Supporting information

A Comparison of $LiVPO_4F$ to $Li_4Ti_5O_{12}$ as Anode Materials for Lithium-Ion Batteries

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Table S1. Structural parameters obtained after Rietveld refinement of XRD data from phase $LiVPO_4F$.

Atom	Wyckoff position	Atomic parameter			occ	B_{iso} (Å^2)
		Atomic position				
		x/a	*y/b*	*z/c*		
V(1)	1a	0	0	0	1.0	3.242
V(2)	1f	0.5	0	0.5	1.0	-7.383
P	2i	0.1060	0.3633	0.2246	1.0	-2.183
O(1)	2i	0.2256	0.1900	0.4276	1.0	5.763
O(2)	2i	0.7926	0.3754	0.3637	1.0	-1.872
O(3)	2i	0.1376	0.2284	0.0527	1.0	-7.575
O(4)	2i	0.1950	0.7103	0.1499	1.0	-7.373
F	2i	0.5750	0.9229	0.2645	1.0	-3.410
Li(1)	2i	0.1488	0.4452	0.3829	1.0	-2.762

Agreement factors: Rw(%)=17.442, Sig=1.754.

Table S2. Structural parameters obtained after Rietveld refinement of XRD data from phase $Li_4Ti_5O_{12}$.

Atom	Wyckoff position	Atomic parameter			occ	B_{iso} (Å^2)
		Atomic position				
		x/a	*y/b*	*z/c*		
Li(1)	8a	0	0	0	1.0	-8.687
Li(2)	16d	0.6250	0.6250	0.6250	0.1667	-8.634
Ti(1)	16d	0.6250	0.6250	0.6250	0.8333	-8.634
O(1)	32e	0.3782	0.3782	0.3782	1.0	-5.999

Agreement factors: Rw(%)=18.187, Sig=1.963.

Table S3. Structural parameters obtained after Rietveld refinement of XRD data from phase Li_2VPO_4F.

Atom	Wyckoff position	Atomic parameter			occ	B_{iso} (Å^2)
		Atomic position				
		x/a	*y/b*	*z/c*		
V(1)	4b	0	0.5	0	1.0	-14.596
P(1)	4e	0.5	0.3455	0.2500	1.0	0.510
O(1)	8f	0.3118	0.4943	0.1054	1.0	-16.583
O(2)	8f	0.0653	0.7339	0.1128	1.0	-17.909
F(1)	4e	0	0.4109	0.2500	1.0	-12.714
Li(1)	8f	0.2154	0.2169	0.4597	0.5	-12.887
Li(2)	8f	0.1800	0.0194	0.5691	0.5	-15.796

Agreement factors: Rw(%)=1.480, Sig=14.930.

Table S4. Structural parameters obtained after Rietveld refinement of XRD data from phase $Li_7Ti_5O_{12}$.

Atom	Wyckoff position	Atomic parameter			occ	B_{iso} (Å^2)
		Atomic position				
		x/a	*y/b*	*z/c*		
Li(1)	16c	0.1250	0.1250	0.1250	1.0	32.230
Li(2)	16d	0.6250	0.6250	0.6250	0.1667	-12.369
Ti(1)	16d	0.6250	0.6250	0.6250	0.8333	-12.369
O(1)	32e	0.3820	0.3820	0.3820	1.0	-13.275

Agreement factors: Rw(%)=17.864, Sig=1.928.

Table S5. Structural parameters obtained after Rietveld refinement of XRD data from phase $Li_{8.5}Ti_5O_{12}$.

Atom	Wyckoff position	Atomic parameter			occ	B_{iso} (Å^2)
		Atomic position				
		x/a	*y/b*	*z/c*		
Li(1)	8a	0	0	0	0.6667	-19.206
Li(2)	16c	0.1250	0.1250	0.1250	1.0	15.530
Li(3)	16d	0.6250	0.6250	0.6250	0.1667	-13.152
Ti(1)	16d	0.6250	0.6250	0.6250	0.8333	-13.152
O(1)	32e	0.3830	0.3830	0.3830	1.0	-13.547

Agreement factors: Rw(%)=17.790, Sig=1.914.

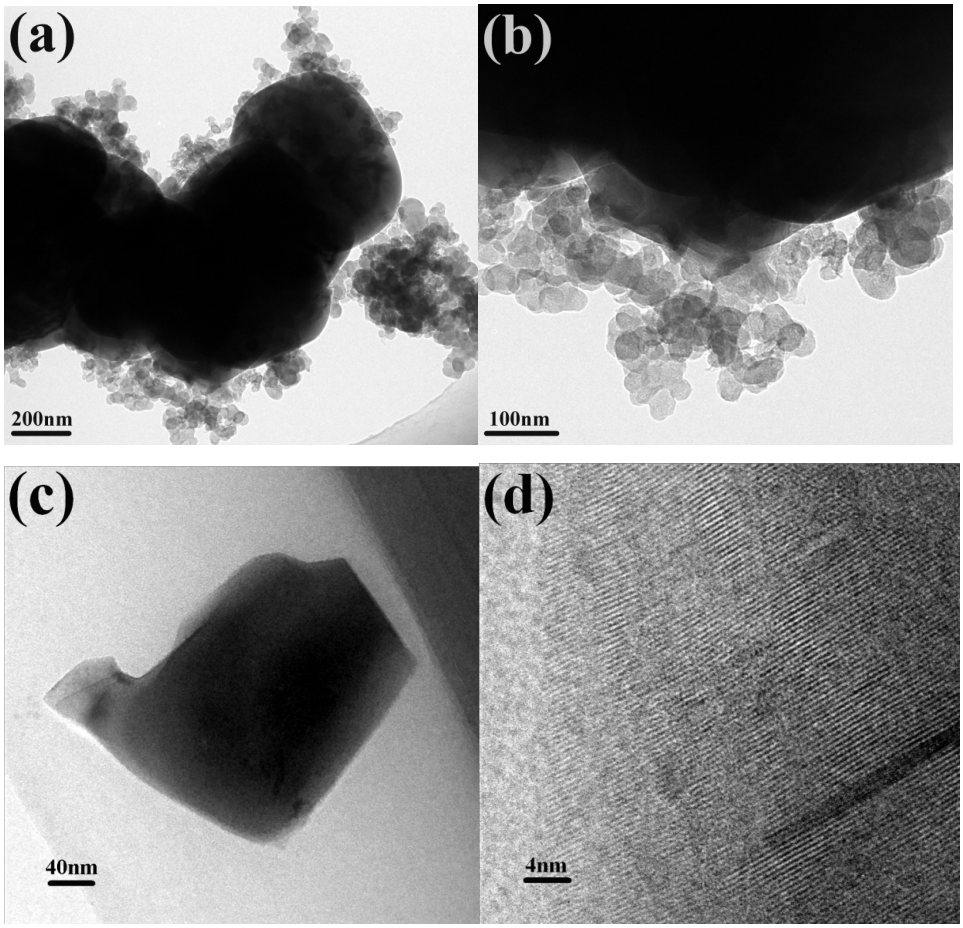

Figure S1. HRTEM images of $LiVPO_4F$ powder (a, b) and $Li_4Ti_5O_{12}$ powder (c, d).

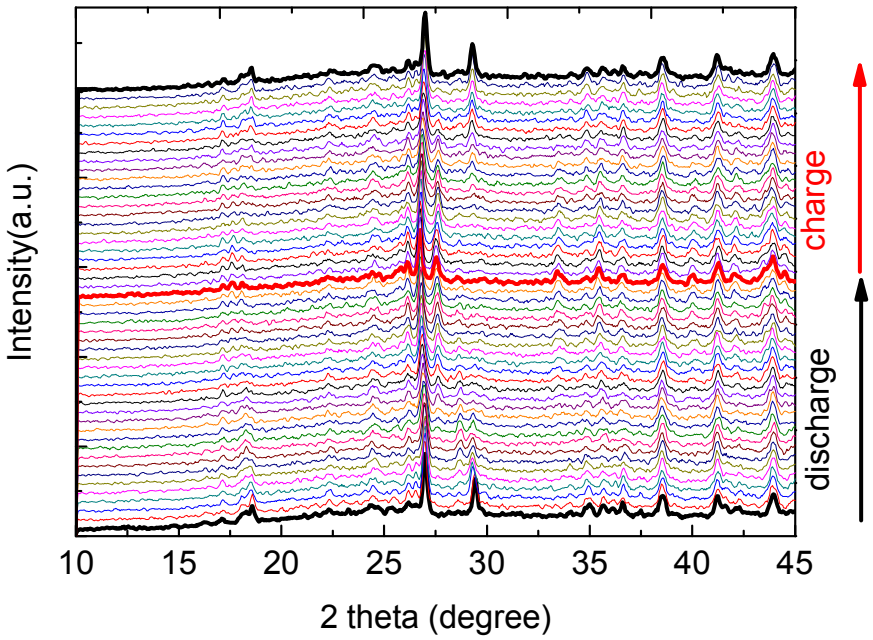

Figure S2. *In-situ* XRD patterns of $LiVPO_4F$ cycled in 1.0-3.0 V.

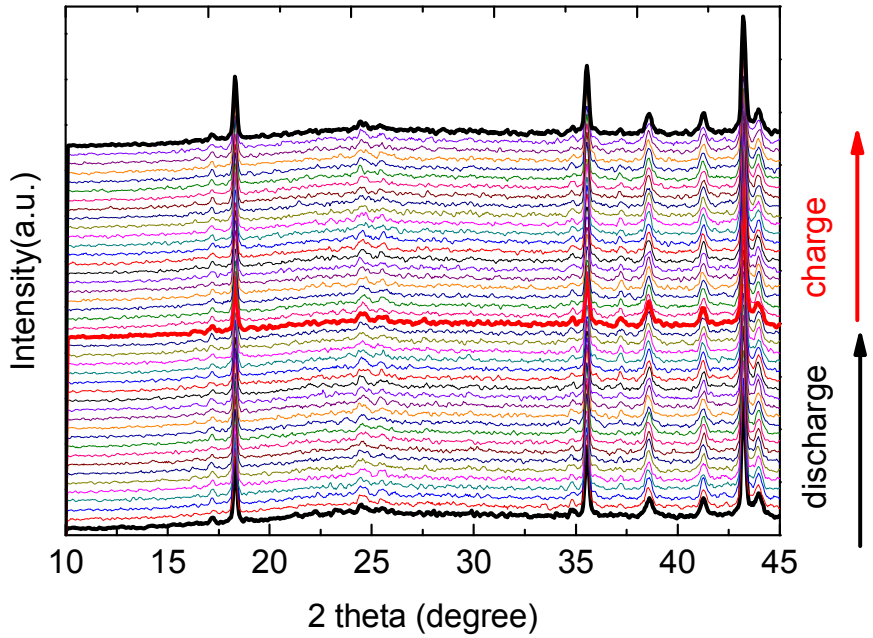

Figure S3. *In-situ* XRD patterns of $Li_4Ti_5O_{12}$ cycled in 1.0-3.0 V.

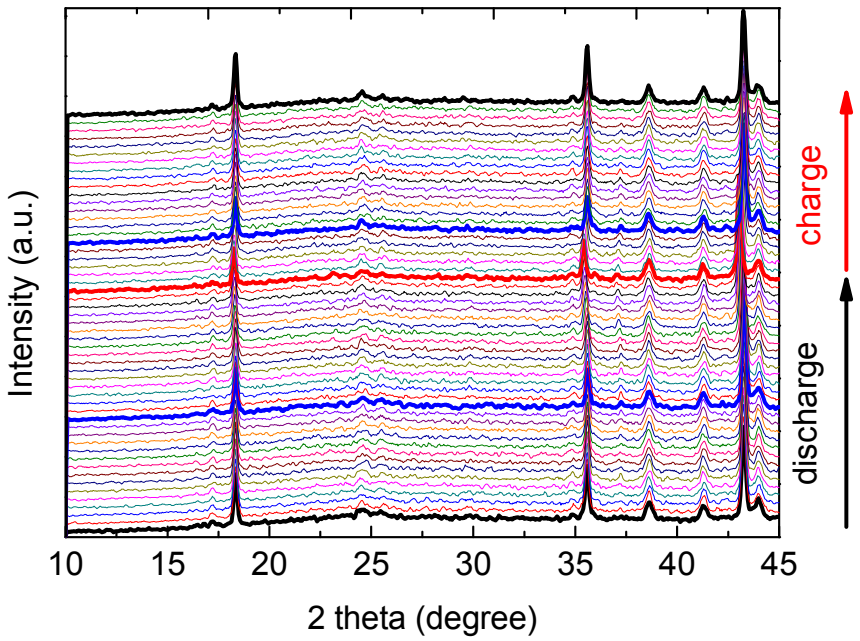

Figure S4. *In-situ* XRD patterns of $Li_4Ti_5O_{12}$ cycled in 0.0-3.0 V.

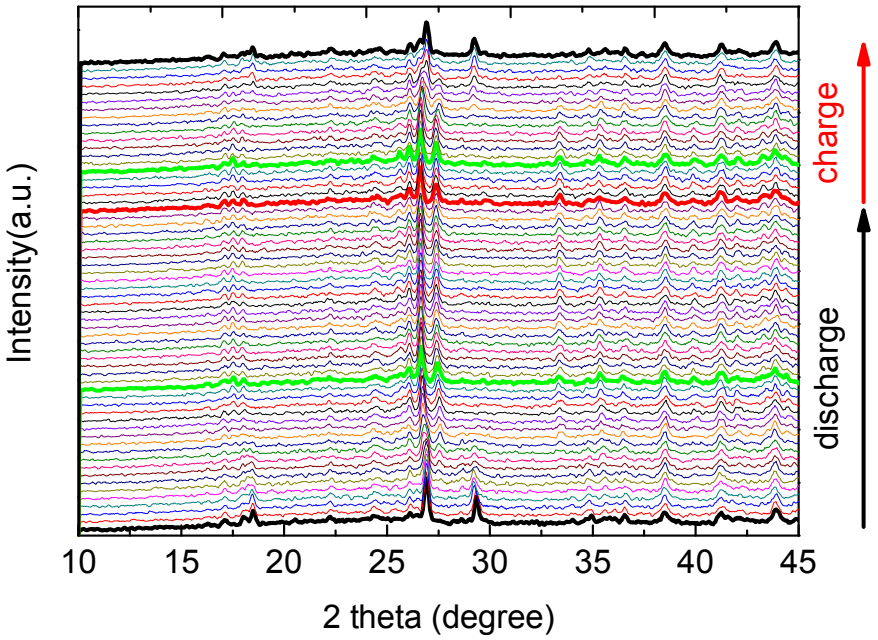

Figure S5. *In-situ* XRD patterns of $LiVPO_4F$ cycled in 0.0-3.0 V.