Supporting Information

$Li_4Ti_5O_{12}$-based anode materials with low working potentials, high rate capabilities and high cyclability for high-power lithium-ion batteries: synergistic effect of doping, incorporating a conductive phase and reducing particle size

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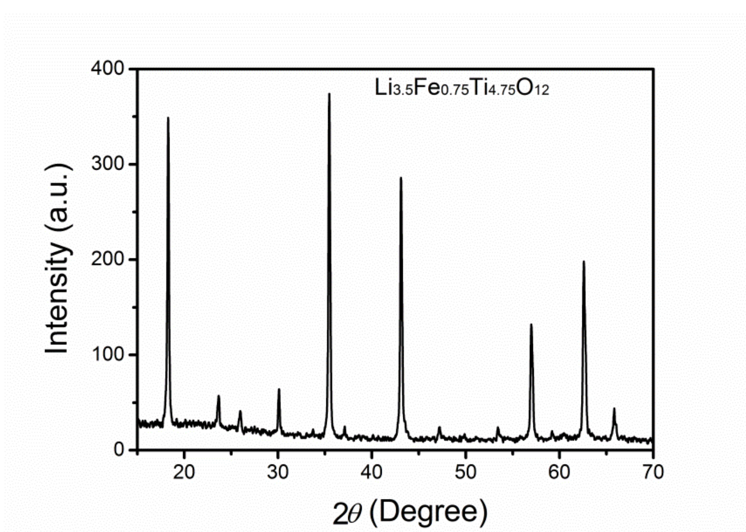

Fig. S1 X-ray diffraction pattern of $Li_{3.5}Fe_{0.75}Ti_{4.75}O_{12}$.

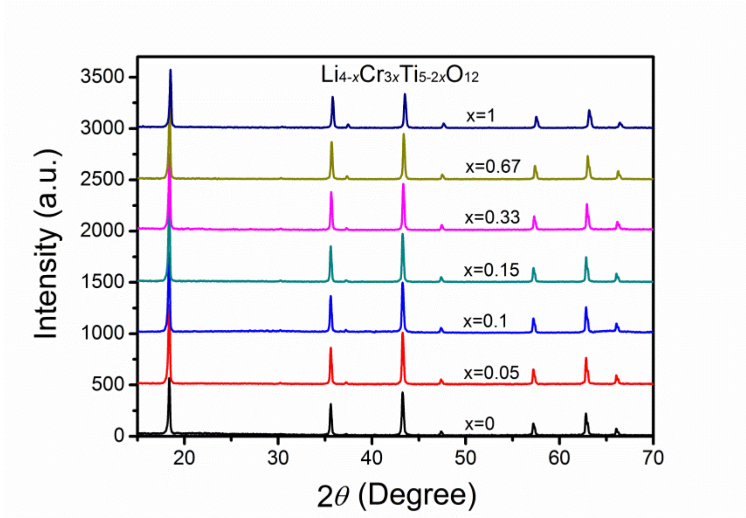

Fig. S2 X-ray diffraction patterns of $Li_{4-x}Cr_{3x}Ti_{5-2x}O_{12}$ ($0 \leq x \leq 1$).

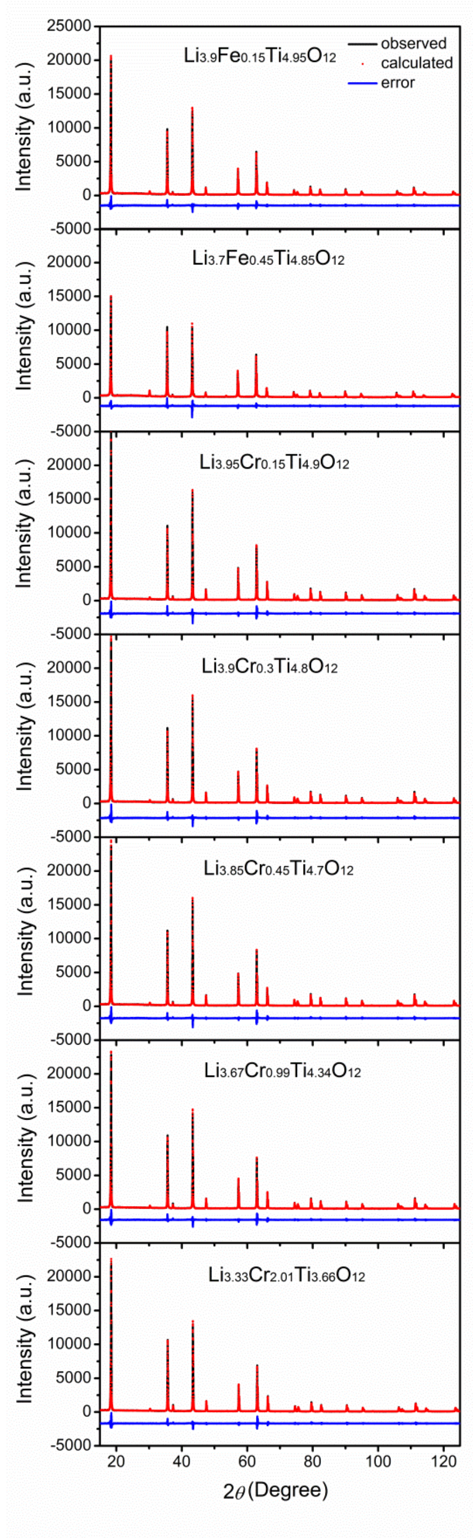

Fig. S3 Rietveld refinement plots of the X-ray diffraction patterns for $Li_{3.9}Fe_{0.15}Ti_{4.95}O_{12}$, $Li_{3.7}Fe_{0.45}Ti_{4.85}O_{12}$, $Li_{3.95}Cr_{0.15}Ti_{4.9}O_{12}$, $Li_{3.9}Cr_{0.3}Ti_{4.8}O_{12}$, $Li_{3.85}Cr_{0.45}Ti_{4.7}O_{12}$, $Li_{3.67}Cr_{0.99}Ti_{4.34}O_{12}$ and $Li_{3.33}Cr_{2.01}Ti_{3.66}O_{12}$.

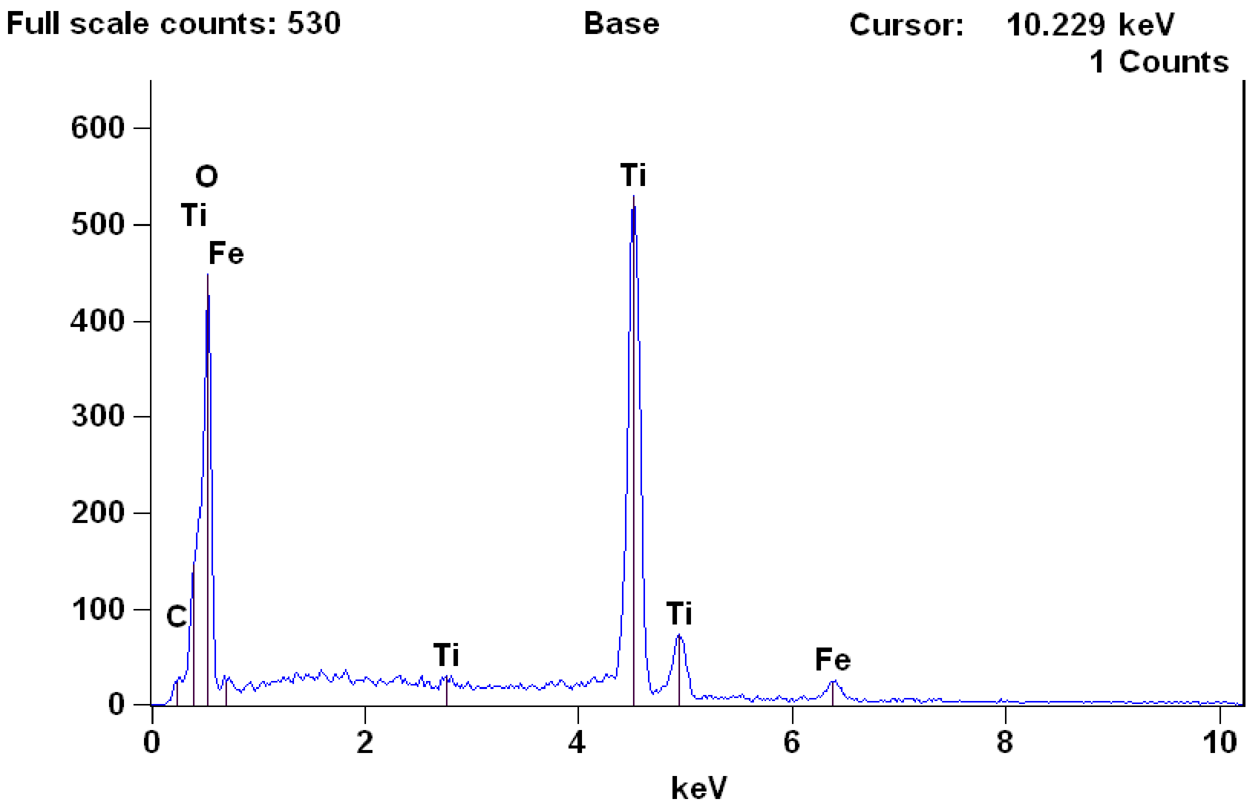

Fig. S4 Energy-dispersive X-ray analysis of $Li_{3.7}Fe_{0.45}Ti_{4.85}O_{12}$ collected from an energy-dispersive X-ray analyzer (NORAN NSS202E). The obvious C peak shows the existence of carbon created in the synthesis of Fe^{2+} doped LTO.

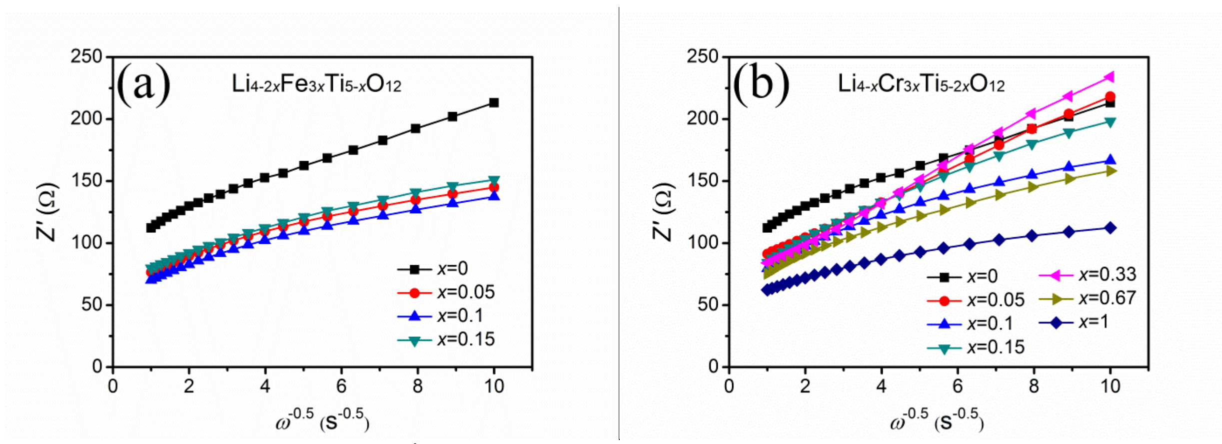

Fig. S5 Relationships between Z' and $\omega^{-0.5}$ of (a) $Li_{4-2x}Fe_{3x}Ti_{5-x}O_{12}$ ($0 \le x \le 0.15$) and $Li_{4-x}Cr_{3x}Ti_{5-2x}O_{12}$ ($0 \le x \le 1$) electrodes at low frequencies.

Table S1 Rietveld refinement results of the X-ray diffraction patterns for $Li_{4-2x}Fe_{3x}Ti_{5-x}O_{12}$ ($0 \leq x \leq 0.15$) and $Li_{4-x}Cr_{3x}Ti_{5-2x}O_{12}$ ($0 \leq x \leq 1$).

Spinel $Li_{4-2x}Fe_{3x}Ti_{5-x}O_{12}$, space group: $Fd\bar{3}m$(cubic)							Spinel $Li_{4-x}Cr_{3x}Ti_{5-2x}O_{12}$, space group: $Fd\bar{3}m$(cubic)					
Composition		x	0	0.05	0.1	0.15	0.05	0.1	0.15	0.33	0.67	1
Nominal composition			$[Li_{2.997}Ti_{0.003}]_{8a}[Li_{1.003}Ti_{4.997}]_{16d}[O_{12}]_{32e}$	$[Li_{2.855}Ti_{0.145}]_{8a}[Li_{1.045}Fe_{0.15}Ti_{4.805}]_{16d}[O_{12}]_{32e}$	$[Li_{2.663}Ti_{0.337}]_{8a}[Li_{1.137}Fe_{0.3}Ti_{4.563}]_{16d}[O_{12}]_{32e}$	$[Li_{2.470}Ti_{0.530}]_{8a}[Li_{1.230}Fe_{0.45}Ti_{4.320}]_{16d}[O_{12}]_{32e}$	$[Li_{2.994}Ti_{0.006}]_{8a}[Li_{0.956}Cr_{0.15}Ti_{4.894}]_{16d}[O_{12}]_{32e}$	$[Li_{2.985}Ti_{0.015}]_{8a}[Li_{0.915}Cr_{0.3}Ti_{4.785}]_{16d}[O_{12}]_{32e}$	$[Li_{2.960}Ti_{0.040}]_{8a}[Li_{0.890}Cr_{0.45}Ti_{4.660}]_{16d}[O_{12}]_{32e}$	$[Li_{2.931}Ti_{0.069}]_{8a}[Li_{0.739}Cr_{0.99}Ti_{4.271}]_{16d}[O_{12}]_{32e}$	$[Li_{2.896}Ti_{0.104}]_{8a}[Li_{0.434}Cr_{2.01}Ti_{3.556}]_{16d}[O_{12}]_{32e}$	$[Li_{2.828}Ti_{0.172}]_{8a}[Li_{0.172}Cr_{3}Ti_{2.828}]_{16d}[O_{12}]_{32e}$
Lattice parameter		a (Å)	8.36122(3)	8.36535(4)	8.36974(4)	8.37460(4)	8.35922(3)	8.35763(3)	8.35616(3)	8.34972(3)	8.33761(3)	8.32699(4)
8a	Li1		0.999(1)	0.952(1)	0.888(1)	0.823(1)	0.998(1)	0.995(1)	0.987(1)	0.977(1)	0.965(1)	0.943(1)
	Ti1		0.001(1)	0.048(1)	0.112(1)	0.177(2)	0.002(1)	0.005(1)	0.013(1)	0.023(1)	0.035(1)	0.057(1)
16d	Li2		0.167(1)	0.174(1)	0.190(1)	0.205(1)	0.159(1)	0.153(1)	0.148(1)	0.123(1)	0.072(1)	0.029(1)
	Ti2	f	0.833(1)	0.801(1)	0.760(1)	0.720(1)	0.816(1)	0.797(1)	0.777(1)	0.712(1)	0.593(1)	0.471(1)
	Fe/Cr		–	0.025(–)	0.05(–)	0.075(–)	0.025(–)	0.05(–)	0.075(–)	0.165(–)	0.335(–)	0.5(–)
32e	O		1(–)	1(–)	1(–)	1(–)	1(–)	1(–)	1(–)	1(–)	1(–)	1(–)
		z	0.26301(7)	0.26296(6)	0.26294(6)	0.26291(7)	0.26297(7)	0.26291(6)	0.26287(7)	0.26279(7)	0.26259(7)	0.26249(7)
R_{wp}			0.1029	0.0953	0.0894	0.0908	0.1030	0.1010	0.1013	0.0995	0.0988	0.0933
R_p			0.0787	0.0744	0.0689	0.0689	0.0787	0.0768	0.0774	0.0760	0.0762	0.0712
χ^2			3.005	2.598	2.271	2.348	3.002	2.896	2.886	2.665	2.589	2.313

f: site occupancy, z: fractional coefficient, R_{wp}: weighted profile residual, R_p: profile residual, and χ^2: goodness of fit.

Table S2 Properties of all the samples.

Sample	Specific surface area (m_2 g^{-1})	R_s (Ω)	R_{ct} (Ω)	σ_w ($\Omega\cdot s^{-0.5}$)	D ($cm^2\cdot s^{-1}$)	Electronic conductivity ($S\cdot cm^{-1}$)	Discharge potential at 0.1 C (mV)	Charge potential at 0.1 C (mV)	Working potential at 0.1 C (mV)	Capacity at 0.5 C (mAh g^{-1})	Capacity at 1 C (mAh g^{-1})	Capacity at 2 C (mAh g^{-1})	Capacity at 5 C (mAh g^{-1})	Capacity at 10 C (mAh g^{-1})	Capacity retention over 200 cycles (%)
$Li_4Ti_5O_{12}$	3.6	3.23	89.3	10.9	5.74×10^{-15}	$<1\times10^{-9}$	1555.9	1574.8	1565.4	166	143	105	33	11	–
$Li_{3.9}Fe_{0.15}Ti_{4.95}O_{12}$	4.4	2.68	62.5	7.78	8.11×10^{-15}	1.9×10^{-8}	1539.2	1583.5	1561.4	161	151	131	82	39	–
$Li_{3.8}Fe_{0.3}Ti_{4.9}O_{12}$	4.0	3.66	58.8	7.58	1.14×10^{-14}	8.9×10^{-8}	1531.4	1581.4	1556.4	152	148	137	100	57	–
$Li_{3.7}Fe_{0.45}Ti_{4.85}O_{12}$	4.3	3.00	64.4	8.22	6.89×10^{-15}	1.7×10^{-7}	1523.4	1578.0	1550.7	149	136	104	61	36	–
$Li_{3.95}Cr_{0.15}Ti_{4.9}O_{12}$	2.6	2.85	81.6	14.4	6.37×10^{-15}	3.4×10^{-8}	1550.7	1574.2	1562.5	158	136	101	50	21	–
$Li_{3.9}Cr_{0.3}Ti_{4.8}O_{12}$	2.4	2.44	62.8	9.87	1.63×10^{-14}	4.7×10^{-8}	1548.8	1571.8	1560.3	154	134	104	58	25	–
$Li_{3.85}Cr_{0.45}Ti_{4.7}O_{12}$	2.0	2.35	65.4	12.9	1.30×10^{-14}	5.5×10^{-8}	1546.6	1570.8	1558.7	147	128	97	43	17	–
$Li_{3.67}Cr_{0.99}Ti_{4.34}O_{12}$	1.9	2.81	74.0	17.3	8.37×10^{-15}	6.7×10^{-8}	1536.1	1566.8	1551.5	145	126	94	47	20	–
$Li_{3.33}Cr_{2.01}Ti_{3.66}O_{12}$	1.9	2.82	61.8	9.23	2.92×10^{-14}	1.1×10^{-7}	1517.5	1552.8	1535.2	141	132	118	83	42	–
$LiCrTiO_4$	2.5	3.96	51.5	5.77	4.25×10^{-14}	1.3×10^{-7}	1503.5	1544.5	1524.0	138	129	118	97	70	–
$Li_{3.8}Fe_{0.3}Ti_{4.9}O_{12}$/MWCNTs	–	–	–	–	–	–	1534.9	1578.0	1556.5	158	154	148	130	106	117
$LiCrTiO_4$/MWCNTs-post	–	–	–	–	–	–	1507.0	1535.9	1521.5	141	137	131	120	106	94.6
$LiCrTiO_4$/MWCNTs	–	–	–	–	–	–	1508.5	1529.9	1519.2	140	137	133	128	120	95.9

Table S3 Electronic conductivities of LTO materials using different dopings, all of which were measured using the same two-probe method [12,13].

Nominal formula	$Li_4Ti_5O_{12}$	$Li_{3.7}Fe_{0.45}Ti_{4.85}O_{12}$	$LiCrTiO_4$	$Li_{3.95}Co_{0.15}Ti_{4.9}O_{12}$	$Li_{3.95}Al_{0.15}Ti_{4.9}O_{12}$	$Li_4Ta_{0.05}Ti_{4.95}O_{12}$	$Li_{3.95}Ga_{0.15}Ti_{4.9}O_{12}$	$Li_{3.9}Mg_{0.1}Al_{0.15}Ti_{4.85}O_{12}$
Electronic conductivity (S cm^{-1})	$<1\times10^{-9}$	1.7×10^{-7}	1.2×10^{-7}	1.3×10^{-9}	1.1×10^{-8}	1.0×10^{-9}	2.0×10^{-9}	7.9×10^{-9}