

## **The Crystal-Structure of Mn-doped LiFePO<sub>4</sub>: A Combined Neutron and X-ray Diffraction Study**

Neeraj Sharma, Vanessa K. Peterson

*The Bragg Institute, Australian Nuclear Science and Technology Organisation,  
Locked Bag 2001, Kirrawee DC NSW 2232, Australia*

Chuanqi Feng, Hua Li,

*Key Laboratory for Synthesis and Applications of Organic Functional Molecules,  
Hubei University, Wuhan 430062, China*

Guodong Du, Zaiping Guo and Huakun Liu

*Institute for Superconducting & Electronic Materials, University of Wollongong,  
NSW 2522, Australia*

Li-ion batteries provide portable power to numerous devices such as mobile phones, media players, and laptop computers. Further research into Li-ion batteries is essential to meet the power demands of modern devices and for use in emerging applications such as electric vehicles and energy storage for smart electricity grids. In this presentation we focus on Mn-doped LiFePO<sub>4</sub>, a potential cathode material for Li-ion batteries.

We use inexpensive starting materials and a one-step reaction method to synthesize carbon-coated LiFePO<sub>4</sub> and Mn-doped LiFePO<sub>4</sub> with particle sizes between 0.5 and 1 μm and a carbon-content of approximately 2 wt.%. For structural characterization we use a combination of synchrotron X-ray diffraction (XRD) and neutron diffraction (ND) data. A number of structural models were tested, featuring permutations of the locations and occupancies of Li, Mn, and Fe cations. Rietveld refinements were conducted separately with XRD and ND data to enable extraction of a starting model for refinements using both XRD and ND, which was refined successfully. The final model contains Mn-dopants that displace Fe from the *M2* site and relocate this fraction of Fe to the Li (*M1*) site. The replacement at the *M2* site is considered isovalent doping (Mn<sup>2+</sup> for Fe<sup>2+</sup>), while the process at the *M1* site is considered supervalent doping (Fe<sup>2+</sup> for Li<sup>+</sup>). The supervalent doping at the *M1* site necessitates the incorporation of Li vacancies for charge balance, in agreement with the final Rietveld-refined structural model. This presentation will highlight how these structural features contribute to the observed enhancement of the electrochemical properties of Mn-doped LiFePO<sub>4</sub> compared to undoped LiFePO<sub>4</sub>.