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Advanced Structural Analysis of Energy Storage Materials

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Abstract : The aim of this research is to conduct X-ray and e-beam characterization techniques on lithium-ion battery materials for the improvement of battery performance. The key characterization techniques employed are the synchrotron X-ray Absorption Spectroscopy (XAS) combined with X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) to obtain a more holistic approach to understanding material properties. This research effort provides additional battery characterization knowledge that promotes the development of new cathodes, anodes, electrolyte and separator materials for batteries, hence, leading to better and more efficient battery performance. Both ex-situ and in-situ synchrotron experiments were performed on $LiFePO_4$, one of the most common cathode material, from different commercial sources and their structural analysis, were conducted using Athena/Artemis software. This analysis technique was then further extended to study other cathode materials like $LiMnxFe_{(1-x)}PO_4$ and even some sulphate systems like $Li_2Mn(SO_4)_2$ and $Li_2Co0.5Mn_{0.5}$ $(SO_4)_2$. XAS data were collected for Fe and P K-edge for LiFePO4, and Fe, Mn and P-K-edge for $LiMnxFe_{(1-x)}PO_4$ to conduct an exhaustive study of the structure. For the sulphate system, $Li_2Mn(SO_4)_2$, XAS data was collected at both Mn and S K-edge. Finite Difference Method for Near Edge Structure (FDMNES) simulations were also conducted for various iron, manganese and phosphate model compounds and compared with the experimental XANES data to understand mainly the pre-edge structural information of the absorbing atoms. The Fe K-edge XAS results showed a charge compensation occurring on the Fe atom for all the differently synthesized $LiFePO_4$ materials as well as the $LiMnxFe_{(1-x)}PO_4$ systems. However, the Mn K-edge showed a difference in results as the Mn concentration changed in the materials. For the sulphate-based system $Li_2Mn(SO_4)_2$, however, no change in the Mn K-edge was observed, even though electrochemical studies showed Mn redox reactions.

Keywords : li-ion batteries, electrochemistry, X-ray absorption spectroscopy, XRD
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