

Li₃V₂(PO₄)₃ Cathode Material: Synthesis Method, High Lithium Diffusion Coefficient and Magnetic Inhomogeneity

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Supplementary Materials

S1. Vanadyl Formate Synthesis

The vanadyl formate synthesis was carried out according to the method described in [54] and showed in Figure S1:

✓ Vanadyl sulfate powder VO(SO₄)₂·3H₂O in an amount of 5 g is dissolved in 100 mL of distilled water.

✓ 90 mL of 12% NH₄OH solution is added to the resulting solution.

✓ The resulting brown oxide precipitate is filtered from the mother liquor using a filter paper with a pore size of 2–3 μm and clean with distilled water until there is no qualitative reaction to SO₄²⁻ ions (on BaCl₂).

✓ The precipitate is transferred to a heat-resistant glass with a volume of 600 ml, after that 100 ml of distilled water and 5 ml of 99.7% formic acid is added. In this case, the ratio of components is following vanadyl sulfate:ammonia (12–14%):formic acid (45–99.7%) = 1:2.0:1.5. After dissolving the brown precipitate, a blue solution is formed, which is evaporated at a temperature of 50°C for 90 minutes until vanadyl formate crystallizes.

✓ The X-ray phase analysis of the dried to constant weight blue crystals showed the resulting product is the single phase sample (Figure S2) with the chemical formula VO(HCOO)₂·H₂O).

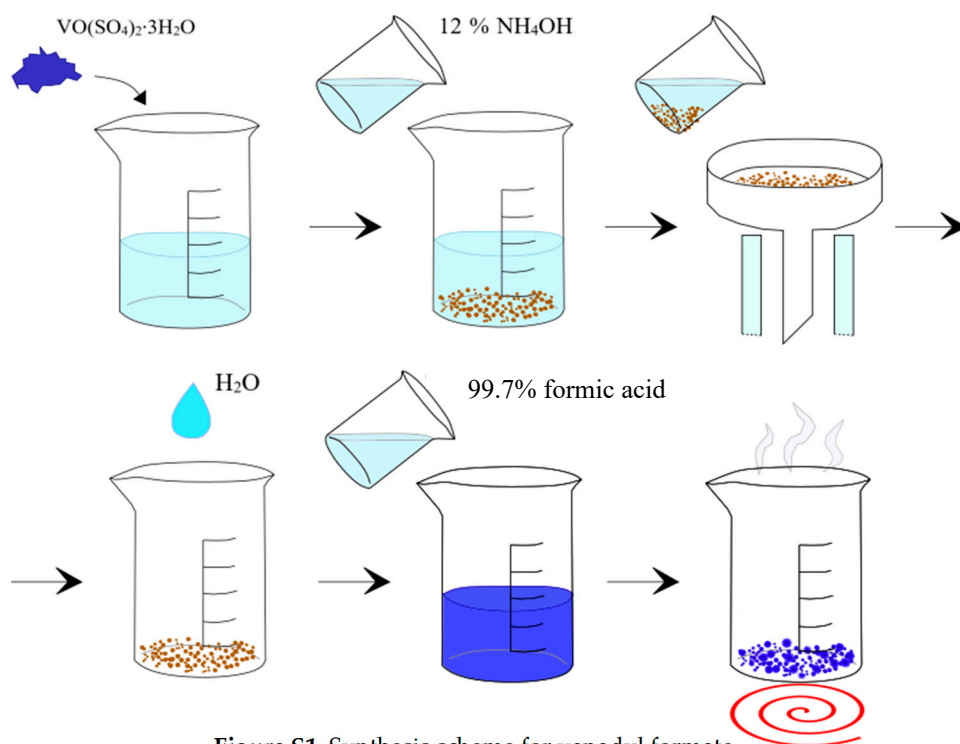


Figure S1. Synthesis scheme for vanadyl formate

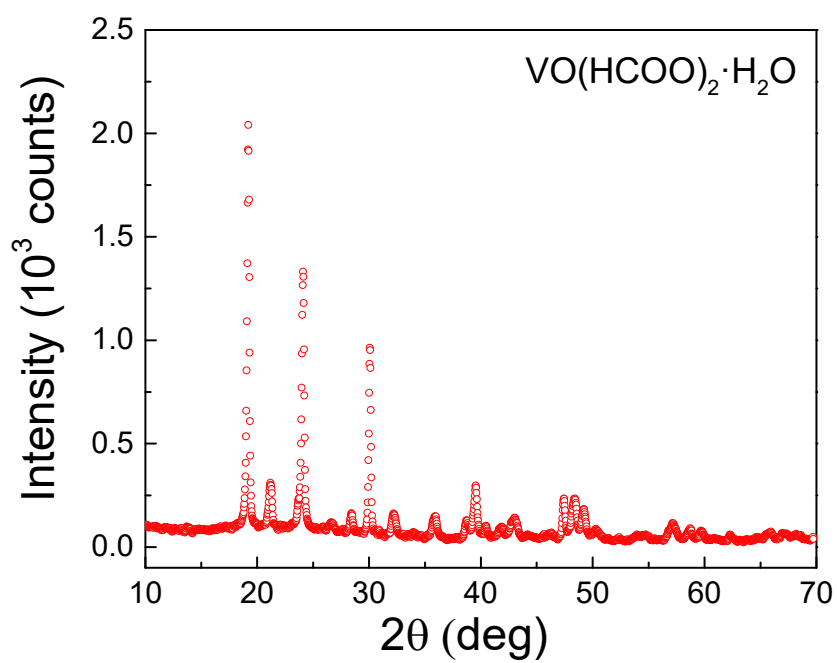


Figure S2. X-ray diffraction pattern of VO(HCOO)₂·H₂O

S2. Phase formation of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ during the heat treatment

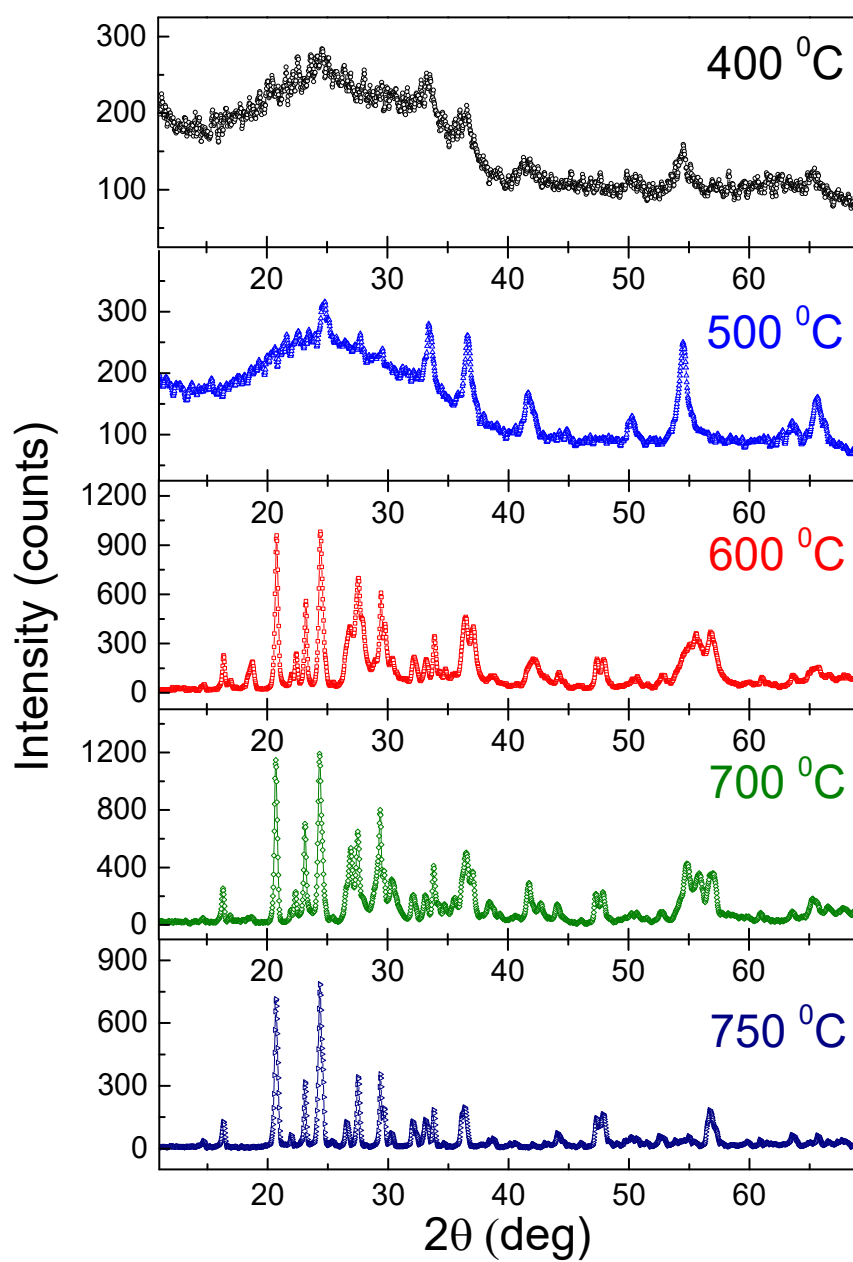


Figure S3. X-ray diffraction patterns of the precursor after thermal hydrolysis during the phase formation process of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ during sequential heat treatment up to 750 °C

S3. X-ray fluorescence analysis

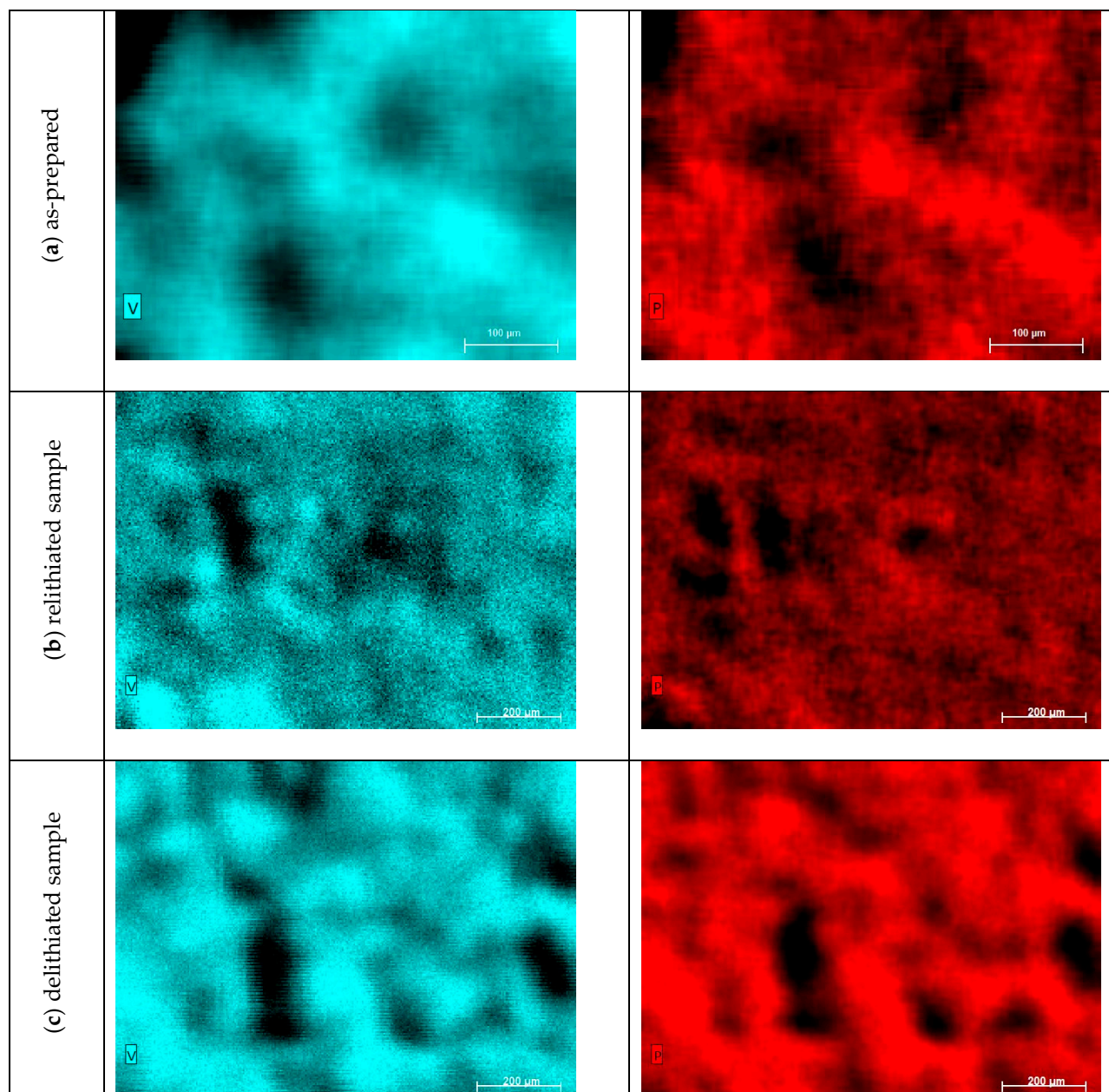


Figure S4. XFA images of LVPO (a) as-prepared sample, (b) relithiated sample and (c) delithiated sample. Dark areas correspond to the absence of a sample

S4. Magnetization measurements of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ -based composites

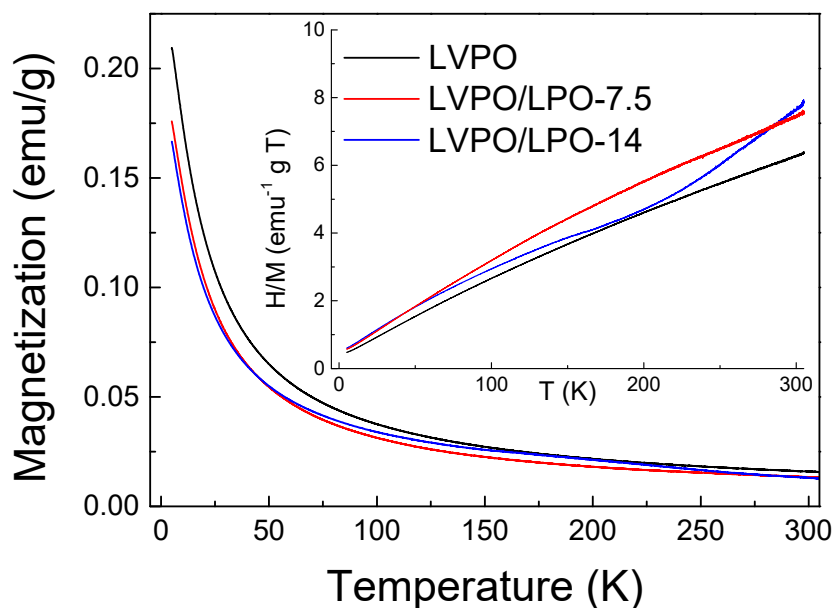


Figure S5. Magnetization M/H as a function of temperature for $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ sample and $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (86 wt.%) / Li_3PO_4 (14 wt.%) and $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (92.5 wt.%) / Li_3PO_4 (7.5 wt.%) composites measured in the FC regime in the external magnetic field $H = 0.1$ T. The composites $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (86 wt.%) / Li_3PO_4 (14 wt.%) and $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (92.5 wt.%) / Li_3PO_4 (7.5 wt.%) are labeled as LVPO/LPO-14 and LVPO/LPO-7.5, respectively. Inset shows the inverse magnetic susceptibility H/M as a function of temperature.

S5. X-ray diffraction analysis

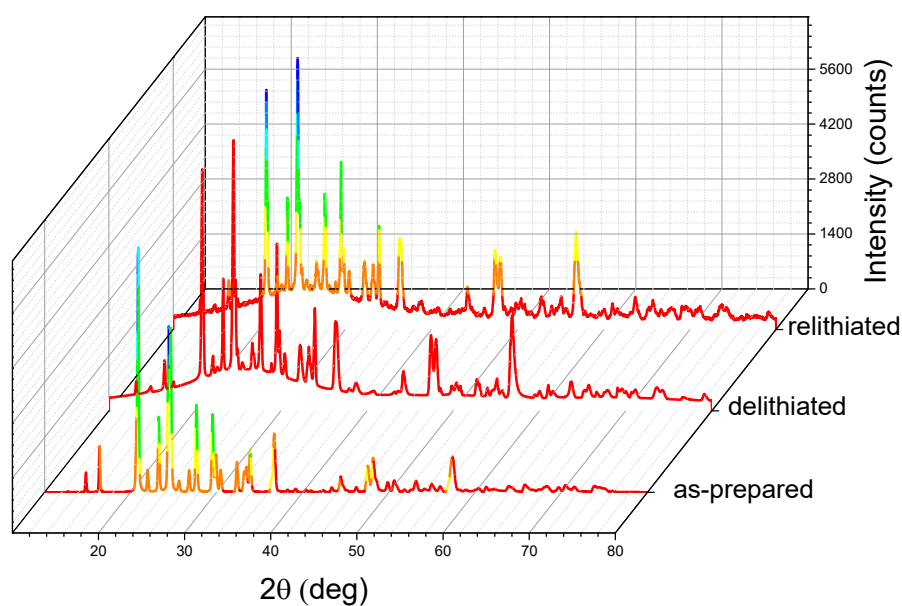


Figure S6. Experimental X-ray diffraction pattern of $\text{Li}_3\text{V}_2(\text{PO}_4)_3$: as-prepared, delithiated and relithiated samples.