Contribution ID: **389** Type: **Poster Presentation**

Computer simulation studies of spinel LiMn₂O₄ and LiNi_xMn_{2-x}O₄ (0≤ x ≤ 2)

Tuesday, 10 July 2012 17:30 (2 hours)

Abstract content
   (Max 300 words)

Spinel LiMn₂O₄ is a low-cost, environmentally friendly, and highly abundant material and is used as a cathode in Li-ion batteries. Doping in batteries improves the efficiency in maintaining electrochemical capacity over a large number of cycles without sacrificing initial reversible capacity at room temperature. We use computer simulation methods to study properties of spinel LiMn₂O₄ and doped LiNi_xMn_{2-x}O₄ (0≤x≤2). In particular, spin density functional theory employing the pseudo-potential plane-wave calculations within the generalized gradient approximation is used to investigate spinel structural and electronic properties; and pressure dependence. The calculated structural parameters are found to be in good agreement with experimental and literature results. In addition, the structural changes and electronic properties of LiMn₂O₄ spinel as a function of nickel content were investigated. The lattice parameters for doped systems are in coherent with the available experimental results. Analysis of electronic properties predicts the nature of bonding for both pure and doped systems.

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

Yes

Level for award
 (Hons, MSc,
   PhD)?

Hons

Main supervisor (name and email)
and his / her institution

Dr RR Maphanga, University of Limpopo

Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

No

Primary author: Mr MALATJI, kemeridge Tumelo (University of Limpopo)

Co-authors: Prof. NGOEPE, Phuti (University of limpopo); Dr MAPHANGA, Rapela (University of Limpopo)

Presenter: Mr MALATJI, kemeridge Tumelo (University of Limpopo)

Session Classification: Poster Session

Track Classification: Track A - Division for Condensed Matter Physics and Materials