

# Aliovalent substitution in $\text{LiFePO}_4$ modifies its phase diagram, thereby enhancing its reactivity in a Li battery

## Scientific Achievement

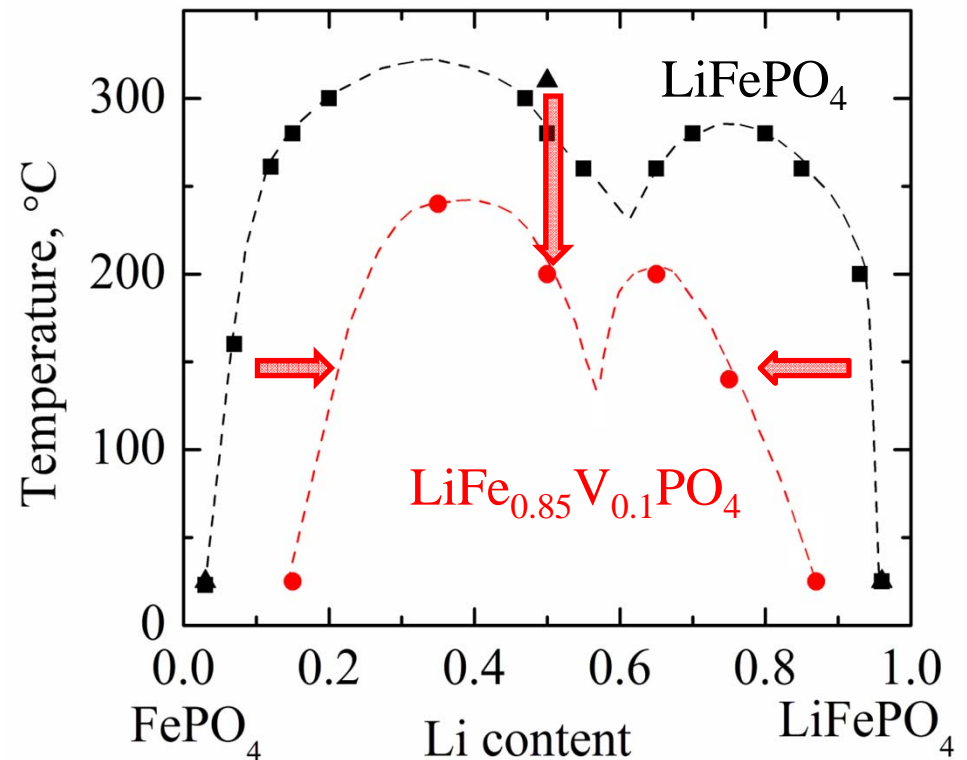
We have shown that aliovalent substitution at the Fe site broadens the single-phase region of the  $\text{LiFePO}_4$ - $\text{FePO}_4$  phase diagram. This explains the enhanced kinetics of substituted  $\text{LiFePO}_4$ , and is consistent with the NECCES pseudo-single-phase reaction mechanism.

## 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

The structure and phase composition of vanadium-substituted  $\text{LiFePO}_4$  was investigated as a function of Li and V contents, as well as temperature using in-situ synchrotron techniques at NSLS.



Phase diagram reveals broader solid solution range in vanadium-substituted  $\text{LiFePO}_4$

R. Malik, F. Zhou, G. Ceder – Nature Materials, 2011, 10, 587. DOI: 10.1038/NMAT3065.

F. Omenya, N. A. Chernova, S. Upreti, P. Y. Zavalij, K.-W. Nam, X.-Q. Yang, M. S. Whittingham – Chem. Mater. 2011, 23, 4733. DOI: 10.1021/cm2017032

F. Omenya, N. A. Chernova, R. Zhang, J. Fang, Y. Huang, F. Cohen, N. T. Dobrzynski, S. D. Senanayake, W. Xu, M. S. Whittingham – Chem. Mater. DOI: 10.1021/cm303259j

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