Contribution ID: **510** Type: **Poster Presentation**

Thermodynamic, structural, electronic and mechanical stability study of olivine LiMPO₄ (M: Mn, Fe, Co)

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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 LiFePO₄ 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 LiMnPO4, LiCoPO₄ and LiNiPO₄. In this study, we investigate the structural, thermodynamic, electronic and mechanical properties of LiMPO₄ (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 LiMnPO₄ has the lowest heat of formation (-1340.5kJ/mol), suggesting stability.

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PhD

Main supervisor (name and email)
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Prof P.E. Ngoepe: phuti.ngoepeQul.ac.za

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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)

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