Spectroscopic fingerprints of site occupancy of Cations in $LiMPO_4$ cathode material for Li-ion batteries

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The ability to store energy of Li-ion batteries depends on the materials used to produce their electrodes. Olivine cathodes $LiMPO_4$ (M=Fe, Mn) are considered safer than conventional cathodes containing Co and Ni. However, this material has poor electronic conductivity and low lithium ion diffusivity [1]. Therefore, we decided to use carbon coating, particle size minimization and doping of metallic elements to improve these drawbacks. Glucose was used as the carbon source. The produced materials have an average particle size of 50 nm. Co and Cr were used as doping elements. Co^{2+} was doped in $LiFePO_4$ and found that it substituted into Fe-site. Fig.1 shown Cr^{3+} was doped in $LiMnPO_4$ and found that it preferred to substitute in to Li-site. These experiments were performed by X-ray Absorption Spectroscopy (XAS).

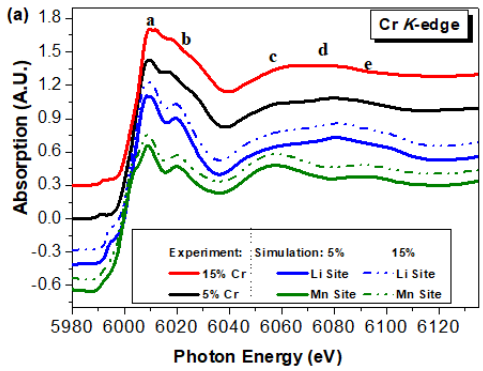

Figure. 1 Experimental Cr K-edge XANES spectrum of the 5% Cr (black line) and the 15% Cr-doped (red line) doped $LiMnPO_4$ sample and simulated XANES spectra with Cr replacing Mn-site (green lines) and Li-site (blue lines).

References:

[1] A.K. Padhi, K. Nanjundaswamy, J.B. Goodenough. J. Electrochem. Soc. 144(4) (1997) 1188-1194.