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Diffusion mechanisms in sodium-ion battery materials using polarized neutrons

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The demand for energy storage is expected to increase dramatically due to the introduction of electric vehicles and the need for load levelling in the wind, tidal and solar renewables industries. The scarcity of lithium together with issues over supply from remote or politically sensitive areas, has led to concerns over cost. Sodium-ion batteries are a particularly attractive alternative for current lithium-ion battery manufacturers, since they are a drop-in replacement. NaxFe1/2Mn1/2O2 has been identified as a potential cathode material for sodium-ion batteries since it has comparable electrochemical performance to commercially available lithium-ion cathodes and it is composed entirely of abundant elements. We have studied the diffusion mechanisms of NaxFe1/2Mn1/2O2 for x=1 and 2/3 using quasi-elastic neutron scattering (QENS) using the ThALES spectrometer with XYZ polarization analysis. In order to perform quantitative modelling of the QENS data we show that it is necessary to isolate the spin incoherent cross section from the spin-independent nuclear and magnetic cross sections. For x = 1 it has the same crystal structure as O3-LixCoO2, whereas for x = 2/3 it has the P2-NaxCoO2 structure. In both cases the planes of sodium ions are sandwiched between oxygen planes, but the difference in the stacking sequence of hexagonal planes leads to very different diffusion mechanisms. We find that the P2 material is a promising cathode material with high rate capability.

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