From the journal:
Journal of Materials Chemistry A

On the dynamics of transition metal migration and its impact on the performance in layered oxides for sodium-ion batteries: $NaFeO_2$ as a case study.

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Electronic Supplementary Information (ESI) available: See DOI: 10.1039/x0xx00000x

Abstract

Transition metal (TM) layered oxides constitute one of the most promising family of compounds for the cathode of Na-ion batteries. However, their structural stability at charged state is a critical performance limiting factor, which is believed to be closely related with irreversible TM migration into the Na layers. Nevertheless, experimental evidence of this TM migration and its influence on the electrochemical performance is still scarce, while the understanding of such a phenomenon constitutes a key step for developing better performing TM layered oxides. Here $NaFeO_2$ has been studied as a model system, since it is expected to produce one of the most pronounced TM migration and provide possibly one of the highest theoretical energy density of TM layered oxides. By combining Potential Intermittent Titration Technique (PITT), Electrochemical Impedance Spectroscopy (EIS) and operando X-ray diffraction it has been possible to analyze the structural evolution of $NaxFeO_2$, track the iron migration and observe their influence on the insertion capacity and Na diffusivity.

Journal of Materials Chemistry A, 2018, DOI: 10.1039/C8TA02473A