SAIP2014

Contribution ID : 113

Computational studies of olivine $NaMPO_4$ (M: Mn, Fe, Co)

Tuesday 08 Jul 2014 at 17:10 (01h50')

Abstract :

Efforts to deal with environmental pollution and exhaustion of oil resources have been the centre of attention throughout the research industry. Hybrid electric vehicles powered by the lithium ion battery have been developed. However, the scarcity of lithium and the possibility of using much safer aqueous electrolytes in sodium ion batteries have shifted interest on sodium ion batteries to ensure sustainability and optimal safety. However, the major drawback for the sodium materials has been their low charge/discharge capacities. Previous studies have shown that $NaFePO_4$ and $NaCoPO_4$ offer charge/discharge capacities of 12 mAh/g and 2.0 mAh/g, respectively, which is very less compare to $LiFePO_4$ (170 mAh/g), $LiMnPO_4$ (70 mAh/g) and $LiCoPO_4$ (70 mAh/g). In this study, we investigate the structural, thermodynamic, electronic and mechanical properties of the olivine $NaMPO_4$ to determine their capabilities as future cathode materials for sodium ion batteries. Calculations have been performed within DFT+U method as implemented in the Vienna Ab initio Simulation Package code. The calculated cell parameters for $NaFePO_4$ and $NaCoPO_4$ were found to be in good agreement to the experimental to within 3%. The heats of formation suggested that $NaMnPO_4$ is the most stable olivine structure, due to the lowest formation energy (-1292 kJ/mol).

Award :
YES

Level :
PhD

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Paper :
YES

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Session classification : Poster1

Track classification : Track A - Division for Physics of Condensed Matter and Materials

Type : Poster Presentation