

Aliovalent substitution for Li in LiFePO_4 forms sarcopside clusters enhancing the reaction rate in a Li battery

Scientific Achievement

We have shown that aliovalent substitution at the Li site is possible, and contrary to belief does not block the 1-d tunnels. Rather the excess metal forms clusters as in the sarcopside structure, $\text{Fe}_{0.5}\text{FePO}_4$. Surprisingly these defects enhanced the kinetics of substituted LiFePO_4 , but at the cost of capacity and is consistent with the NECCES pseudo-single-phase reaction mechanism. Such defects reduce the overpotential for single phase formation, and thus enable the diffusion of the lithium ions.

Significance and Impact

Understanding $\text{LiFePO}_4/\text{FePO}_4$ transformation and why substitution accelerates it will help in designing the next generation battery materials.

Research Details

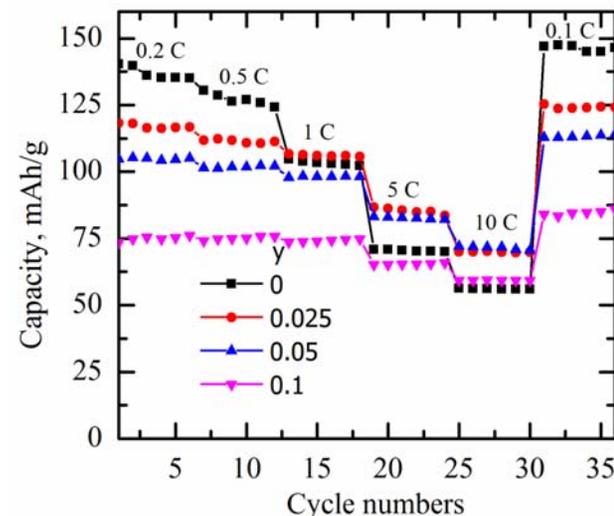
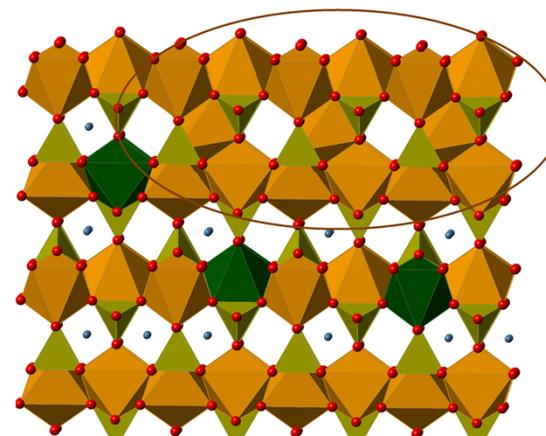
Single crystals of $\text{Li}_{1-2y}\text{Fe}_{1+y}\text{PO}_4$ were grown, and V-substituted powder materials, $[\text{Li}_{1-3y}\text{Fe}_y]\text{Fe}_{1-y}\text{V}_y\text{PO}_4$ synthesized. These were characterized by x-ray and neutron diffraction, and TEM.

Y. Janssen, D. Santhanagopalan, D. Qian, M. Chi, X. Wang, C. Hoffmann, Y. S. Meng, P. G. Khalifah – Chem. Materials, 2013, 25, 4574. DOI: 10.1021/cm4027682

F. Omenya, N. A. Chernova, Q. Fang, R. Zhang, M. S. Whittingham – Chem. Mater. 2013, 25, 2691. DOI: 10.1021/cm401293r

This work was performed at Binghamton University, Brookhaven National Laboratory, Stony Brook University, UC San Diego, Oak Ridge National Laboratory and NIST.

sarcopside defect



Capacity as a function of rate of reaction and of vanadium content



U.S. DEPARTMENT OF
ENERGY

Office of
Science

