

Synthesis and Structure of Novel Battery Materials

Lithium transition metal fluorophosphates with a tavorite structure have been recognized as promising electrode materials for lithium-ion batteries because of their good energy storage capacity combined with electrochemical and thermal stability.

The structure of the pure single phase end-member $\text{Li}_2\text{FePO}_4\text{F}$ was synthesized by lithiation of LiFePO_4F , and solved via Rietveld refinement of the combined X-ray and neutron diffraction data, showing that Li^+ occupies multiple sites in the tavorite lattice.

Neutron powder diffraction data were collected at the HFIR HB-2A diffractometer and in this study highlight the critical need for neutron diffraction to accurately and quantitatively “see” the light atoms such as Li, which is crucial to understanding the microscopic behavior of Li battery materials.

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