanically stable under the strain 0.001 as it obeys the mechanical stability criteria for triclinic crystals. The Pugh ratio predicts the material to be ductile. The density of states shows no band gap at the fermi level confirming the conductivity of the generated material. In conclusion, the addition of fluorine to Li1.2Mn0.8O2 confirms its potential in improving the issues surrounding the Li-rich Mn-based cathodes.

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

yes

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

MSc

Primary author: MIKOSI, Vusani

Co-authors: Dr MALATJI, Kemeridge (Supervisor); Dr NGOEPE, Noko (supervisor); Prof. NGOEPE, Phuti (supervisor)

Presenter: MIKOSI, Vusani

Session Classification: Physics of Condensed Matter and Materials Track 2

Track Classification: Track A - Physics of Condensed Matter and Materials