

SAIP2013



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

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Abstract :

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.

Award :

yes

Level :

PhD

Supervisor :

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Paper :

yes

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