Contribution ID: **112**

Type: **Poster (sponsored)**

Investigation of Operating Voltage during Electrochemical Lithiation of LixMn2O4 (1 ≤ x ≤ 2) composite cathode material.

The synergetic effects of incorporating layered-spinel components as bi-functional composite cathode materials has demonstrated an improvement on the structural stability and cycling performance, making this type of composite material a viable option in advancing lithium ion batteries to cater for the growing energy demand. In particular, the 0.7Li2MnO3.0.3Li4Mn5O12 composite material delivered a higher specific capacity, > 250 mAh/g. Recent studies have focused mainly on enhancing the specific capacity of layered-spinel composites. However, there is limited knowledge on how such layered-spinel composite electrodes affect the working voltage of lithium ion batteries. All the intensive calculations in this study are carried out on the Lengau cluster of the Centre for High Performance Computing (CHPC), whereby we use the DL_POLY standalone code, and the CASTEP and the ONETEP codes embedded in Material Studio. The DL_POLY code was employed to generate the nanoarchitectures of layered (Li2MnO3)-spinel (LiMn2O4) composite, with different lithium concentrations, under the NVE and NVT ensembles using the amorphisation and recrystallisation technique. RDFs and XRDs were used for characterization of the materials and structural changes were observed. Average lithium intercalation voltages have also been calculated for the layered (LixMnO3)-spinel (LixMn2O4) composites. The average voltage was found to increases with an increase in lithium concentration, as such the (LixMnO3)-spinel (LixMn2O4) composite material is a better cathode material as it shows a good behavior in terms of average voltage than LiMn2O4.

Presenter Biography

Primary author: HLUNGWANI, DONALD (UNIVERSITY OF LIMPOPO)

Co-authors: NGOEPE, Phuti (University of Limpopo); LEDWABA, Raesibe Sylvia (University of Limpopo)

Presenter: HLUNGWANI, DONALD (UNIVERSITY OF LIMPOPO)

Session Classification: Poster session

Track Classification: Materials Science