

Structure-property relationship and structural dynamics of layered transition metal oxides for sodium-ion battery applications

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In recent years, the family of layered sodium-containing transition metal oxides, Na_xMO_2 , where $M=\text{Ti}, \text{V}, \text{Cr}, \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}$ (or mixture of 2-3 of these elements), have attracted a great deal of attention due to their fascinating electronic, chemical and mechanical properties.[1, 2] Notably, $\text{Na}_x\text{Mn}_{1-y}\text{MyO}_2$, where $M=\text{Fe}, \text{Ni}, \text{Mg}, \text{Ti}$, are amongst the leading cathode materials for sodium-ion batteries (SIBs).[3] SIBs are particularly interesting, as they represent a low cost alternative to the ubiquitous lithium-ion batteries, owing to the larger abundance of sodium in the earth's crust. At ambient conditions, the Na_xMO_2 compounds adopt various structural polymorphs (i.e. the so called O2-, O3-, P2- and P3-type structures) depending on the constituent transition metal(s), M , and the Na content.[4] Interestingly, the P2-type materials typically exhibit a higher capacity and cycle life, while the O2-type delivers a higher operating voltage.[5, 6] Recent determinations of the Na diffusion coefficient in these materials yield differences of up to five orders of magnitude depending on phase, composition and experimental technique.[7] It has been proposed that the electrochemical differences may be related to a higher Na-ion mobility in the P2-type structure, due to the presence of a more energetically favorable migration pathway.[8] In the present work, the structure, structural dynamics and electrochemical properties of P2-type $\text{Na}_{0.67}\text{Mn}_{0.8}\text{M}_{0.2}\text{O}_2$, $M=\text{Mg}^{2+}, \text{Fe}^{3+}, \text{Ti}^{4+}$, are proposed to be investigated. In particular, the effect of the imposed change in Mn oxidation state as a result of the different valences of the substituted transition metals, M , and the associated variation in Jahn-Teller distortions from the Mn^{3+} ions in the structure is examined. In addition, the ability of crystal water to alter the Na diffusion rates by tuning the interlayer distances in the structure in hydrated versions of the compounds, $\text{Na}_{0.67}\text{Mn}_{0.8}\text{M}_{0.2}\text{O}_2 \cdot y\text{H}_2\text{O}$, will be studied.

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Speakers Gender

Male

Travel Funding

No

Level of Expertise

Early Career <5 Years since PdD

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No

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