IN SITU Fe K-EDGE XAS STUDY DURING CYCLING OF Li₂FeSiO₄

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Lithium iron silicates (Li₂FeSiO₄) offer many benefits as novel cathode materials in Li-ion batteries. By using abundant elements, like iron and silicon, they offer an economic alternative to the Co based system currently employed in most commercial batteries. Another driving factor in battery development is associated with their safety and the Si–O bond provides stability similar to the P–O bond in LiFePO4 compounds [1].

Another advantage of the iron silicates, is the theoretical possibility to remove two Li ions from Li2FeSiO₄, by utilizing the Fe⁺²/Fe⁺³ and the Fe⁺³/Fe⁺⁴ redox couples, thus, producing a higher capacity than 166 mAh/g for one Li ion. Although capacities greater than 200 mAh/g have been reported by several groups [2-4] it has yet to be clarified whether it was due to Fe⁺⁴ formation or electrolyte degradation [1]. Pouch cells were made to study the XANES and EXAFS of the Fe K-edge of Li2FeSiO₄-based batteries cycled between 3.5 and 4.8 V, so as to show the eventual suggested Fe⁺³/Fe⁺⁴ redox couples or wether the additional capacity originates from electrolyte degradation [5]. In addition, the pre-edge features of the XANES signal will be used in that regard.



XANES spectra of the Fe K-edge for Li2FeSiO4, cycled between 3.5 and 4.8V and measured at various state of charge.

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