Structure, defects and thermal stability of delithiated olivine phosphates

Scientific Achievement
We have revealed that water catalyzes the conversion of Mn-rich olivine (Fe,Mn)MPO₄ to sarcopside (Fe,Mn)₃(PO₄)₂ upon heating.

Significance and Impact
Controversial data on thermal stability of delithiated Mn-rich olivines used as cathodes in Li-ion batteries is explained by detrimental role of water uncontrollably reacting with sample upon air exposure. Dry samples are stable up to 400 °C, which is safe for most applications and will allow greater energy storage than the common LiFePO₄.

Research Details
We investigated structural changes upon heating of delithiated olivine phosphates under variety of conditions using in-situ x-ray diffraction at NSLS. This was complemented by thermal gravimetric analysis with mass spectrometry and calorimetry. Li and H NMR also gave key information about the reactions.

In-situ high-temperature synchrotron diffraction of dry and moist Fe₀.₃Mn₀.₇PO₄ indicating that moisture exposure compromises thermal stability

This work was performed at Binghamton University, Stony Brook University, Cambridge University and Brookhaven National Laboratory