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Revisiting the Alluaudite $NaMnFe_2(PO_4)_3$ Sodium Insertion Material: Structural, Diffusional and Electrochemical Insights

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Abstract

Among the gamut of sodium battery insertion materials, $NaMnFe_2(PO_4)_3$ was reported as the first alluaudite framework compound albeit with poor electrochemical activity [Chem. Mater. 22 (2010) 5554]. We hereby report auto-combustion synthesis of carbon coated $NaMnFe_2(PO_4)_3$ alluaudite and its Na^+ diffusion, ionic conductivity and electrochemical activity synergizing experiments with bond valence site energy (BVSE) modelling. It registered a 2.8 V redox activity with a reversible capacity of ~60 mAh g^{-1} with good cycling stability. BVSE calculations revealed an exceptionally low one-dimensional migration barrier of 0.31 eV for Na-ion diffusion. It was in sync with the low activation energy barrier of 0.162 eV derived from ac impedance spectroscopy. $NaMnFe_2(PO_4)_3$ alluaudite cathode was found to have conductivity value of 0.5×10^{-6} S cm^{-1} at room temperature. Among the PO_4-based sodium battery insertion materials, $NaMnFe_2(PO_4)_3$ alluaudite shows excellent ionic conductivity with very low Na^+ migration barrier. It can lead to the realization of superior reversible capacity in this alluaudite cathode comparable to $LiFePO_4$.

Keywords: Sodium-ion battery, alluaudite, combustion, bond valence site energy, conductivity.