



Contribution ID: 510

Type: Poster Presentation

Thermodynamic, structural, electronic and mechanical stability study of olivine LiMPO_4 (M: Mn, Fe, Co)

Tuesday, 9 July 2013 17:40 (1 hour)

Abstract content
 (Max 300 words)

The ever growing demand of portable electronic devices and the vision of massive commercial use of electric powered vehicles have led to a call to pursue more effective batteries. These batteries should contain vital socio-economic and useful physical properties. Amongst these batteries lithium rechargeable batteries have shown great signs in achieving desired performance. Previous investigations have shown the olivine LiFePO_4 is of interest in portable electronic appliances as a future cathode battery material. Consequently, attention has also been shifted to other olivine lithium transition metal phosphates such as LiMnPO_4 , LiCoPO_4 and LiNiPO_4 . In this study, we investigate the structural, thermodynamic, electronic and mechanical properties of LiMPO_4 (M; Fe, Mn, Co) to determine their stability. Calculations have been performed within DFT+U method as implemented in the Vienna Ab initio Simulation Package code. The lattice parameters were found to be in good agreement with the experimental results. According to our DFT+U calculations, olivine LiMnPO_4 has the lowest heat of formation (-1340.5kJ/mol), suggesting stability.

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

yes

Level for award
 (Hons, MSc,
 PhD)?

PhD

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

Prof P.E. Ngoepe: phuti.ngoepe@ul.ac.za

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

yes

Primary author: Mr LETHOLE, NDANDULENI LESLEY (SAIP)

Co-authors: Prof. CHAUKE, Hasani (University of Limpopo); Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Mr LETHOLE, NDANDULENI LESLEY (SAIP)

Session Classification: Poster1

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