Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

A Better Understanding of the Capacity Fading Mechanisms of $Li_3V_2(PO_4)_3$

Liping Wang*, Jin Xu, Chong Wang, Xumei Cui, Jingze Li, Yong-Ning Zhou*

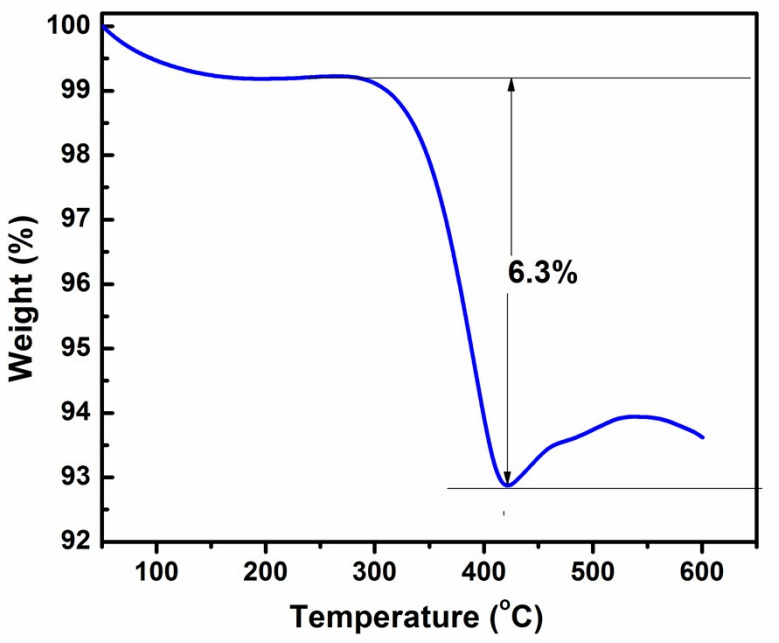

Figure S1 Thermo-gravimetric analyzer (TGA) curves of as-obtained $Li_3V_2(PO_4)_3$ during heating in air at a heating rate of 10 °C/minutes.

* Corresponding author. +86 28 83207620. Fax: +86 28 83202569.

E-mail addresses: lipingwang@uestc.edu.cn (L. Wang), ynzhou@fudan.edu.cn (Y. N. Zhou)

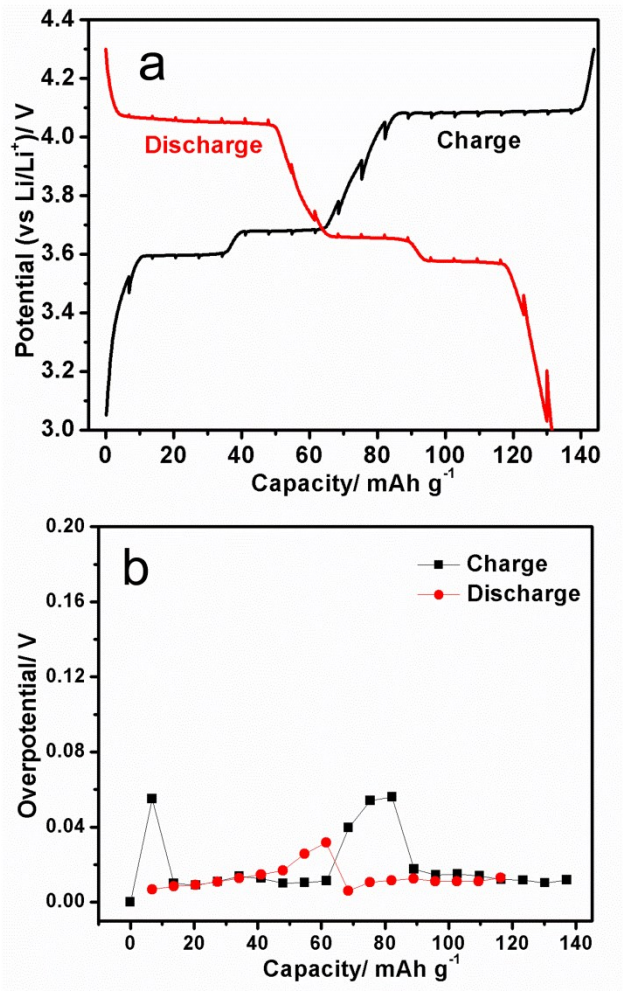

Figure S2 (a) GITT curves plotted with the voltage as a function of specific capacity in the voltage window 3.0-4.3 V. The current density is set at 13 mA g^{-1} with a relaxation time of 4 hours; (b) The overpotential value as a function of specific capacity in the charge process.

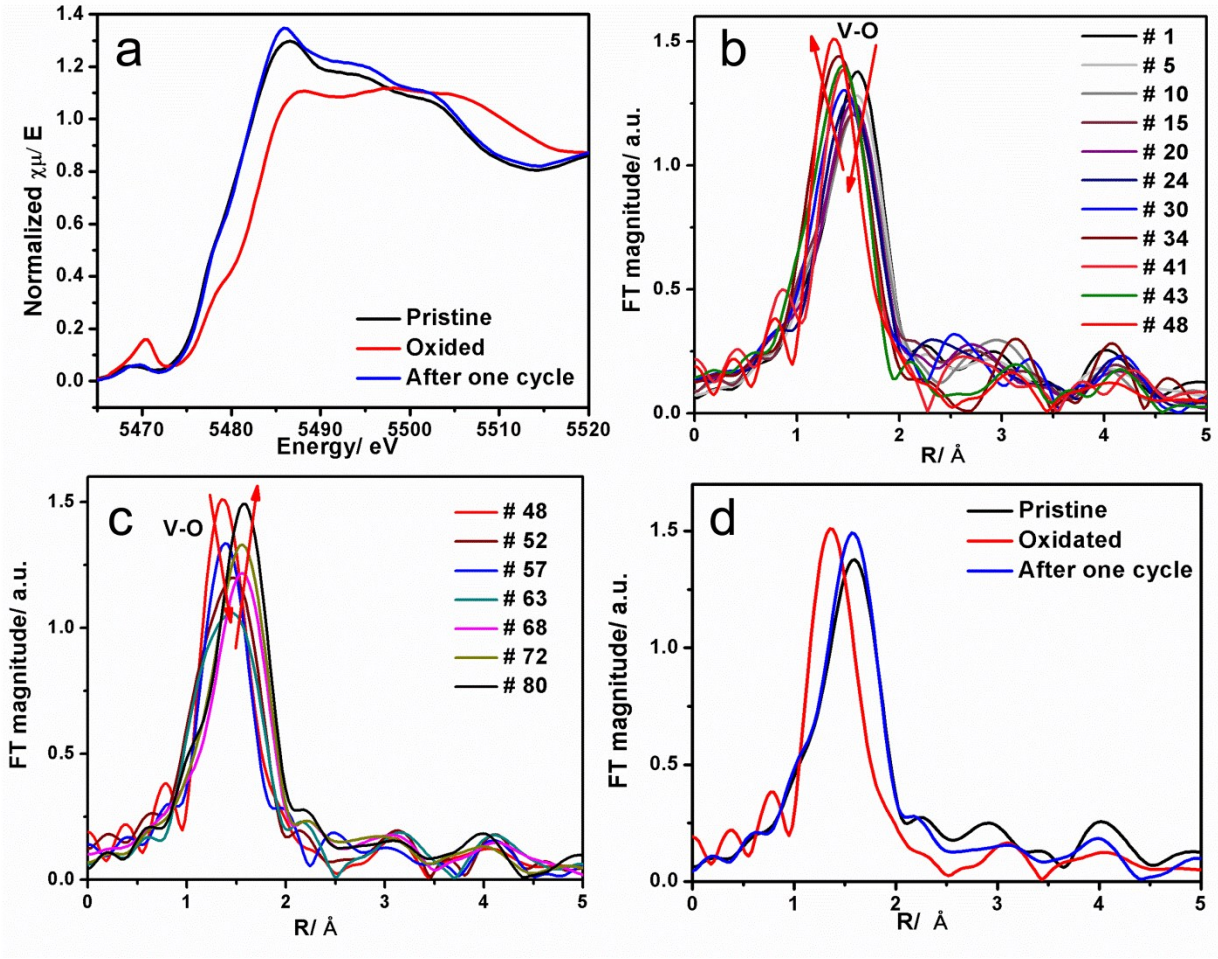

Figure S3 (a) V-K edge XANES spectra of LVP for the pristine, charge to 4.8 V and discharge to 3.0 V; (b) Selected Fourier transform spectra of k^3-weighted V EXAFS spectra of LVP during charge process; (c) Selected Fourier transform spectra of k^3-weighted V EXAFS spectra of LVP during discharge process; (d) Comparison of the Fourier transform spectra of k^3-weighted V EXAFS spectra of LVP for the pristine, charged to 4.8 V and discharge to 3.0 V.

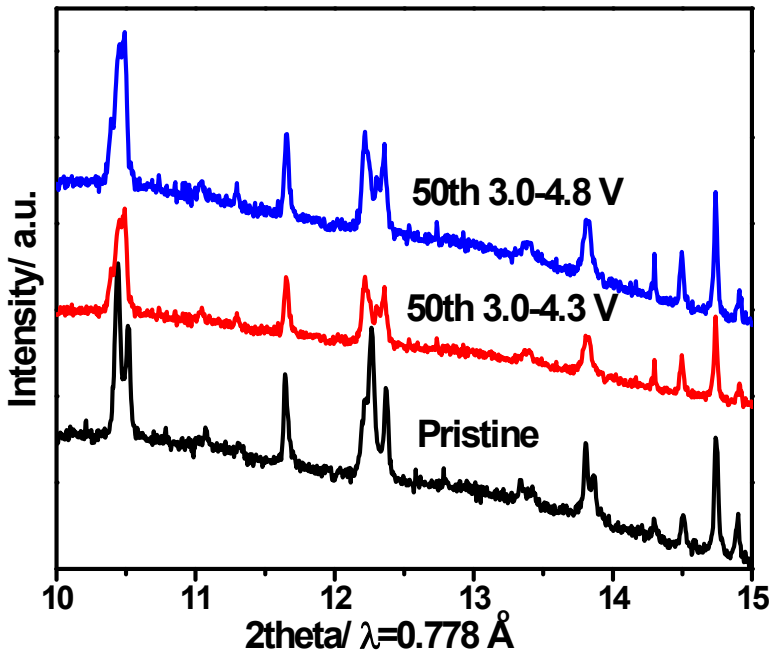

Figure S4 XRD patterns of the pristine LVP electrode and the electrodes after 50 cycles in the voltage windows: 3.0-4.3 V and 3.0-4.8 V.

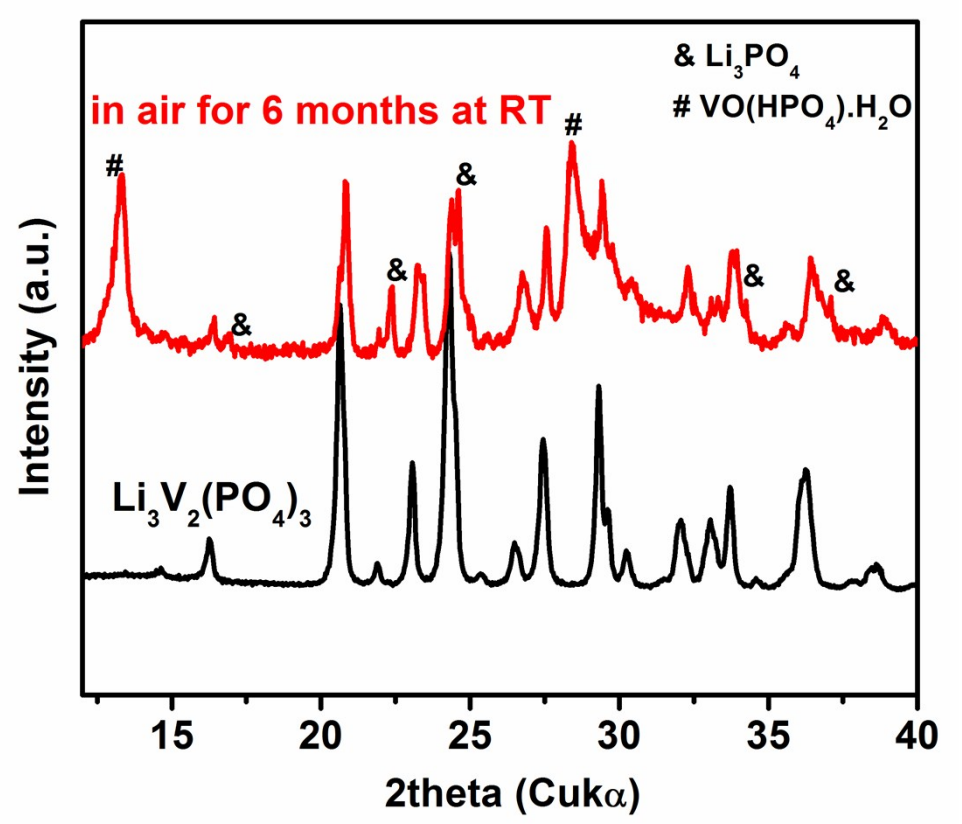

Figure S5 XRD patterns of $Li_3V_2(PO_4)_3$ exposed in air at room temperature after 6 months.

Table S1 V K-edge EXAFS structure parameters of LVP at different charge-discharge states.

Samples	Path	r/Å	σ^2 /10^{-3}Å^2	ΔE/eV	R
LVP_pristine	V-O1	1.91(6) ± 0.027	7.22 ± 4.21	17.43 ± 3.58	0.008
	V-O2	2.06(8) ± 0.025	5.10 ± 3.86		
	V-P	3.43(1) ± 0.044	1.82 ± 5.04		
LVP_ch 4.0V	V-O1	1.86(6) ± 0.027	7.25 ± 3.72	15.29 ± 3.84	0.015
	V-O2	2.01(8) ± 0.027	4.75 ± 3.67		
	V-P	3.40(1) ± 0.047	0.92 ± 5.38		
LVP_ch 4.8V	V-O1	1.79(3) ± 0.018	11.08 ± 2.26	9.76 ± 3.48	0.011
	V-O2	1.94(3) ± 0.020	8.00 ± 2.47		
	V-P	3.27(1) ± 0.120	9.93 ± 18.40		
LVP_disch 3.9V	V-O1	1.81(2) ± 0.028	4.78 ± 3.66	16.87 ± 3.57	0.008
	V-O2	1.97(3) ± 0.027	2.61 ± 3.49		
	V-P	3.31(4) ± 0.062	5.78 ± 7.50		
LVP_disch 3.0V	V-O1	1.91(6) ± 0.027	7.38 ± 4.46	10.48 ± 4.38	0.007
	V-O2	2.06(5) ± 0.025	5.18 ± 4.04		
	V-P	3.43(7) ± 0.062	1.94 ± 7.93		

r: bond length; σ^2: Debye-Waller factor (disorder); ΔE: inner shell potential shift; R: R-factor.

Table S2 Lattice parameters of LVP before and after 50 cycles.

	a (Å)	*b* (Å)	*c* (Å)	*β*	*V* (Å^3)
pristine	8.61	8.59	12.04	90.57	890.70
After 50 cycles (3.0-4.3 V)	8.51	8.55	11.87	90.55	863.53
After 50 cycles (3.0-4.8 V)	8.49	8.73	11.87	90.52	879.34