Low Loss Electron Energy Spectroscopy on $LiFePO_4$ for Li ion Battery Applications

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Keywords: EELS, DFT, $LiFePO_4$, Li ion batteries

$LiFePO_4$ is a potential cathode material for high energy Li ion battery applications. The potential of this material in Li ion battery applications is hindered by its low electronic and ionic conductivity [1]. Doping $LiFePO_4$ with multivalent cations has been one of the proposed methods to improve $LiFePO_4$ electron properties [2]. This requires a fundamental understanding of the electronic structure and conduction properties of $LiFePO_4$. Band structure calculations derived from Density Functional Theory (DFT) calculations have produced controversial results that predict $LiFePO_4$ as being semi-metallic with a small band gap of ~ 0.1 eV or an insulator characterized by a large band gap ~ 4 eV band gap [3, 4, 5]. There is also a lack of conclusive experimental studies on the electronic properties of $LiFePO_4$.

The low loss region (0-50eV) of an Electron Energy Loss Spectrum contains information about valence electron excitations and thus the electronic structure of a specimen. Here we present results from a low-loss electron energy-loss spectroscopic (EELS) study of $LiFePO_4$. The low loss EELS spectra were acquired at 80 KV (with an energy resolution of 0.5 eV) in order to reduce the influence from the relativistic Cerenkov losses. Zero loss peak de-convolution and Kramers-Kronig transformations have been used to analyze the low-loss EELS spectrum from which the real part and imaginary parts of the energy loss spectrum, ε_1, ε_2 respectively, were extracted. Figure 1(a) shows the derived real ε_1 and imaginary ε_2 parts of the low loss EELS spectrum while Figure 1(b) shows plots of the calculated optical absorption spectrum and imaginary ε_2 of the energy loss spectrum. The obtained results are in good agreement with first principles calculations and Ultraviolet-Visible-Infrared (UV-Vis-IR) optical measurements [3] supporting the argument of $LiFePO_4$ as a wide gap insulator. We discuss these results vis-à-vis, the EELS methods used and *ab initio* modelling of the low loss properties. We put these results into context of $LiFePO_4$ electronic properties and its application as a cathode material for Li ion batteries.

M. Luysberg, K. Tillmann, T. Weirich (Eds.): EMC 2008, Vol. 1: Instrumentation and Methods, pp. 395–396, DOI: 10.1007/978-3-540-85156-1_198,

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6. The authors acknowledge the BMBF for the partial funding of the project REALIBATT

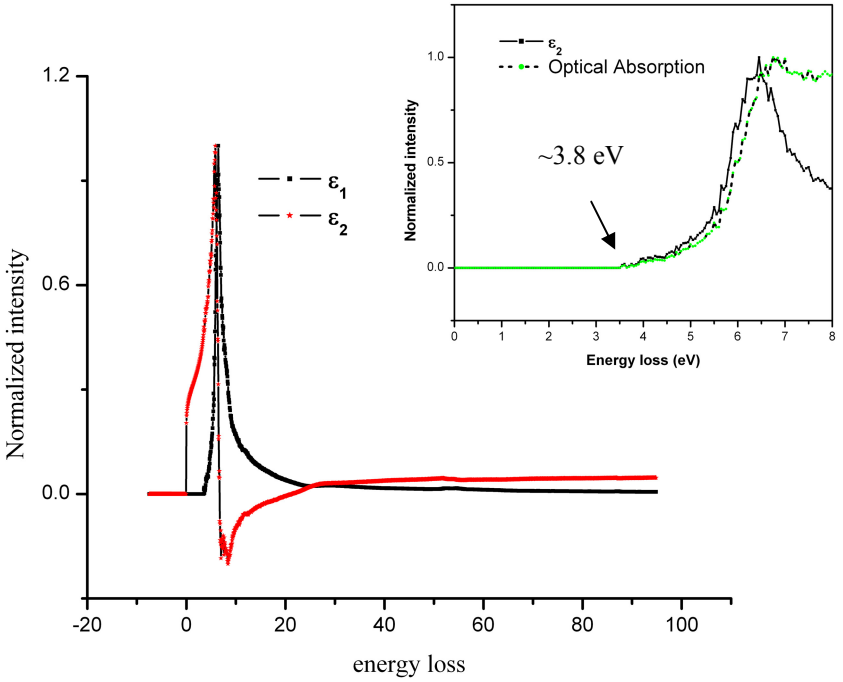

Figure1. (a) A plot of the obtained real ε_1 and imaginary ε_2 parts of the low loss $LiFePO_4$ EELS spectrum (b) Plots of the calculated optical absorption spectrum and imaginary ε_2 of the energy loss spectrum showing the onset of the obtained spectral intensity at ~ 3.8 eV.