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Phase transformations during battery operation in vanadium phosphate cathode materials probed by operando synchrotron X-ray diffraction

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Phosphate based cathode materials has seen great success following the demonstration of LiFePO4 as a functioning Li-ion battery cathode material, especially due to its very low cost and high safety compared with the previously used oxide based materials. However, despite the inductive effect of the phosphate group, LiFePO4 has a relatively low discharge potential compared with materials based on other transition metals, such as vanadium, cobalt and nickel. The capacity is also low due to the limited number of oxidation states for iron, yielding only a single Li-ion per formula unit.

An interesting alternative to LiFePO4 is Li3V2(PO4)3 as it has the highest gravimetric capacity among the known phosphates (197 mAh g-1). The material displays a complex series of phase transformations during charge and discharge, and interestingly, these transformations are very dependent on the number of Li-ions extracted during charging

In recent years, new methods have been developed to investigate the dynamic structural behavior of battery materials during operation using synchrotron X-ray diffraction. The methods are expected to give a more realistic view of the behavior of batteries in operation. In this study, we investigate the dynamic structural behavior of Li3V2(PO4)3 as a function of extracted Li-ions using in-situ synchrotron diffraction. The detailed structural information of the phase transformations in this material clearly demonstrates the strength of in-situ diffraction methods.

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