

Electrochemical properties and first-principle analysis of $\text{Na}_x[\text{M}_y\text{Mn}_{1-y}]\text{O}_2$ (M = Fe, Ni) cathode

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Abstract

Sodium-ion batteries are the commercially and environmentally viable next-generation candidates for automobiles. Structural and electrochemical aspects are greater concerns towards the development of a stable cathode material. Selecting transition metals and their composition greatly influences charge order, superstructures, and different voltage plateaus. This, in turn, influences transport properties and cyclic performance. This article aims to study the electrochemical performance, diffusivity, and structural stability of $\text{Na}_x[\text{M}_y\text{Mn}_{1-y}]\text{O}_2$ (M = Fe, Ni) as cathode. Both experimental and DFT-based calculations apprehend the voltage plateaus due to redox reactions. The rate of cycling and the initial structure also influence the cycle life. The diffusion coefficient of P2-type $\text{Na}_{0.67}\text{Fe}_{0.5}\text{Mn}_{0.5}\text{O}_2$ for $\text{Mn}^{3+/4+}$ redox reactions is more than that of the O3-type $\text{NaFe}_{0.5}\text{Mn}_{0.5}\text{O}_2$ while it is less for $\text{Fe}^{3+/4+}$ redox reactions, because of structural transition. The diffusion coefficient of $\text{NaNi}_{0.5}\text{Mn}_{0.5}\text{O}_2$ is less for $\text{Ni}^{2+/4+}$ redox reaction and is up to the order of $10^{-11} \text{ cm}^2 \text{ s}^{-1}$.