

X-ray absorption spectroscopy of changes in Ti sites during Li insertion in nanostructured anatase.

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Anatase TiO₂ has been found to exhibit a good ability to store Li for use in lithium ion batteries. TiO₂ has also been shown to have a good particle size-dependent insertion capacity for Li. This would allow much higher capacities batteries to be produced if the TiO₂ was processed in a nanostructured form. This was achieved using a modified sol-gel method. The resulting anatase samples had a varying range of nanostructures. In situ XAS, X-ray absorption spectroscopy, measurements of the samples during electrochemical Li insertion were made in order to measure the change of valence and local environment of the Ti. The X-ray Absorption Near-Edge Structure, XANES, region shows change in valence. The Ti³⁺ and Ti⁴⁺ XANES spectrums display a fundamental difference in the shape and therefore the derivative of the absorption edge. This gives a new method to measure the changing valence during in situ measurements by combining different ratios of Ti³⁺ and Ti⁴⁺ reference curves. Using this technique each of the anatase samples were analysed to determine the change in valence and thus the lithium capacity of each of the different samples. This new technique is supplemented with an extended x-ray absorption fine structure, EXAFS, study of the changing bond length between the Ti and O which can also be used to determine the valence of the Ti.