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Mechanistic Insights into the Electrochemical Lithiation of $Ag_2VO_2PO_4$

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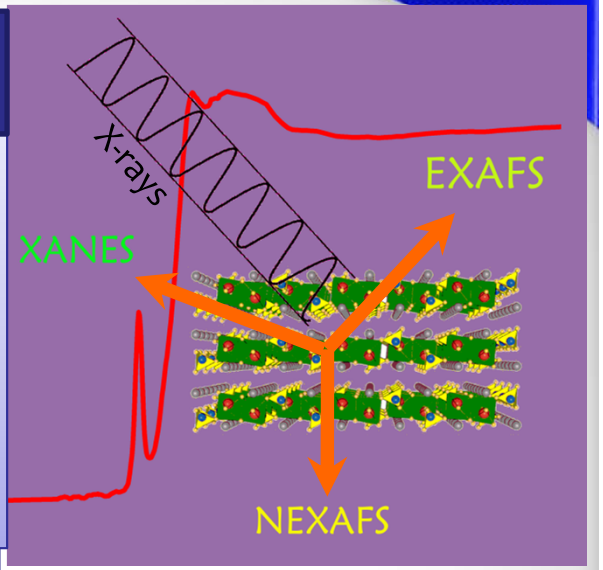
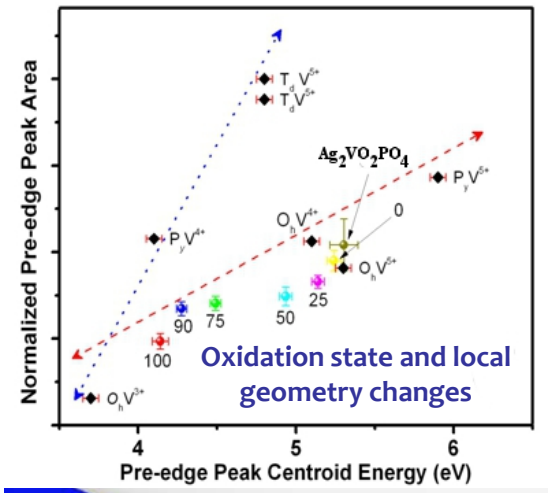
- Amorphization often accompanies electrochemical discharge of cathode materials in Li-ion batteries, leaving the material highly disordered and precluding the application of standard diffraction tools.
- We have used multiple-edge X-ray absorption fine structure (XAFS) spectroscopy in conjunction with density functional theory to identify intermediate phases and elucidate the mechanism of electrochemical lithiation for $Ag_2VO_2PO_4$, a promising bimetallic vanadium phosphate cathode material.





Findings

- Concomitant, not sequential reduction of vanadium and silver during discharge
- Quantitative description of stoichiometry and valence at various depths of discharge
- Stability of PO_4^{3-} groups to lithiation and inductive impact on V-O bonds raising V potential
- The sequence of V 3d states occupied upon electrochemical reduction follows: V $3d_{zy}$ then $3d_{zx}$, and finally $3d_{xy}$