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Delithiated $Fe_{1-x}Mg_xPO_4$ cathode materials: Structural, magnetic, and Mössbauer studies

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ABSTRACT

$Fe_{1-x}Mg_xPO_4$ (x = 0.01, 0.05, and 0.1) cathode materials are synthesized by a two-step method, which combines the solid-state reaction method and the chemical lithium deintercalation method. A study was conducted to investigate the structural and the magnetic properties of $Fe_{1-x}Mg_xPO_4$. The crystalline structure of the samples was analyzed by X-ray diffractometer (XRD) using the Rietveld refinement. The magnetic properties of the samples were determined from vibrating sample magnetometer (VSM) and Mösssbauer spectroscopy, including their magnetic interactions, Fe ion states, and structural ordering. The Néel temperature (T_N) of $Fe_{1-x}Mg_xPO_4$ decreases with the increase of the Mg content due to the weakening of the antiferromagnetic exchange. Furthermore, for $Fe_{1-x}Mg_xPO_4$, the effective moment value decreases as expected with increasing Mg content. Mössbauer spectroscopy measurements at different temperatures were made. The spectrum at 295 K was fitted with a doublet, which has an isomer shift of δ = 0.32 – 0.43 mm/s (Fe^{3+}). The large value of the electric quadrupole splitting (ΔE_Q = 0.95 – 1.87 mm/s) is explained by the asymmetric local environment of the Fe ions. Below the T_N, the spectra of $Fe_{1-x}Mg_xPO_4$ in the eight resonance absorption lines (including two relatively small intensities) were analyzed. We can obtain a spin value for Fe ions (S = 5/2) of $Fe_{0.9}Mg_{0.1}PO_4$ from the Brillouin functional analysis.