Electronic Supplementary Information (ESI)

Defect-free solvothermally assisted synthesis of microspherical mesoporous $LiFePO_4/C$

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The synthesis method of $LiFePO_4$ precursor using water solvent

Stoichiometric amounts of 0.028 mol lithium acetate hydrate ($CH_3COOLi \cdot 2H_2O$), iron(III) nitrate hydrate ($Fe(NO_3)_3 \cdot 9H_2O$), and phosphoric acid (85 wt.%, H_3PO_4) were dissolved in 40 mL distilled water. The mixture was stirred for 0.5 h and transferred to a 100 mL Teflon-lined autoclave. The autoclave was sealed and heated to 160 °C for 2 h. After cooling to room temperature, the precursor was obtained by filtration, washed with distilled water, and dried in air at 80 °C for 24 h.

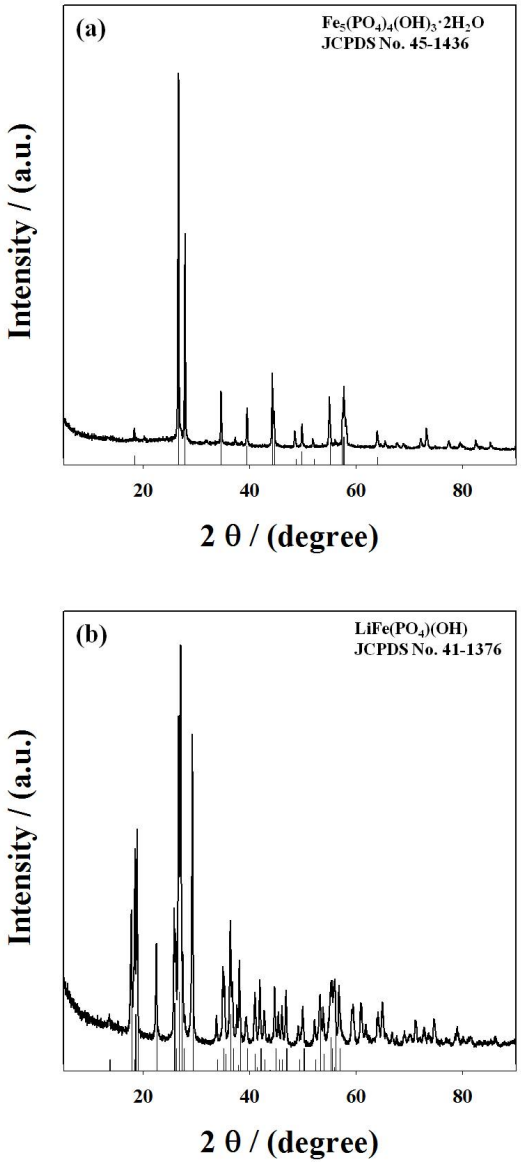

Fig. S1. XRD patterns of the precursors prepared using (a) water or (b) ethanol as the solvent.

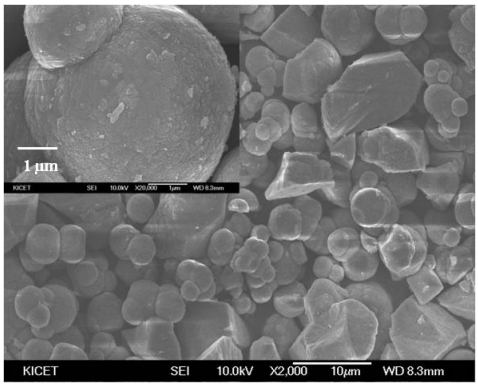

Fig. S2. FE-SEM imaging of the precursor prepared using water as the solvent.

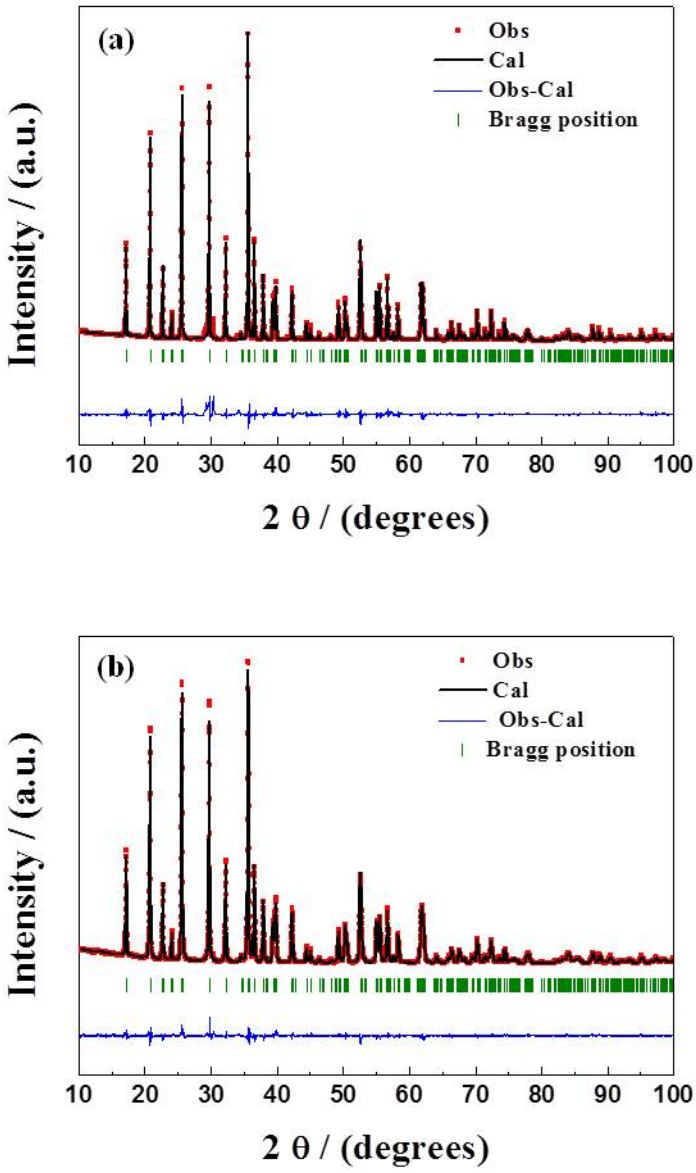

Fig. S3. Rietveld refinement of XRD spectra of (a) bare $LiFePO_4$ and (b) $LiFePO_4$/C. R-factors are R_p = 8.49%, R_I = 7.90%, R_F = 3.83% and S = 2.65 for bare $LiFePO_4$, and R_p = 4.67%, R_I = 8.02%, R_F = 1.70%, and S = 0.639 for $LiFePO_4$/C.

Table S1. Lattice parameters and Rietveld refinement results for bare $LiFePO_4$ and $LiFePO_4$/C

	a (Å)		b (Å)	c (Å)		Volume (Å^3)	Antisite defects (%)	
Bare $LiFePO_4$	10.321014(7)		6.001056(4)	4.687696(3)		290.3418	0.992	
	Atom	Site	Multiplicity	X	y	Z	Biso	Occupancy
	Li^{+1}	Li1	4	0	0	0	2.2(3)	0.495040(12)
	Fe^{+2}	Li1	4	0	0	0	2.2(3)	0.004960(12)
	P	P1	4	0.0950(2)	0.25000	0.4184(5)	1.38(7)	0.50000
	O^{-2}	O1	4	0.0968(6)	0.25000	0.7432(12)	1.68(15)	0.50000
	O^{-2}	O2	4	0.4573(7)	0.25000	0.2084(11)	1.27(15)	0.50000
	O^{-2}	O3	8	0.1639(5)	0.0483(7)	0.2829(7)	1.52(11)	1.00000
$LiFePO_4$/C	a (Å)		b (Å)	c (Å)		Volume (Å^3)	Antisite defects (%)	
	10.317427(8)		5.999850(4)	4.688508(4)		290.2328	0.990	
	Atom	Site	Multiplicity	x	y	z	Biso	Occupancy
	Li^{+1}	Li1	4	0	0	0	2.5(2)	0.495050(8)
	Fe^{+2}	Li1	4	0	0	0	2.5(2)	0.004950(8)
	P	P1	4	0.09525(16)	0.25000	0.4182(4)	1.37(5)	0.50000
	O^{-2}	O1	4	0.0950(4)	0.25000	0.7425(8)	1.34(10)	0.50000
	O^{-2}	O2	4	0.4565(4)	0.25000	0.2066(7)	1.11(9)	0.50000
	O^{-2}	O3	8	0.1645(3)	0.0486(4)	0.2853(4)	1.09(7)	1.00000

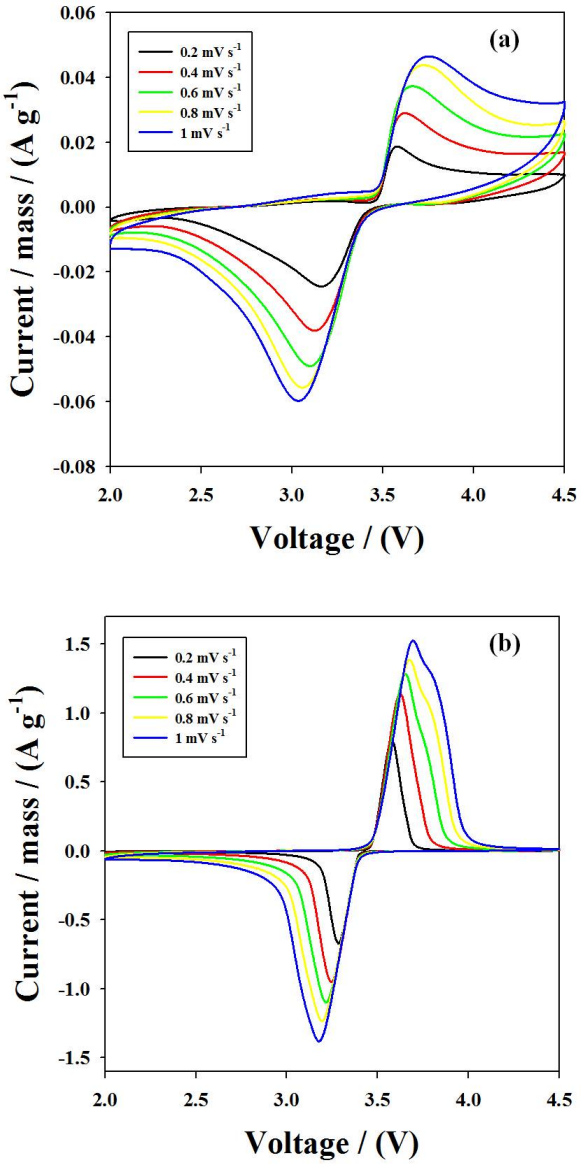

Fig. S4. Cyclic voltammograms for (a) bare $LiFePO_4$ and (b) $LiFePO_4$/C (scan rate: 0.2–1 mV s^{-1}, voltage range: 2.0–4.5 V).