High voltage $Na_3Fe_{0.3}V_{1.7}O(PO_4)_2F_2$ cathode material for sodium ion batteries

Rachid Essehli [a], Hamdi ben Yahia [a], Kenza Maher [a], MD Ruhul Amin [a]
[a] *Qatar Environment and Energy Research Institute (QEERI) at Hamad Bin Khalifa University (HBKU), Doha, Qatar.*

E-mail: ressehli@hbku.edu.qa

Sodium-ion batteries (NaIBs) are very promising for large-scale energy storage system due to their cost and safety potency. However, challenges remain in the development of suitable electrode materials to enable high-power and -energy density, and long lifespan. Several vanadium phosphate-based materials have been extensively studied as cathode and anode in Na-ion batteries because of their potential stability at $V^{2+,3+,4+,5+}$ oxidation states.[1] The fluorophosphates compounds with the general formula $Na_3V_2(PO_4)_2F_{3-x}O_x$, have also been investigated due to their excellent electrochemical performance. In this work focus was dedicated to the synthesis of impurity free $Na_3Fe_{0.3}V_{1.7}O(PO_4)_2F_2$ phase through a facile hydrothermal route. The morphology of the materials is analyzed by Scanning Electron Microscopy (SEM). The material exhibits a specific reversible capacity of 110 $mAhg^{-1}$ between 4.5 and 2 V versus Na^+ /Na, at C/10 rate. The cell exhibits excellent cycling stability and rate performances. The interfacial charge transfer resistance (R_{ct}), at the cathode-electrolyte interface, and ionic diffusivity have been measured as a function of lithium concentration. The diffusivity and R_{ct} values are almost constant as a function of sodium content except the decrease of diffusivity at the transition between first and second plateaus regime. The obtained results indicate that the rate performance of the material is limited by interfacial resistance in the submicron scale particle size. The isothermal calorimetery is used to investigate the in situ heat generation and thermal stability of $Na/Na_3Fe_{0.3}V_{1.7}O(PO_4)_2F_2$ during charge/discharge, and the results is quantitatively analyzed.

[1] M. Bianchini, F. Fauth, N. Brisset, F. Weill, E. Suard, C. Masquelier, L. Croguennec, Chem. Mater. 2015, 27, 3009