

Interfacial effects in ϵ -Li_xVOPO₄ and evolution of the electronic structure

Scientific Achievement

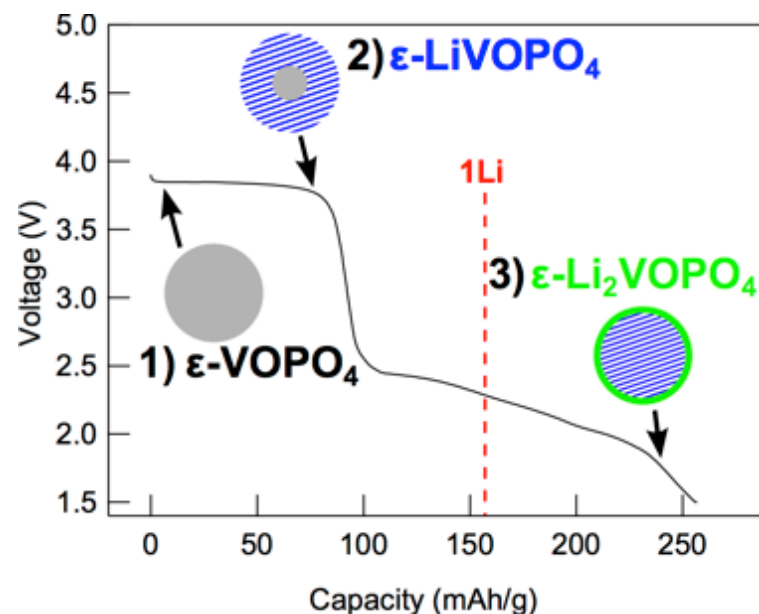
Identified disrupted kinetics in the high voltage reaction as a main contributor limiting the realized capacity in hydrothermally synthesized ϵ -VOPO₄, a promising multi-electron lithium ion battery (LIB) cathode.

Significance and Impact

Provides a mesoscopic description of how phase segregation can evolve in multi-electron LIB cathode nanoparticles.

Research Details

- Used variable photon-energy x-ray photoelectron spectroscopy to chemically distinguish and depth-resolve the interfacial phase transitions in hydrothermal ϵ -VOPO₄ electrodes as function of Li intercalation
- Confirmed endpoint phases by direct comparison with hybrid density functional theory



Findings: Our analysis shows that the second lithium reaction begins before the full incorporation of the first lithium. This results in a pronounced lithium gradient within the nanoparticles, with the ϵ -Li₂VOPO₄ phase only forming near the surface.

N. F. Quackenbush et al., Chem. Mater. 2015
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Work performed at Binghamton, NSLS and UC San Diego