

Synthesis and electrochemical studies of layer-structured metastable α -LiVOPO₄

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Table S1 Crystallographic data and structure refinement details for LiVOPO₄·2H₂O

Formula	H4 Li O7 P V
Formula weight	204.88
T (K)	223(2)
Crystal system	Orthorhombic
Space group	Cmca
Unit cell dimensions (Å)	$a = 8.9454(7)$ $b = 9.0406(7)$ $c = 12.7473(10)$
V/ Å ³	1030.90(14)
Z	8
Density (calculated, g. cm ⁻³)	2.640
μ (mm ⁻¹)	2.206
Crystal size (mm ³)	0.40 x 0.36 x 0.16
Theta range	3.20 to 27.48°
Reflections collected	3374
Independent reflections	633 [R(int) = 0.0230]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7192 and 0.4724
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	633 / 0 / 61
Goodness-of-fit on F ²	1.175
Final R indices [I>2sigma(I)]	R ₁ = 0.0250, wR ₂ = 0.0679
R indices (all data)	R ₁ = 0.0252, wR ₂ = 0.0681
Largest diff. peak and hole	0.261 and -0.718 e.Å ⁻³

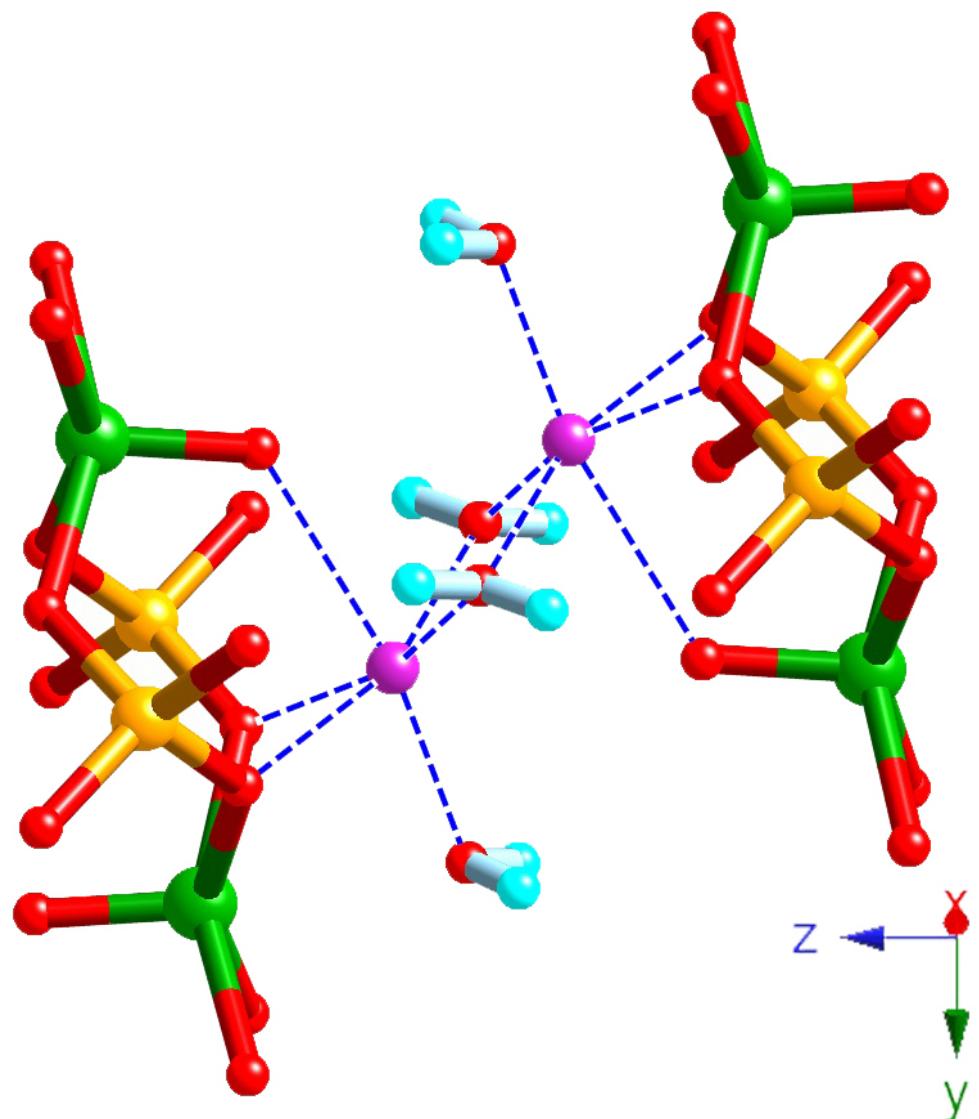


Fig. S2 Crystal structure of $\text{LiVOPO}_4 \cdot 2\text{H}_2\text{O}$ showing coordination of lithium with oxygen atoms. The V, P, O, H and Li atoms are shown in green, orange, red, blue and purple respectively.

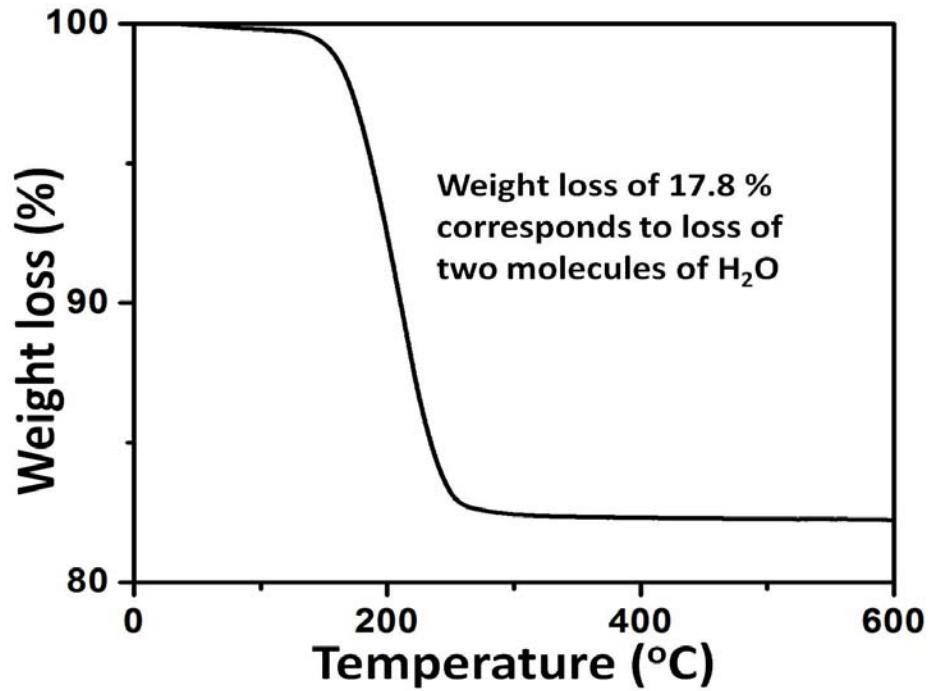


Fig. S3 TGA of $\text{LiVOPO}_4 \cdot 2\text{H}_2\text{O}$ in air at a rate of 5°C min^{-1}

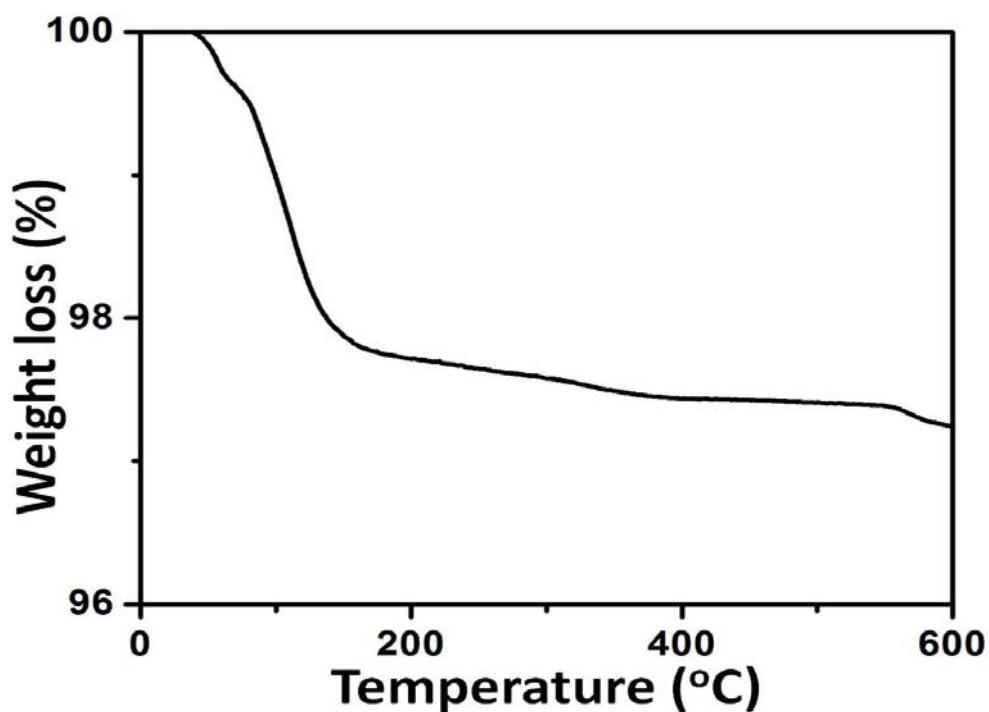


Fig. S4 TGA of compound obtained by dehydration of $\text{LiVOPO}_4 \cdot 2\text{H}_2\text{O}$ in air at a rate of 5°C min^{-1}

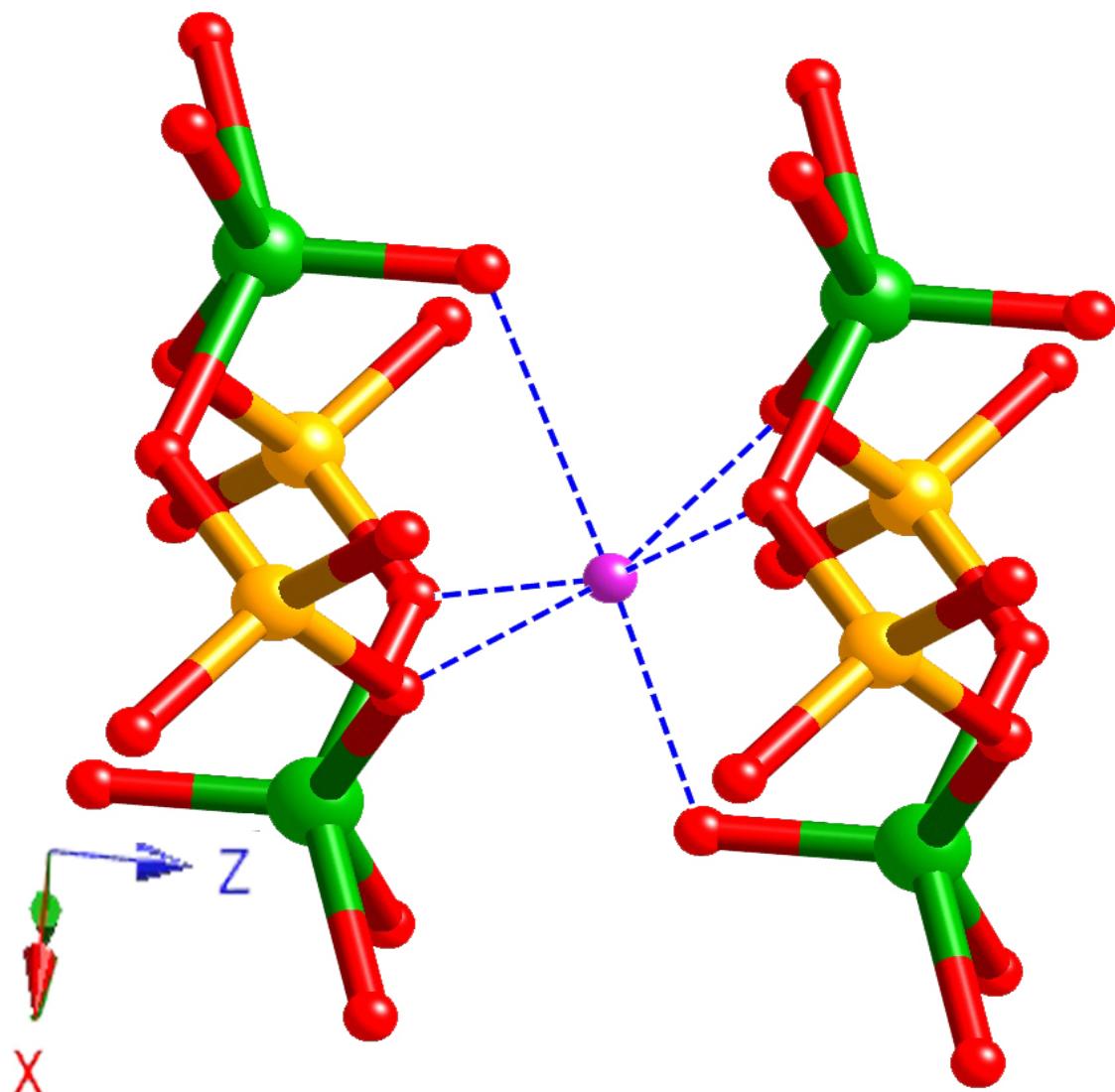


Fig. S5 Crystal structure of α -LiVOPO₄ showing coordination of lithium with oxygen atoms. The V, P, O and Li atoms are shown as green, orange, red and purple colored balls respectively.

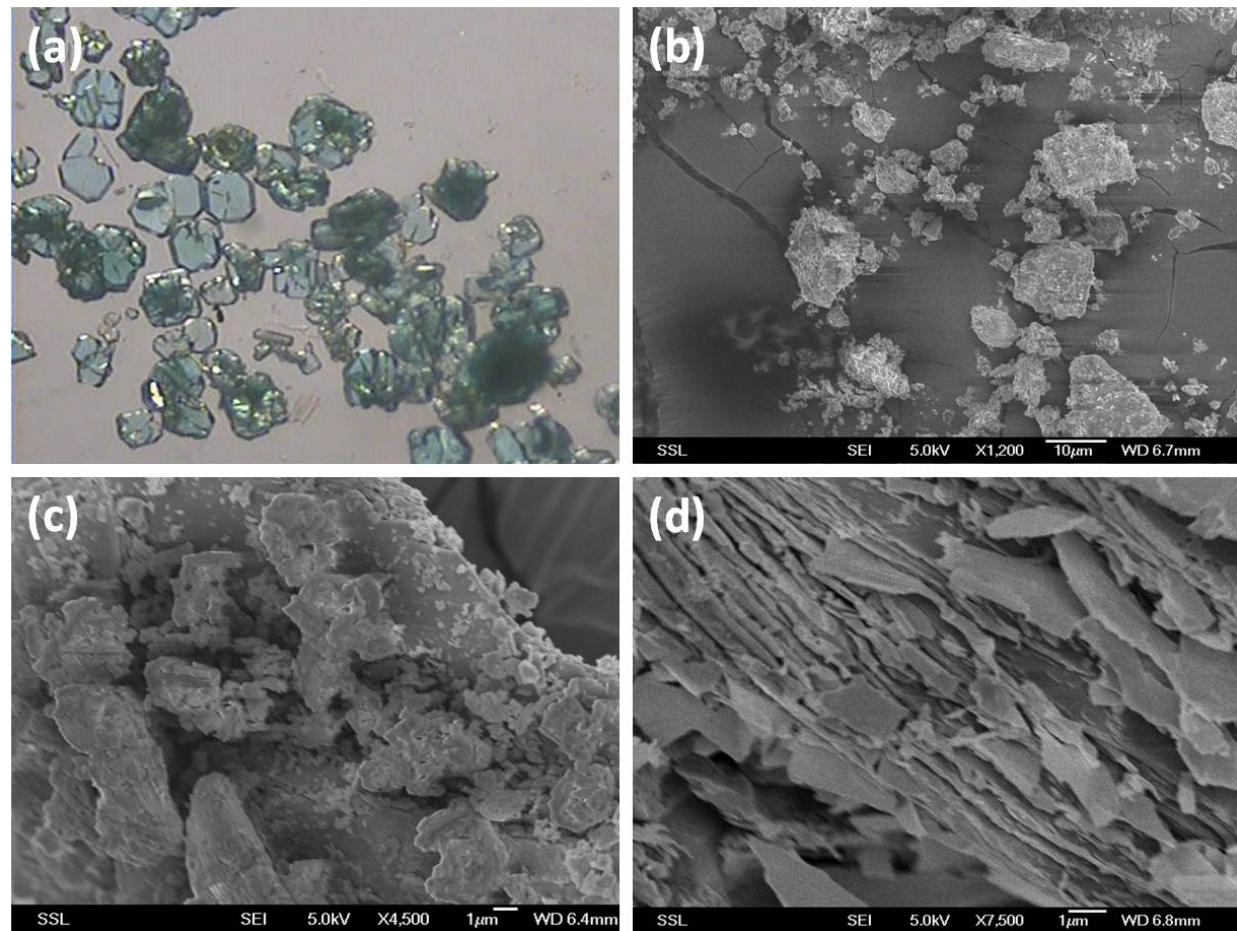


Fig. S6. SEM micrographs of (a) single crystals of LiVOPO₄·2H₂O, (b) ball-milled LiVOPO₄·2H₂O, (c) α_I-LiVOPO₄ obtained by dehydration of ball-milled LiVOPO₄·2H₂O at low magnification and (d) α_I-LiVOPO₄ at high magnification

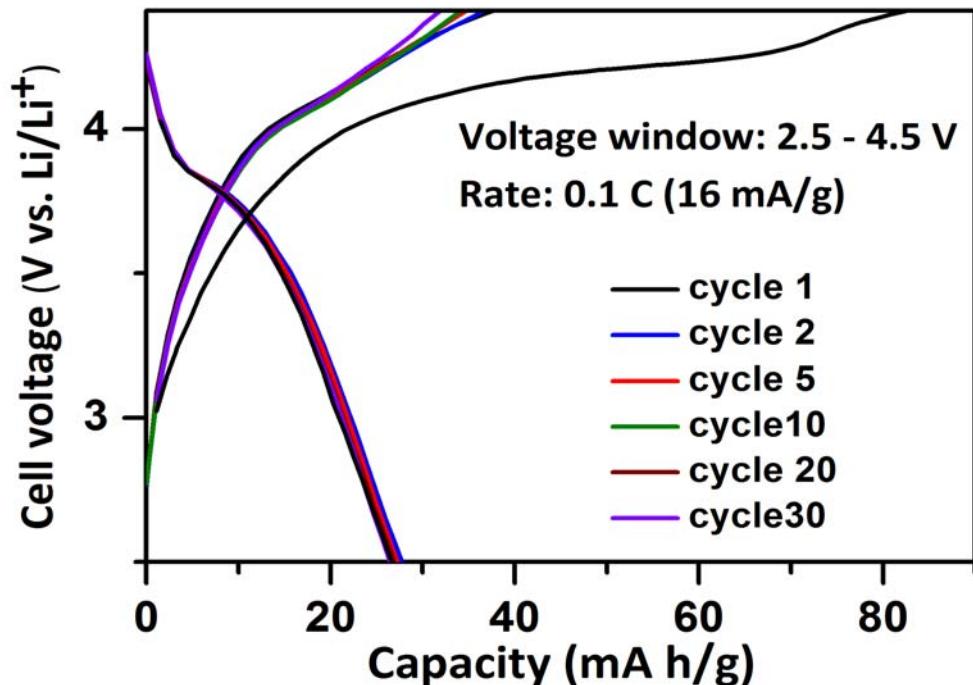


Fig. S7 Galvanostatic charge-discharge cycles of α -LiVOPO₄ obtained from as synthesized LiVOPO₄·2H₂O

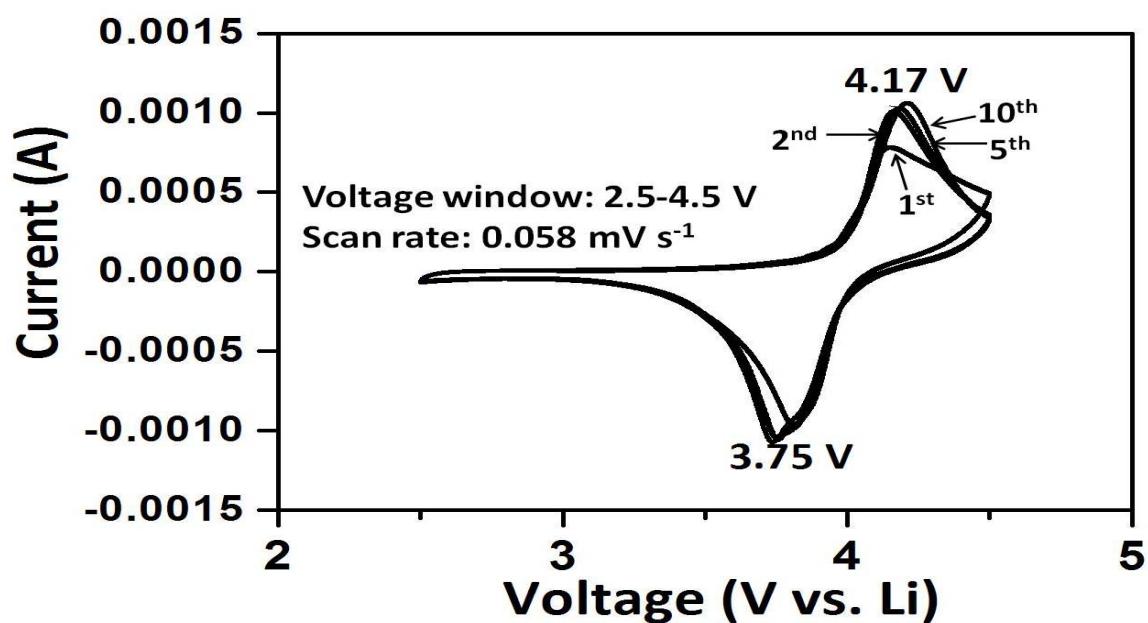


Fig. S8 Cyclic voltammograms of α -LiVOPO₄ in the voltage window of 2.5-4.5 V at a scan rate of 0.058 mV s⁻¹

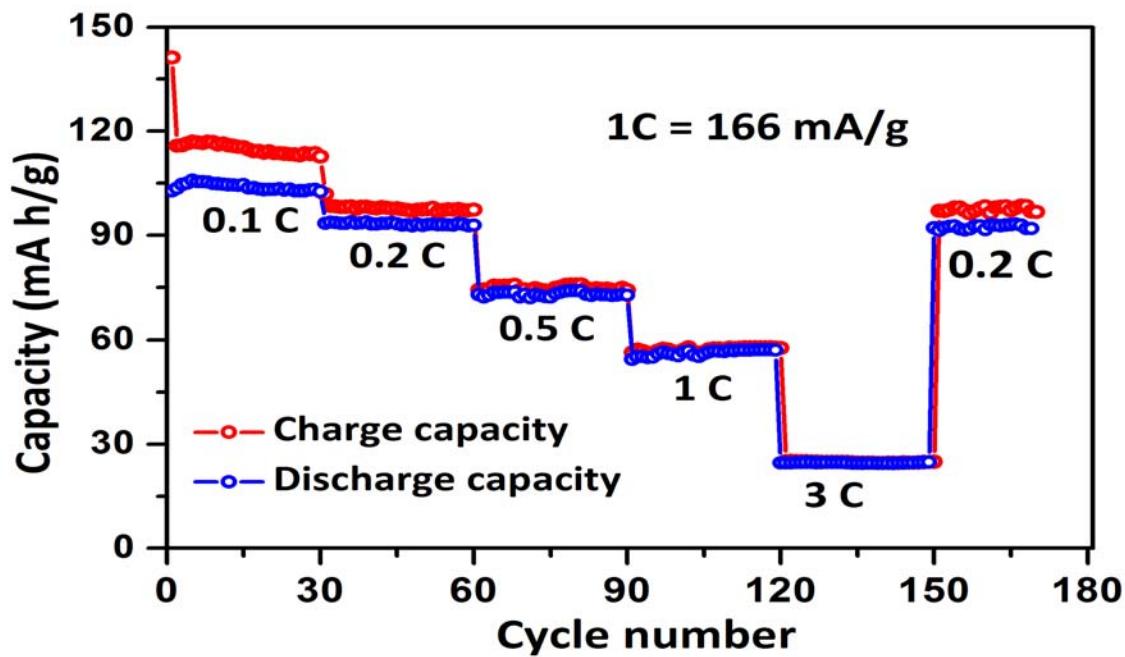


Fig. S9 Rate capability study of α -LiVOPO₄ at various current rates