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Computational studies of olivine NaMPO₄ (M: Mn, Fe, Co)

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Abstract content
   (Max 300 words)
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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 NaFePO₄ and NaCoPO₄ offer charge/discharge capacities of 12 mAh/g and 2.0 mAh/g, respectively, which is very less compare to LiFePO₄ (170 mAh/g), LiMnPO₄ (70 mAh/g) and LiCoPO₄ (70 mAh/g). In this study, we investigate the structural, thermodynamic, electronic and mechanical properties of the olivine NaMPO₄ 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 NaFePO₄ and NaCoPO₄ were found to be in good agreement to the experimental to within 3%. The heats of formation suggested that NaMnPO₄ is the most stable olivine structure, due to the lowest formation energy (-1292 kJ/mol).

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