Electronic Supplementary Information

Y-doped P2-$Na_{0.6}Li_{0.11}Fe_{0.27}Mn_{0.62}O_2$ cathode with improved high-rate capability and cycling stability for Na-ion batteries

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Table S1. Stoichiometry from inductively coupled plasma-atomic emission spectrometry (ICP-AES) results of NLFM.

Elements	Content(mg/kg)	mol ratio
Na	13.70	0.59(7)
Li	0.76	0.10(8)
Fe	15.28	0.27(4)
Mn	34.10	0.61(8)

Table S2. Stoichiometry from inductively coupled plasma-atomic emission spectrometry (ICP-AES) results of NLFMY-1.

Elements	Content(mg/kg)	mol ratio
Na	13.68	0.59(5)
Li	0.77	0.10(9)
Fe	14.96	0.26(7)
Mn	33.90	0.61(6)
Y	0.43	0.004(8)

Table S3. Stoichiometry from inductively coupled plasma-atomic emission spectrometry (ICP-AES) results of NLFMY-2.

Elements	Content(mg/kg)	mol ratio
Na	13.75	0.59(8)
Li	0.78	0.11(2)
Fe	14.46	0.25(8)
Mn	33.83	0.61(5)
Y	0.86	0.009(7)

Table S4. Stoichiometry from inductively coupled plasma-atomic emission spectrometry (ICP-AES) results of NLFMY-3.

Elements	Content(mg/kg)	mol ratio
Na	13.87	0.60(3)
Li	0.75	0.10(7)
Fe	14.13	0.25(2)
Mn	34.27	0.62(3)
Y	1.73	0.019(4)

Table S5. Refined crystallographic parameters of NLFMY-1 with the Rietveld method. S.G. *P63/mmc*, $a = b = 2.88(7)$ Å, $c = 11.21(9)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$, R_{wp}=3.39%, $\chi^2 = 0.5284$.

Sample	Atom	Site	x	y	z	Occupancy
NLFMY-1	Mn	2a	0	0	0	0.62(3)
	Fe	2a	0	0	0	0.265(4)
	Li	2a	0	0	0	0.112(3)
	Y	2a	0	0	0	0.005(2)
	Na1	2b	0	0	0.25	0.298(4)
	Na2	2d	0.3333	0.6667	0.75	0.302(6)
	O	4f	0.3333	0.6667	0.0872	1
P63/mmc : $a = b = 2.8876(3)$ Å $c = 11.2193(4)$ Å V= 81.02(2) Å^3						
$R_p = 2.65\%$ $R_{wp} = 3.39\%$ GOF(χ^2) = 0.5284						

Rietveld refinement was conducted using hexagonal space group P63/mm and by placing Mn, Fe, Li, Y ions in octahedral sites of the transition-metal layer and Na ions at the two trigonal prismatic sites in the alkaline metal layer. ~0.5% of Y^{3+} occupies the octahedral site and has no occupancy in the Na layer. The refinement shows excellent goodness of fit with this model (GOF(χ^2) = 0.5284), which confirms the proposed structural model.

Table S6. Refined crystallographic parameters of NLFMY-2 with the Rietveld method. S.G. *P63/mmc*, $a = b = 2.89(1)$ Å, $c = 11.24(7)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$, R_{wp}=3.37%, $\chi^2 = 0.5032$.

Sample	Atom	Site	x	y	z	Occupancy
NLFMY-2	Mn	2a	0	0	0	0.62(3)
	Fe	2a	0	0	0	0.26(7)
	Li	2a	0	0	0	0.113(4)
	Y	2a	0	0	0	0.01(1)
	Na1	2b	0	0	0.25	0.297(5)
	Na2	2d	0.3333	0.6667	0.75	0.303(4)
	O	4f	0.3333	0.6667	0.0872	1
P63/mmc : $a = b = 2.8914(2)$ Å $c = 11.2478(1)$ Å V= 81.43(5) Å^3						
$R_p = 2.65\%$ $R_{wp} = 3.37\%$ GOF(χ^2) = 0.5032						

Rietveld refinement was conducted using hexagonal space group P63/mm and by placing Mn, Fe, Li, Y ions in octahedral sites of the transition-metal layer and Na ions at the two trigonal prismatic sites in the alkaline metal layer. ~1% of Y^{3+} occupies the octahedral site and has no occupancy in the Na layer. The refinement shows excellent goodness of fit with this model (GOF(χ^2) = 0.5032), which confirms the proposed structural model.

Table S7. Refined crystallographic parameters of NLFMY-3 with the Rietveld method. S.G. *P63/mmc*, $a = b = 2.89(7)$ Å, $c = 11.21(7)$ Å, $\alpha = \beta = 90°$, $\gamma = 120°$, R_{wp}=3.65%, $\chi^2 = 0.7043$.

Sample	Atom	Site	x	y	z	Occupancy
NLFMY-3	Mn	2a	0	0	0	0.62(3)
	Fe	2a	0	0	0	0.25(8)
	Li	2a	0	0	0	0.111(7)
	Y1	2a	0	0	0	0.0162(3)
	Na1	2b	0	0	0.25	0.298(8)
	Na2	2d	0.3333	0.6667	0.75	0.258(2)
	Y2	2d	0.3333	0.6667	0.75	0.0039(2)
	O	4f	0.3333	0.6667	0.0872	1
P63/mmc : $a = b = 2.8973(6)$ Å $c = 11.2176(2)$ Å V= 80.98(3) Å^3						
R_p =2.84% R_{wp} =3.65% GOF(χ^2) = 0.7043						

Rietveld refinement was conducted using hexagonal space group P63/mm and by placing Mn, Fe, Li, Y ions in octahedral sites of the transition-metal layer and Na ions at the two trigonal prismatic sites in the alkaline metal layer. ~1.6% of Y^{3+} occupies the octahedral site and ~0.4% of Y^{3+} enters the Na layer. The refinement shows excellent goodness of fit with this model (GOF(χ^2) = 0.7043), which confirms the proposed structural model.

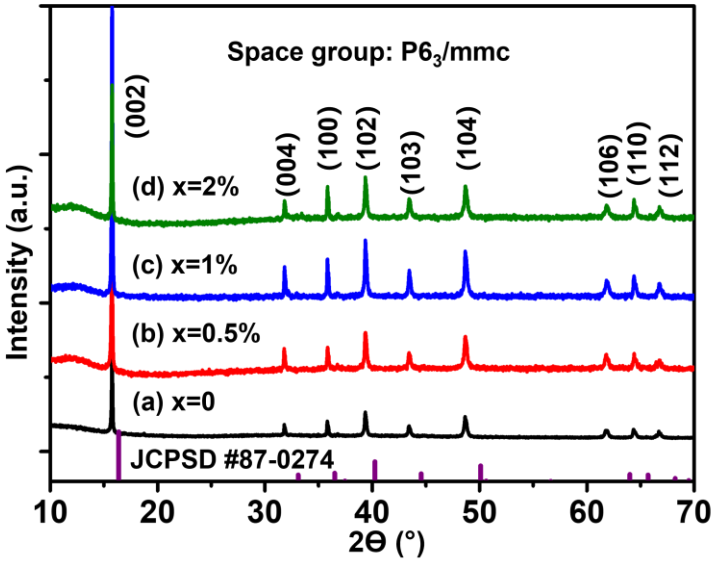

Fig. S1. XRD patterns were collected for $Na_{0.6}Li_{0.11}Fe_{0.27-x}Mn_{0.62}Y_xO_2$ samples with different Y^{3+} doping amounts (x=0, 0.5%, 1%, 2%).

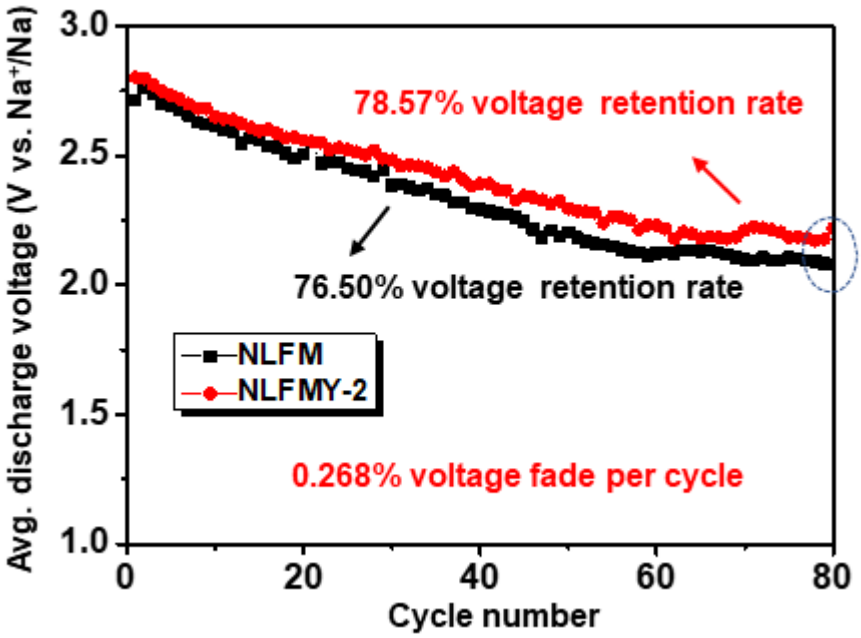

Fig. S2. Average discharge voltage vs. cycle number plot of NLFM and NLFMY-2.

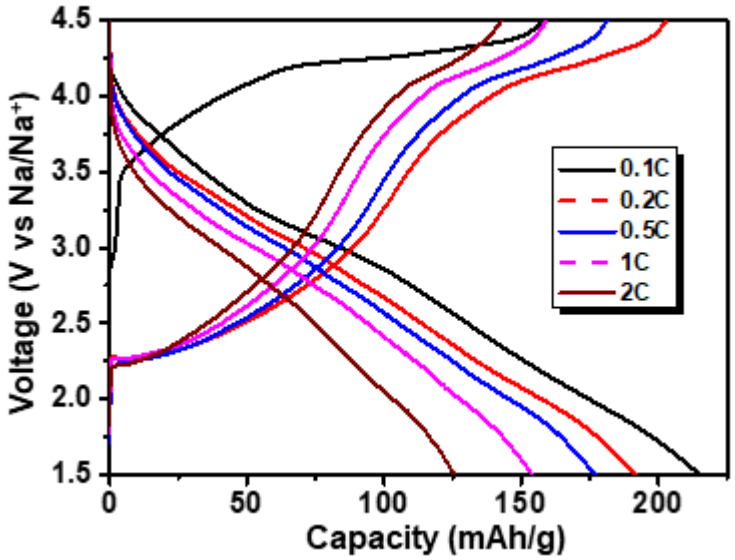

Fig. S3. The charge and discharge voltage profiles with different current rate (0.1C-2C) for the NLFMY-2 electrode.

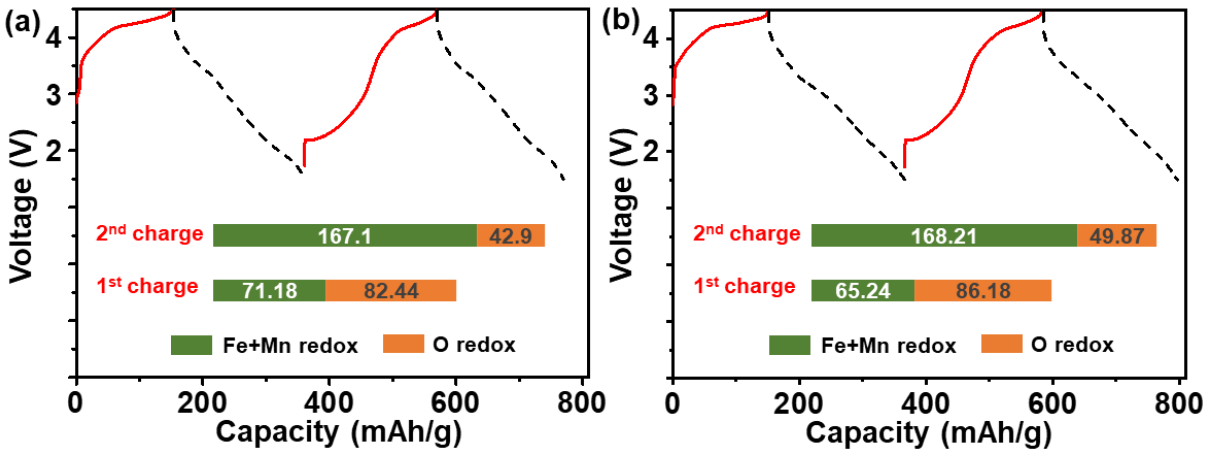

Fig. S4. The capacity contributions of Fe redox, Mn redox and O redox in the (a) NLFM and (b) NLFMY-2 electrodes during the initial two charging processes.