EELS study of Li-based materials: ELNES at the lithium K-edge and low energy losses.

V. Mauchamp, P. Moreau, F. Boucher, and G. Ouvrard

Institut des Matériaux Jean Rouxel, 2 rue de la Houssinière, 44322 Nantes cedex 3, France.

Within the broad field of research devoted to the Li-ion batteries, EELS has come to be considered a powerful tool in the determination of electronic properties. To date, although many studies have focused on the core losses of metals or anions which constitute such materials, there has been little detailed EELS research concerning the lithium atom itself. We feel that a better understanding of the electronic structure of this atom is crucial in determining its insertion sites. We therefore performed various experiments on lithium-based materials displaying diverse electronic behaviors, such as insulators (Li$_2$O and LiOH,H$_2$O) as opposed to metals (Li and LiMn$_2$O$_4$). We obtained the lithium K-edges (Fig 1) and low losses for these compounds. Understanding the differences between the electronic structure of Lithium in these various materials (in terms of oxidation state changes, solid state effects and core hole effects) requires theoretical support. We therefore performed electronic structure calculations using WIEN2k [1] (a code based on the Density Functional Theory) and the simulated Li K-edges and low losses for each of these compounds were then determined.

A comparison between experimental spectra and simulations, including band structure analysis, allows for a better understanding of the variable electronic properties of lithium as a function of its environment.

![Fig 1: experimental lithium K-edge in various model compounds](image)

Reference