



Contribution ID: 123

Type: Oral Presentation

Phase Stability of $\text{Li}_{2-\text{x}}\text{MnO}_3$ (TM= Ni, Co, Cr and Ru) Cathode Material Using Cluster Expansion and Monte Carlo Simulations

Monday, 4 July 2022 15:00 (15 minutes)

$\text{Li}_{2-\text{x}}\text{MnO}_3$ has received great attention as potential cathode material due to its higher capacity, low cost and non-toxicity. However, its application is obstructed by its poor rate performance and structural degradation during cycling. Cationic dopants have been used to reduce the collapse of the structure and they tend to improve the performance of cathode materials. As such, it is highly desirable to identify new doped structures as a remedial technique to optimize the properties of $\text{Li}_{2-\text{x}}\text{MnO}_3$. In the current study, Cluster Expansion and Monte Carlo simulations were utilized to investigate the phase stability of $\text{Li}_{2-\text{x}}\text{Mn}_{1-\text{x}}\text{TM}_\text{x}\text{O}_3$ system (TM=Ni, Co, Cr and Ru). The binary ground state diagrams generated using Cluster Expansion yielded 73, 65, 90 and 83 new stable phases of $\text{Li}_{2-\text{x}}\text{Mn}_{1-\text{x}}\text{Ni}_\text{x}\text{O}_3$, $\text{Li}_{2-\text{x}}\text{Mn}_{1-\text{x}}\text{Co}_\text{x}\text{O}_3$, $\text{Li}_{2-\text{x}}\text{Mn}_{1-\text{x}}\text{Cr}_\text{x}\text{O}_3$ and $\text{Li}_{2-\text{x}}\text{Mn}_{1-\text{x}}\text{Ru}_\text{x}\text{O}_3$ respectively. Monte Carlo simulations were used to determine high temperature properties for entire range of TM concentrations ($0 \leq x \leq 1$) and phase diagrams were constructed. The findings predicted $\text{Li}_{2-\text{x}}\text{Mn}_{0.83-\text{x}}\text{Ni}_{0.17}\text{O}_3$, $\text{Li}_{2-\text{x}}\text{Mn}_{0.5-\text{x}}\text{Co}_{0.5}\text{O}_3$, $\text{Li}_{2-\text{x}}\text{Mn}_{0.5-\text{x}}\text{Cr}_{0.5}\text{O}_3$ and $\text{Li}_{2-\text{x}}\text{Mn}_{0.5-\text{x}}\text{Ru}_{0.5}\text{O}_3$ as the most stable phases of doped $\text{Li}_{2-\text{x}}\text{MnO}_3$. These structures may be useful in future applications as electrode materials for lithium-ion batteries.

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

Yes

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

MSc

Primary author: MPAHLELE, Mamonamane (university of Limpopo)

Co-authors: Dr MASEDI, Clifton (University of Limpopo); Dr MALATJI, Kemeridge; Prof. NGOEPE, Phuti (University of Limpopo); Prof. LEDWABA, Raesibe Sylvia (University of Limpopo)

Presenter: MPAHLELE, Mamonamane (university of Limpopo)

Session Classification: Physics of Condensed Matter and Materials

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