

Local environment and structure of ϵ -VOPO₄ cycled with graphene

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In the quest to improve electrochemical performance of energy storage materials, a potential avenue to increase the energy density of Li-ion batteries is the use of cathode materials that are capable of intercalating more than 1 Li⁺ per redox center in a fully reversible fashion. One group of compounds that exhibit these desirable characteristics are vanadyl phosphates.

The vanadate phosphate (VOPO₄) compounds are a class of multi-electron materials that have been demonstrated to successfully utilize multiple redox couples (V³⁺ ↔ V⁴⁺ ↔ V⁵⁺.) To enable fully reversible intercalation of two Li ions and reach the theoretical capacity of 305 mAh/g sample morphology and particle size has to be closely controlled. In addition, electrochemical efficiency is highly dependent on type of carbon used to prepare electrode – the reason yet not understood.

Here, we presents results of a multifaceted investigation into the local structural ordering of vanadate phosphate compounds, that enables reversible cycling over the 2-lithium range, employing X-ray powder diffraction, pair distribution function (PDF) analyses and NMR measurements.