Supporting information

Improvement of the electrochemical performance by partial chemical substitution into the lithium site of titanium phosphate-based electrode materials for lithium-ion batteries: $LiNi_{0.25}Ti_{1.5}Fe_{0.5}(PO_4)_3$

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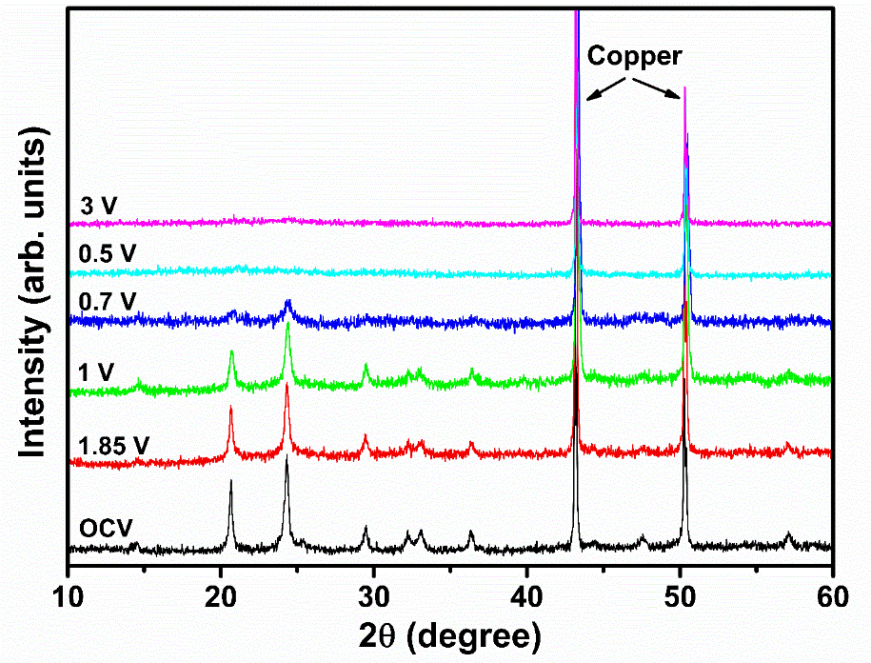

Figure SI-1: Ex-situ XRD patterns of the LNFTP electrodes at different states of charge

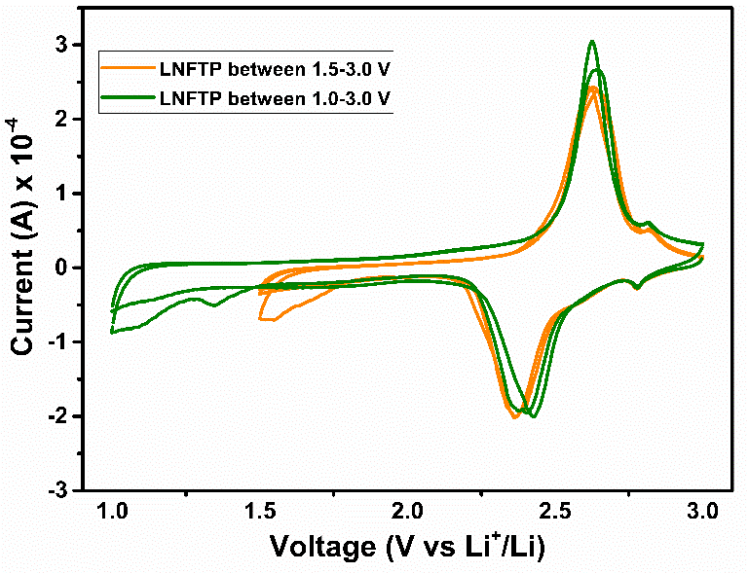

Figure SI-2: CV curves of the LNFTP at both voltage ranges 1.5-3.0 V and 1.0-3.0 V measured at slow scan rates of 0.02 mV/s

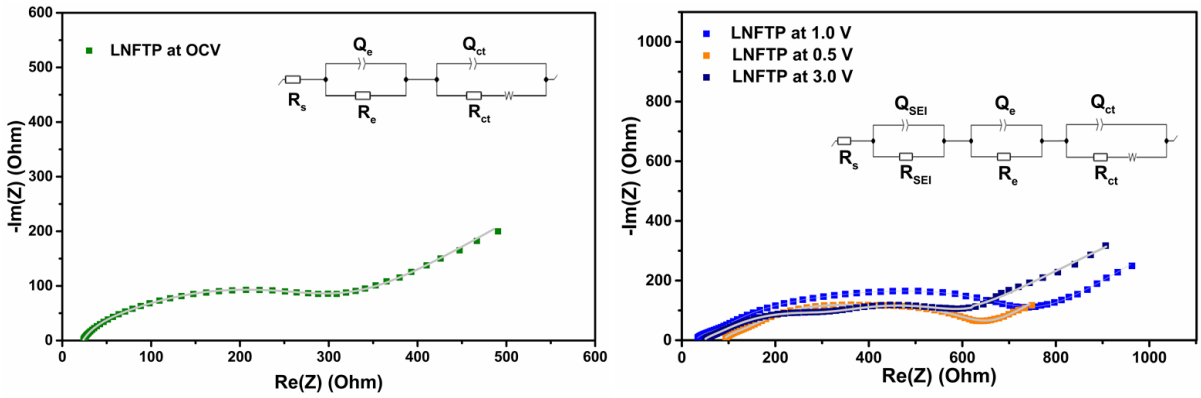

Figure SI-3: Nyquist plots of the LNFTP@C material at different states of discharge/charge: at the OCV (left) at 1.0V, 0.5V and 3.0V (right).

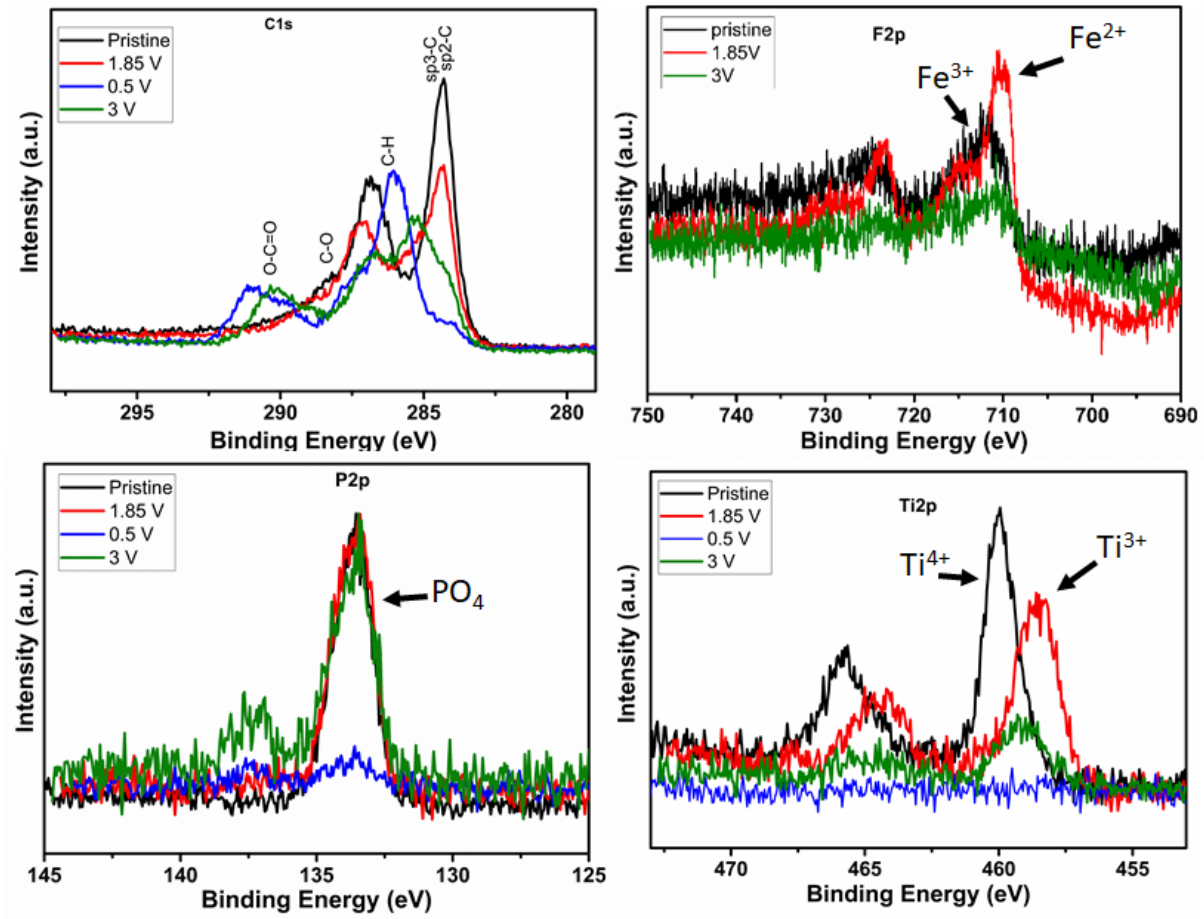

Figure SI-4: XPS data of C1s, F2p, Ti2p and P2p at different states of charge

Table SI-1: Atomic positions of the LNFTP material obtained via Rietveld Refinement

LNFTP	Atoms	x	y	z	B	Occ.	Mult
R-3c	Ni	0.0000	0.0000	0.0000	1	0.5	6
	Li1	0.0000	0.0000	0.0000	1	0.5	6
	Li2	0.5962(4)	0	0.25	1	0.25	18
	Fe	0.0000	0.0000	0.1394(2)	1.08(1)	0.5	12
	Ti	0.00000	0.0000	0. 1394(2)	1.08(1)	1.5	12
	P	0.2906(6)	0.0000	0.25000	3.2(2)	3.0	18
	O1	0.1754(8)	-0.0195(9)	0.1892(4)	1.9 (2)	6.0	36
	O2	0.1915(8)	0.1688(5)	0.0809(5)	1	6.0	36
Rp: 9.11 %			**Rwp: 8.14 %**				

Table SI-2: Calculated interatomic distances (Å) of the LNFTP material

(M)-(O)	d (Å)
(Li1)-(O2) <Li-O>	2.28(9) x6 2.28
(Ni)-(O2) <Ni-O>	2.28(9) x6 2.28
(Li2)-(O1) (Li2)-(O1) (Li2)-(O2) (Li2)-(O2) <Li-O>	3.103(9) x2 2.429(8) x2 2.112(7) x2 2.397(5) x2 2.5103
(Fe)-(O1) (Fe)-(O2)	1.889(8) x3 1.963(9) x3
(Ti)-(O1) (Ti)-(O2) <Fe,Ti-O>	1.889(8) x3 1.963(9) x3 1.926
(P)-(O1) (P)-(O2) <P-O>	1. 556(9) x2 1. 493(7) x2 1.5245

Table SI-3:R value of the fitted Nyquist curves of the carbon coated LNFTP@C electrode at different states of charge/discharge

	R_s	R_{SEI}	R_e	R_{ct}
OCV	23.1	-	46.7	240.4
1.0 V	28.8	352.5	38.7	307.8
0.5 V	87.3	247	53	255
3.0 V	46.2	247.3	43.8	236.1