

## Supporting Information

# Y-F co-doping behavior of LFP/Carbon nanocomposites for high-rate lithium-ion batteries.

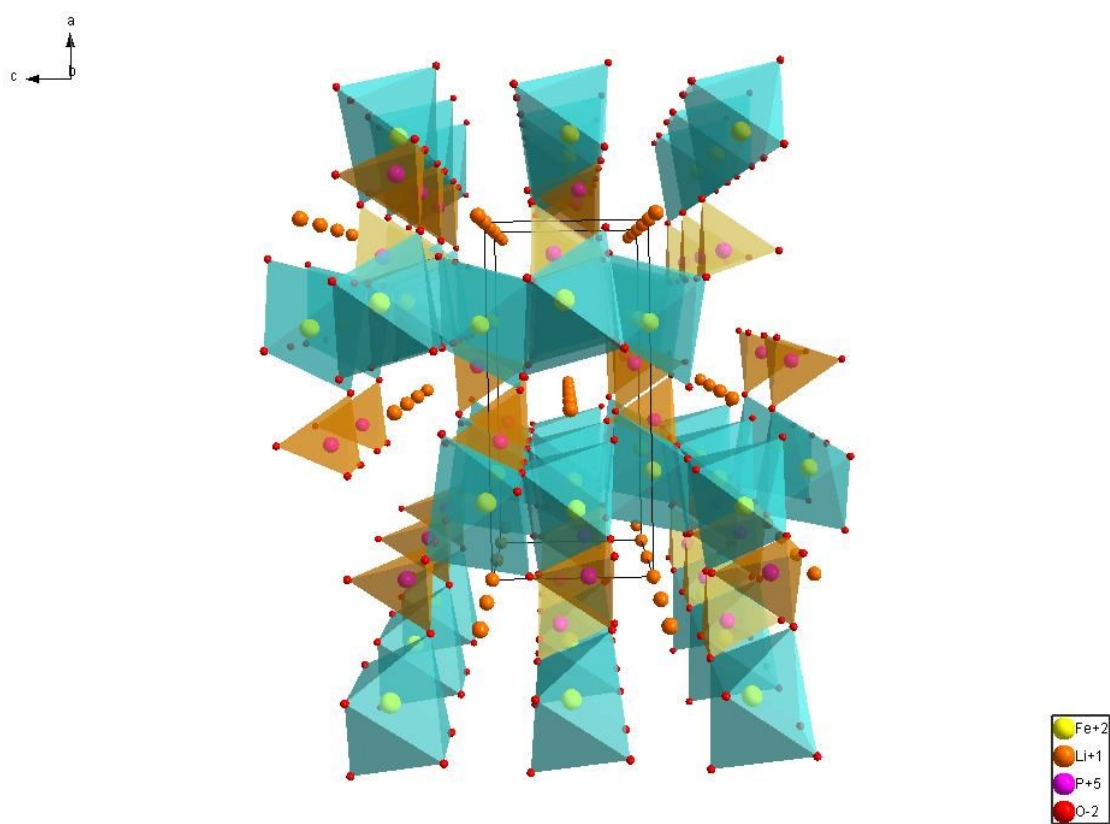


Fig. S1 Schematic diagram of the LFP structure along the b-axis (010) direction.

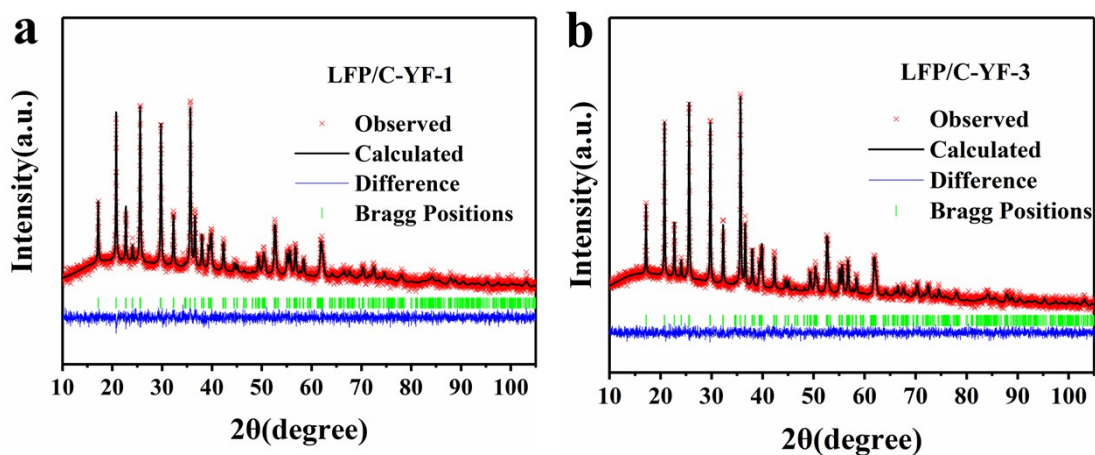


Fig. S2 XRD powder pattern (red points) and Rietveld fit (black lines) of a) LFP-YF-1 and b) LFP-YF-3.

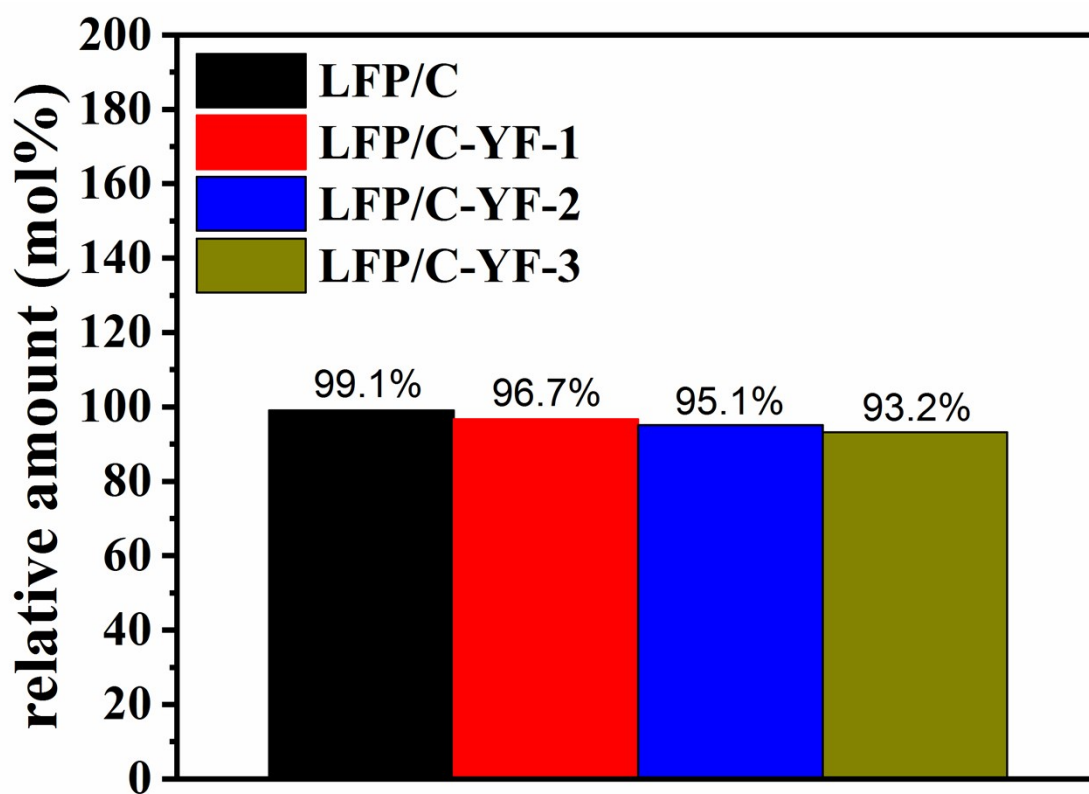


Fig. S3 ICP-OES plot of the molar percentage of Li of all samples.

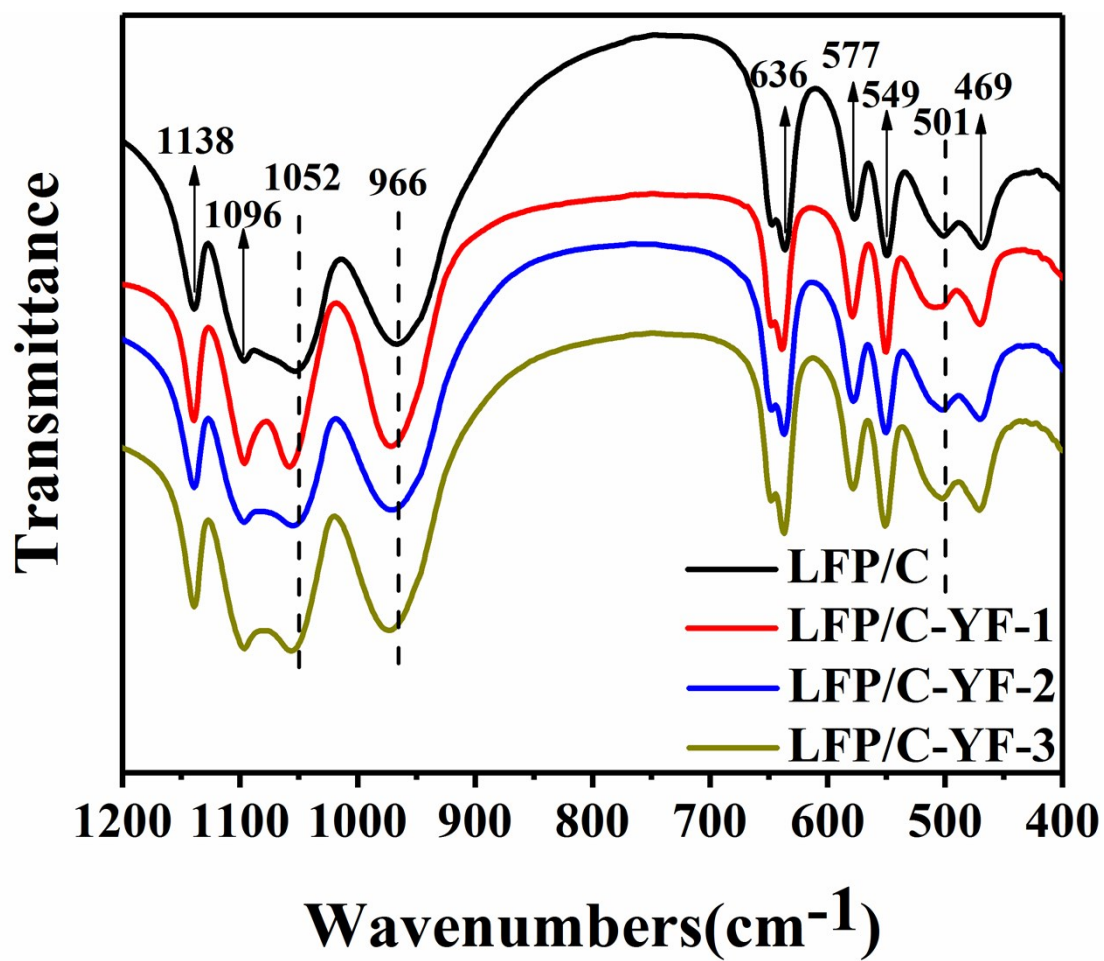


Fig. S4 FTIR spectrum of all the samples recorded in the wavenumber region of 400-1200 cm<sup>-1</sup>.

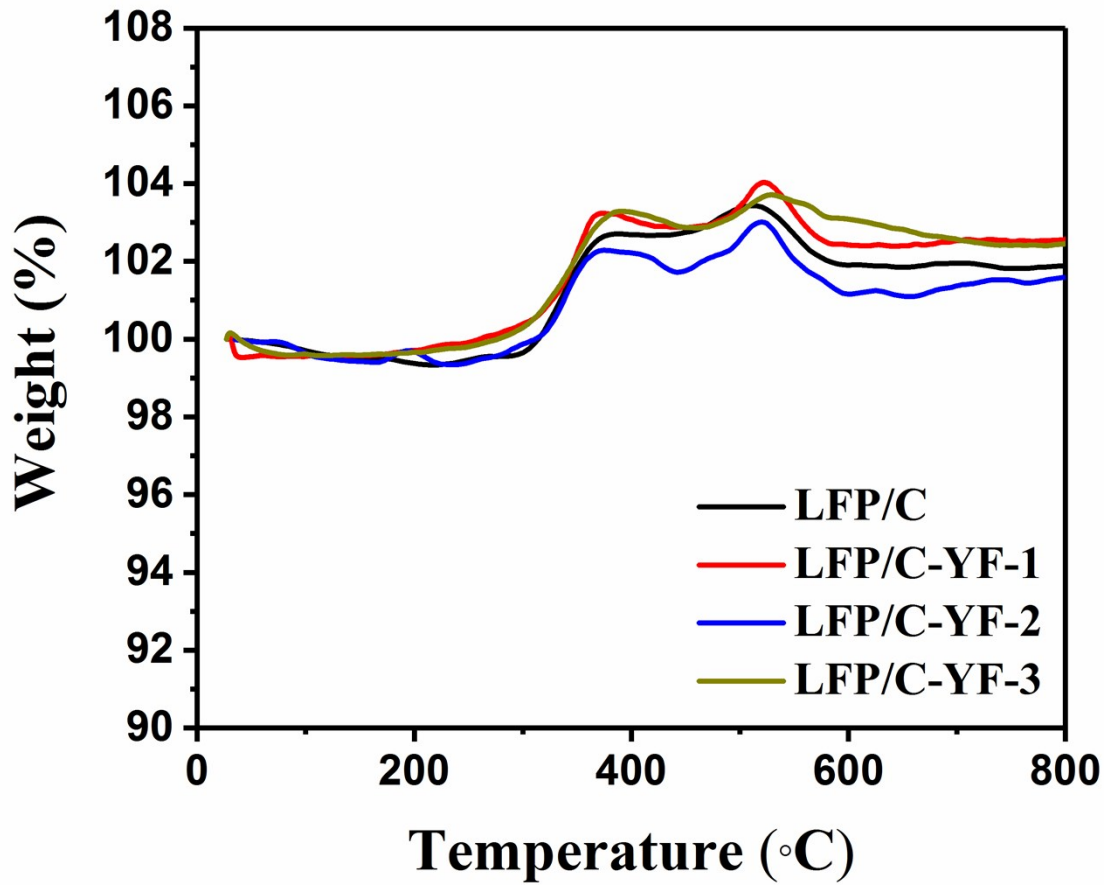


Fig. S5 TGA profiles of all the samples composites under air atmosphere with a heating rate of 10°C/min.

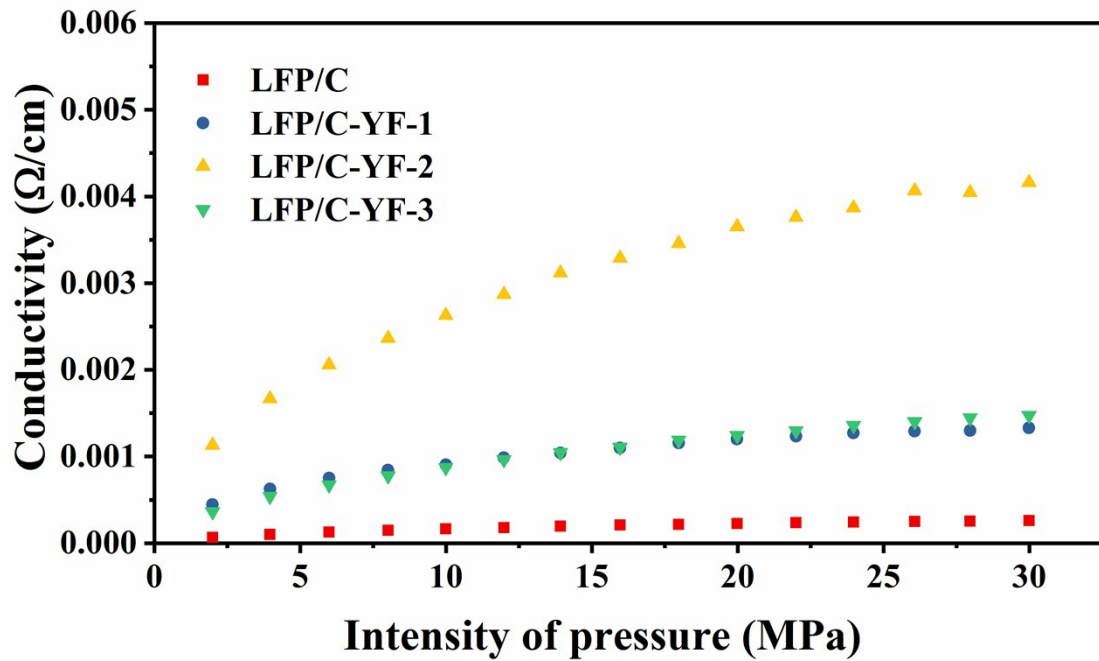


Fig. S6 The pressure-conductivity graph of all samples measured by the four-probe method.

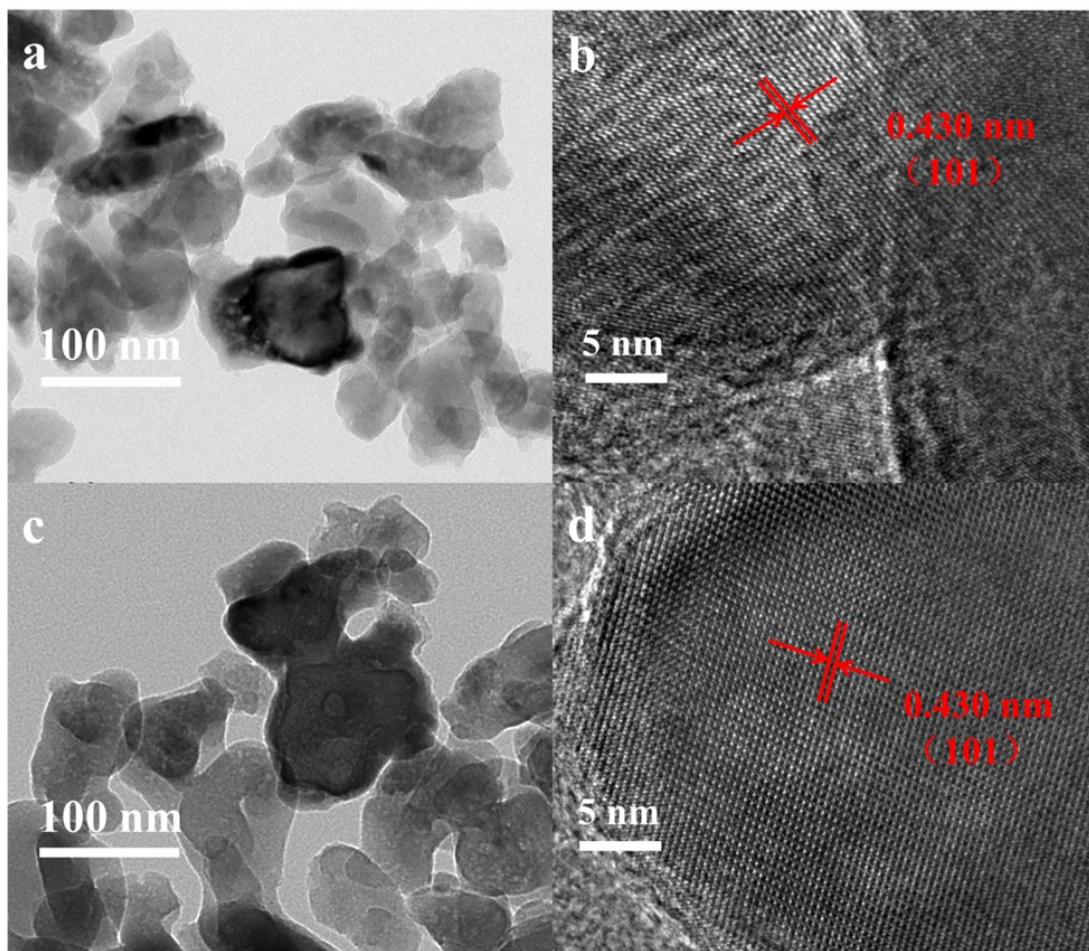


Fig. S7 TEM images and HRTEM images of a) b) LFP/C-YF-1 and c) d) LFP/C-YF-3.

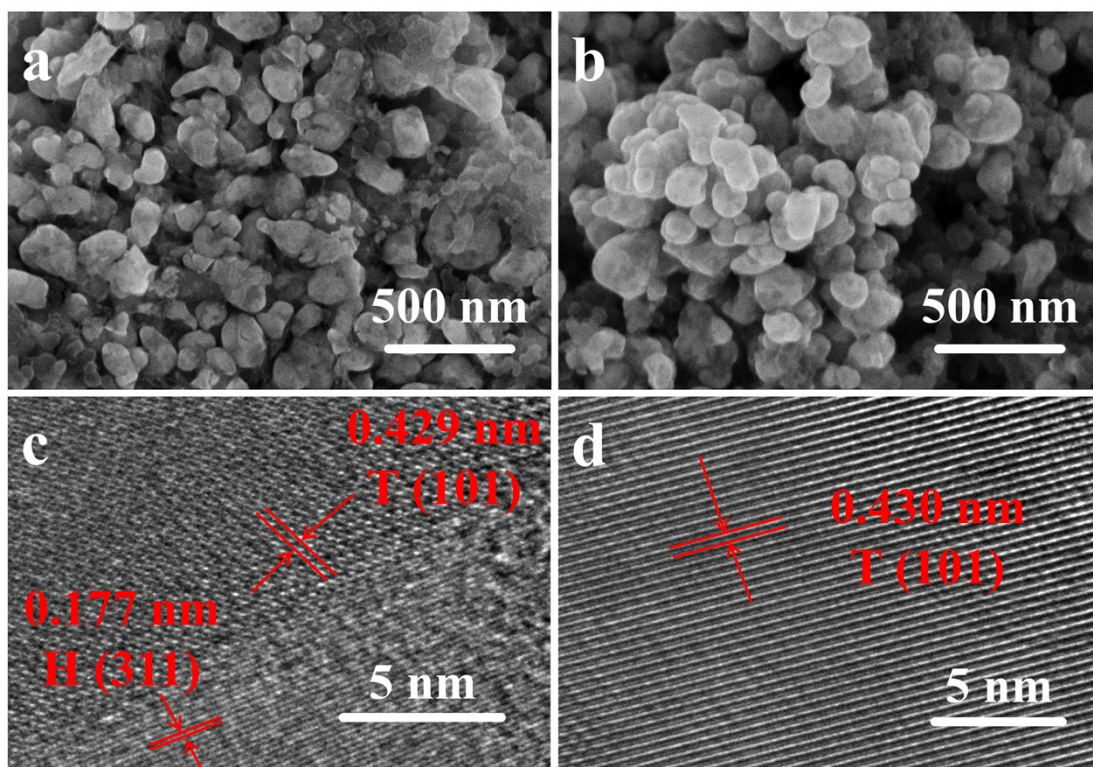


Fig. S8 SEM images and HRTEM images of a) c) LFP/C and b) d) LFP/C-YF-2 after 700 cycles at 5C.

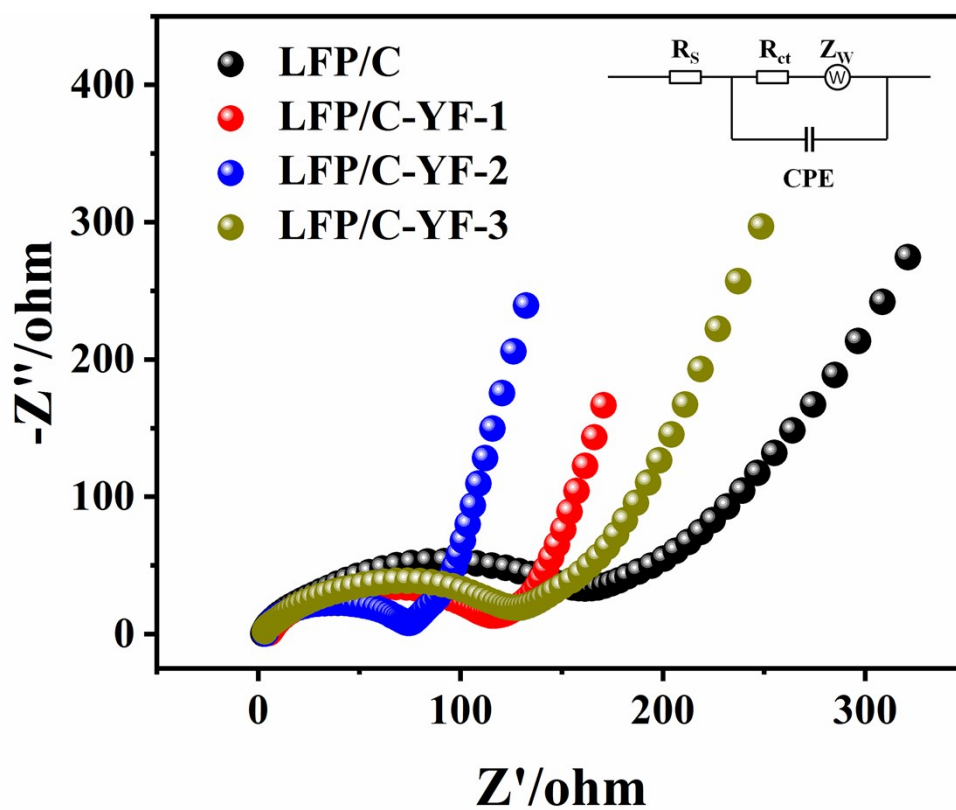


Fig. S9 Nyquist plots of all the samples with a frequency range of 0.1 Hz–100 kHz.

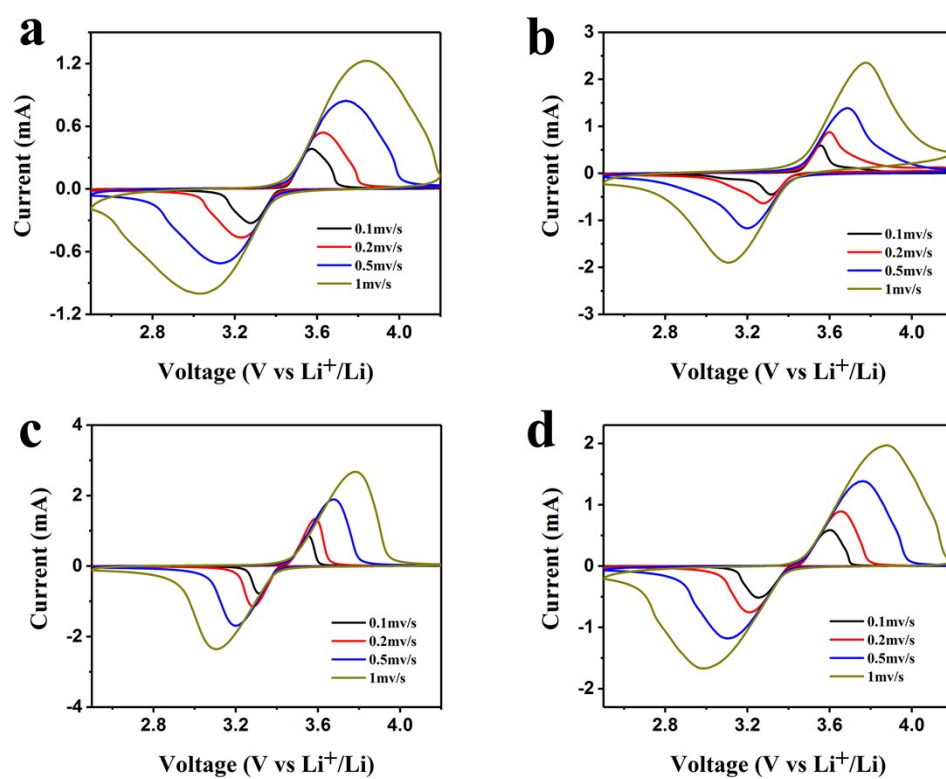


Fig. S10 the CV curves of a) LFP/C; b) LFP/C-YF-1; c) LFP/C-YF-2 and d) LFP/C-YF-3 composites at different scanning rates.

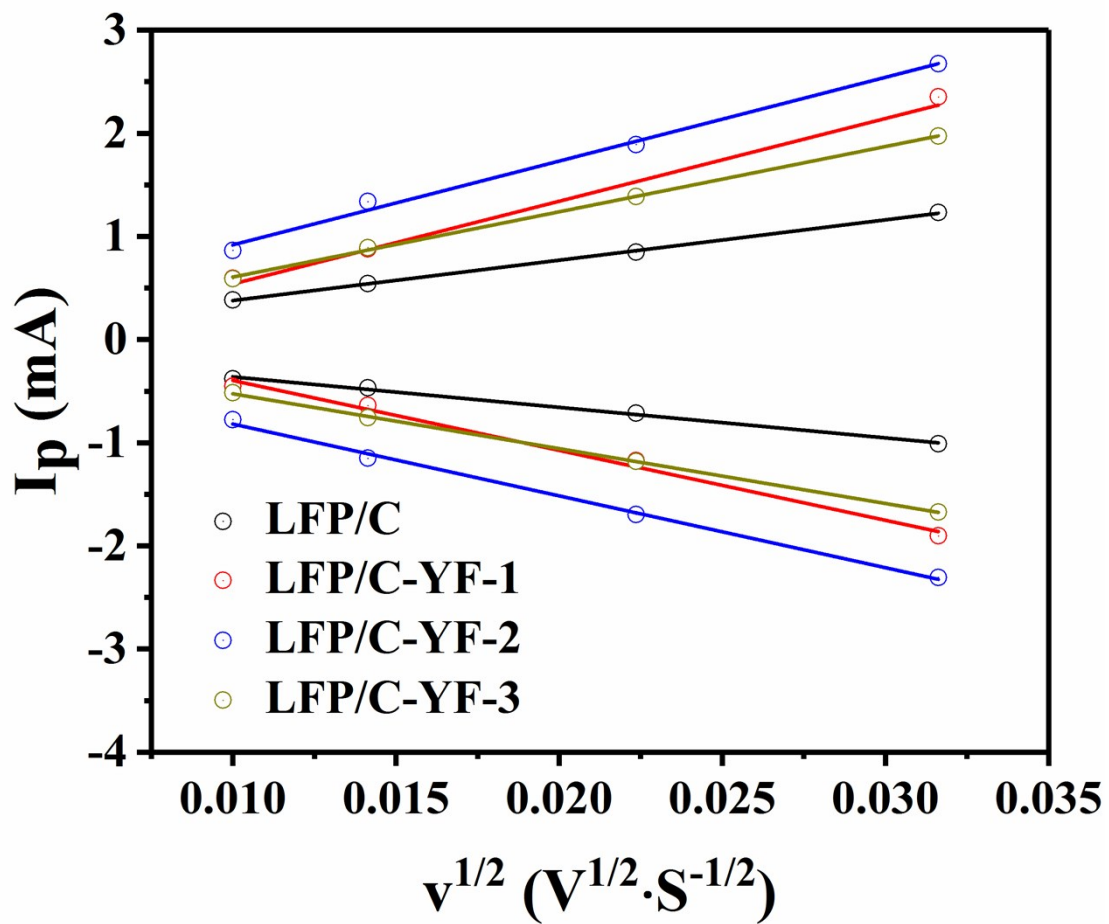


Fig. S11 relationship between the peak current and the square root of the scan rate.



Table S1 Selected bond lengths (in Å).

M-O bond	LFP/C	LFP/C-YF-1	LFP/C-YF-2	LFP/C-YF-3
Li-O(1)	2.1367	2.1794	2.1838	2.1678
Li-O(2)	2.0866	2.0947	2.0860	2.1178
Li-O(3)	2.1508	2.1891	2.1773	2.1891
ΣLi-O	2.1247	2.1544	2.1490	2.1582
P-O(1)	1.5311	1.5244	1.5141	1.5406
P-O(2)	1.5741	1.4859	1.5238	1.4646
P-O(3)	1.5188	1.5633	1.5712	1.5599
ΣP-O	1.5413	1.5245	1.5364	1.5217

Table S2 Calculated the Rs, Rct and DLi of all samples.

Sample	Rs/Ω	Rct/Ω	State	Slope	DLi/cm <sup>2</sup> ·s
LFP/C	2.2	143.5	Oxidation	39.10	5.08×10 <sup>-10</sup>
			Reduction	-29.58	2.91×10 <sup>-10</sup>
LFP/C-YF-1	5.2	99.1	Oxidation	80.22	1.70×10 <sup>-9</sup>
			Reduction	-67.75	1.22×10 <sup>-9</sup>
LFP/C-YF-2	3.4	57.2	Oxidation	81.22	2.26×10 <sup>-9</sup>
			Reduction	-69.64	1.66×10 <sup>-9</sup>
LFP/C-YF-3	2.1	113.1	Oxidation	63.30	8.89×10 <sup>-10</sup>
			Reduction	-57.17	7.25×10 <sup>-10</sup>

Table S3. LFP/C -related atomic occupancy information and calculation error value.

Sample	Atom	occupancy	x	y	z	Rwp	Rp	χ <sup>2</sup>
LFP/C	Li1	1	0	0	0	1.71%	1.36%	0.967
	Fe1	1	0.2821(5)	0.25	0.9744(5)			
	P1	1	0.0959(3)	0.25	0.4209(8)			
	O1	1	0.0918(2)	0.25	0.7470(4)			
	O2	1	0.4550(7)	0.25	0.2076(8)			
	O3	1	0.1609(5)	0.0501(6)	0.2838(4)			

Table S4 LFP/C-YF-1 -related atomic occupancy information and calculation error value.

Sample	Atom	occupancy	x	y	z	Rwp	Rp	χ <sup>2</sup>			
LFP/C-YF-1	Li1	1	0	0	0	1.77%	1.40%	1.022			
	Fe1	0.9948(6)	0.2822(1)	0.25	0.9737(6)						
	P1	1	0.0948(9)	0.25	0.4155(1)						
	O1	1	0.0979(5)	0.25	0.7404(6)						
	O2	0.9959(8)	0.4607(3)	0.25	0.2003(9)						
	O3	1	0.1665(5)	0.0445(8)	0.2840(1)						
	Y1	0.0051(3)	Fe1 occ. By Y1						0.0051(3)		
	F1	0.0040(2)	O2 occ. By F1						0.0040(2)		

Table S5 LFP/C-YF-2 -related atomic occupancy information and calculation error value.

Sample	Atom	occupancy	x	y	z	Rwp	Rp	$\chi^2$
LFP/C-YF-2	Li1	1	0	0	0	1.78%	1.43%	1.037
	Fe1	0.9934(8)	0.2823(5)	0.25	0.9749(6)			
	P1	1	0.0939(3)	0.25	0.4170(1)			
	O1	1	0.0986(4)	0.25	0.7398(4)			
	O2	0.9909(5)	0.4570(2)	0.25	0.2054(5)			
	O3	1	0.1658(9)	0.0446(5)	0.2818(1)			
	Y1	0.0065(1)	Fe1 occ. By Y1			0.0065(1)		
	F1	0.0090(4)	O2 occ. By F1			0.0090(4)		

Table S6 LFP/C-YF-3 -related atomic occupancy information and calculation error value.

Sample	Atom	occupancy	x	y	z	Rwp	Rp	$\chi^2$
LFP/C-YF-3	Li1	1	0	0	0	1.75%	1.39%	1.017
	Fe1	0.9878(6)	0.2821(8)	0.25	0.9746(3)			
	P1	1	0.0957(3)	0.25	0.4161(2)			
	O1	1	0.0972(1)	0.25	0.7435(1)			
	O2	0.9896(8)	0.4633(7)	0.25	0.1914(4)			
	O3	1	0.1666(1)	0.0444(1)	0.2839(3)			
	Y1	0.0121(3)	Fe1 occ. By Y1			0.0121(3))		
	F1	0.0103(1)	O2 occ. By F1			0.0103(1)		

Table S7 The ICP analysis of LFP/C and LFP/C-YF-2composites after cycling, respectively (fully charged/discharge).

samples	Percentage of lithium in LiFePO <sub>4</sub> /mol/% (after 700 cycles)	
	charge	discharge
LFP/C	13.46	78.72
LFP/C-YF-2	11.36	96.88