

Relating ϵ -LiVOPO₄ performance to local environment dynamics and hysteresis

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The vanadyl phosphates (VOPO₄) are a class of multi-electron materials that have been demonstrated to successfully utilize multiple redox couples ($V^{3+} \leftrightarrow V^{4+} \leftrightarrow V^{5+}$.) The electrochemical efficiency of these reactions however, is highly dependent on the synthetic method used to prepare the material – the reason yet not understood. The source of material is potentially one of the factors contributing towards conflicting reports in the literature as to the nature of second Li insertion. Several studies have conclude the reaction proceeds via a two-phase mechanism, while others identified only one intermediate phase.

Here, we combine operando pair distribution function (PDF) measurements and analysis along with X-ray diffraction in an attempt to identify potential structural differences between LiVOPO₄ synthesized via solid state and hydrothermal method, which might affect the diffusion pathways and ultimately limit the cycling efficiency.