Electronic Supplementary Information (ESI)

Suppressing multiphase transitions of O3-$NaNi_{0.5}Mn_{0.5}O_2$ cathode by iron and magnesium co-doping towards sodium-ion batteries

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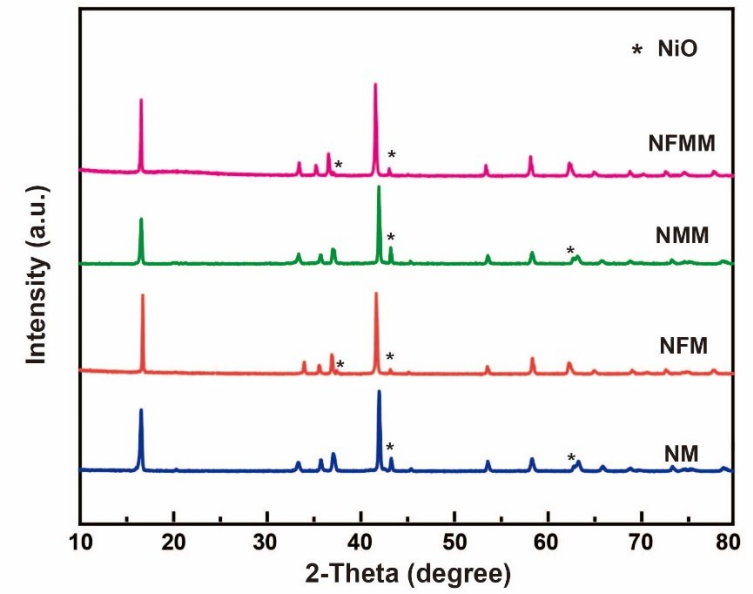

Figure S1. XRD patterns of the prepared samples.

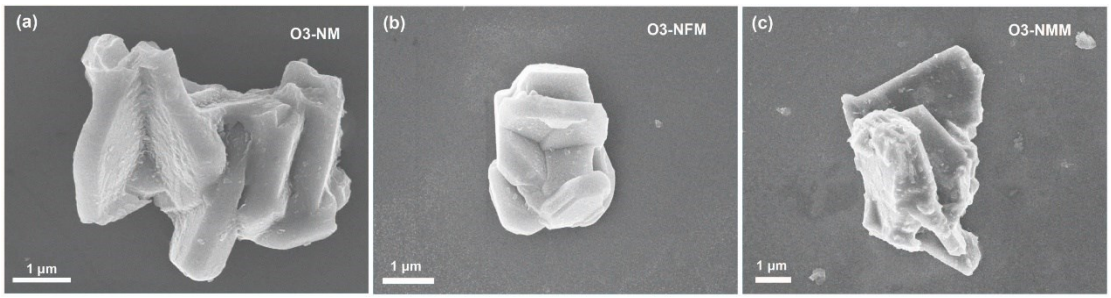

Figure S2. SEM images of (a) O3-NM, (b) O3-NFM, and (c) O3-NMM material for comparison.

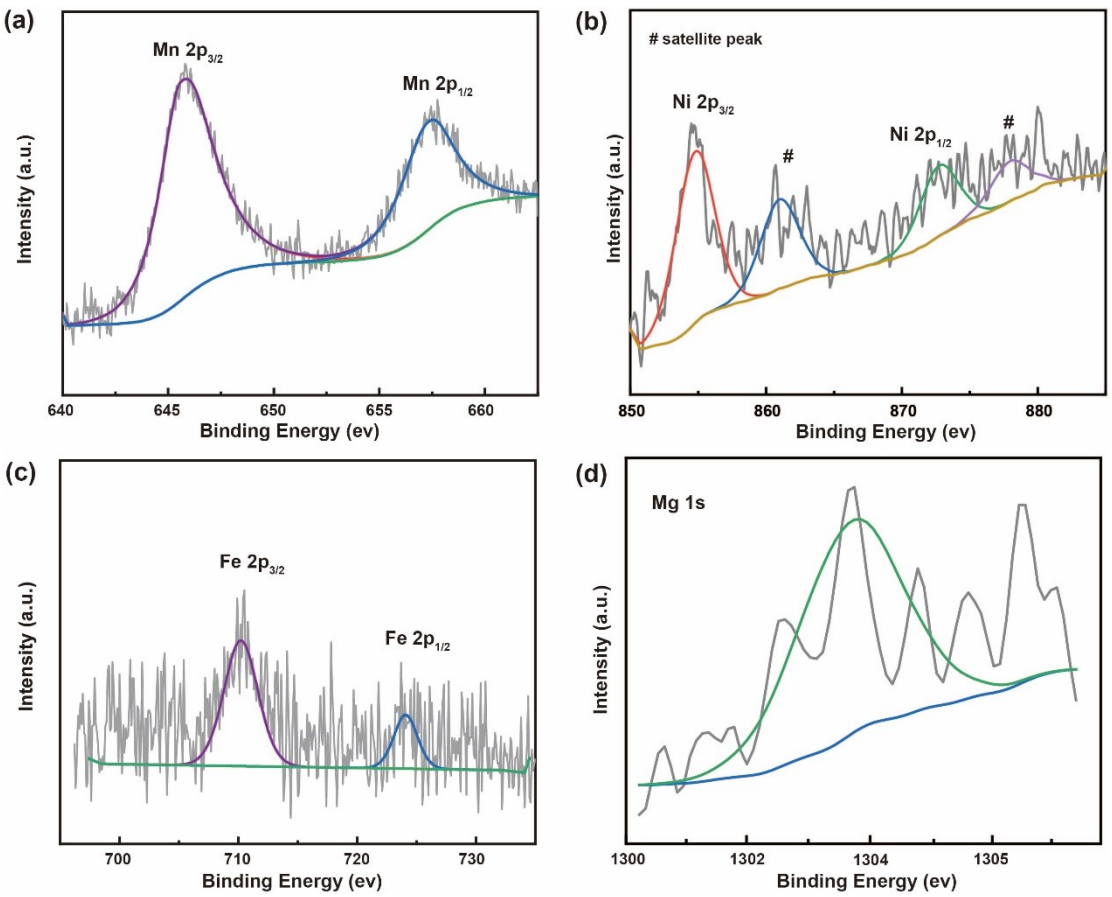

Figure S3. XPS spectra of (a) Mn 2p , (b) Ni 2p, (c) Fe 2p, and (d) Mg 1s for the O3-NFMM material.

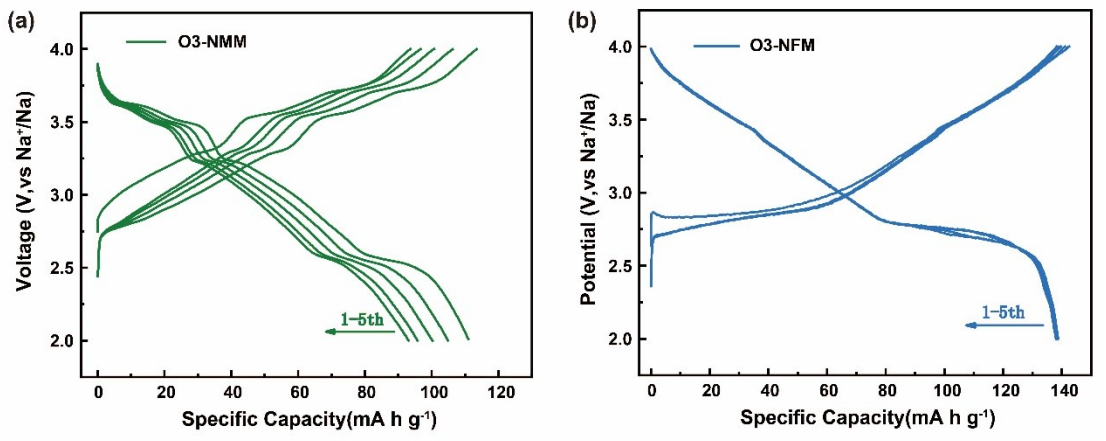

Figure S4. The charge/discharge curves of (a) O3-NMM and (b) O3-NFM for comparison.

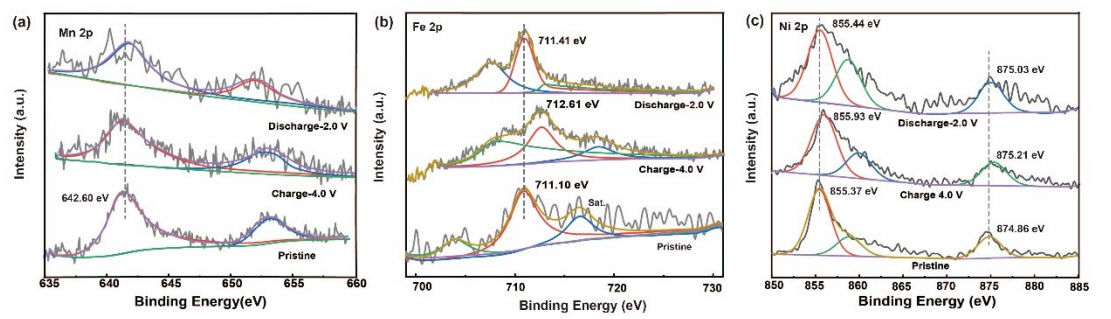

Figure S5. XPS spectra of (a) Mn 2p, (b) Fe 2p and (c)Ni 2p in O3-NFMM at different state during the first charge/discharge process.

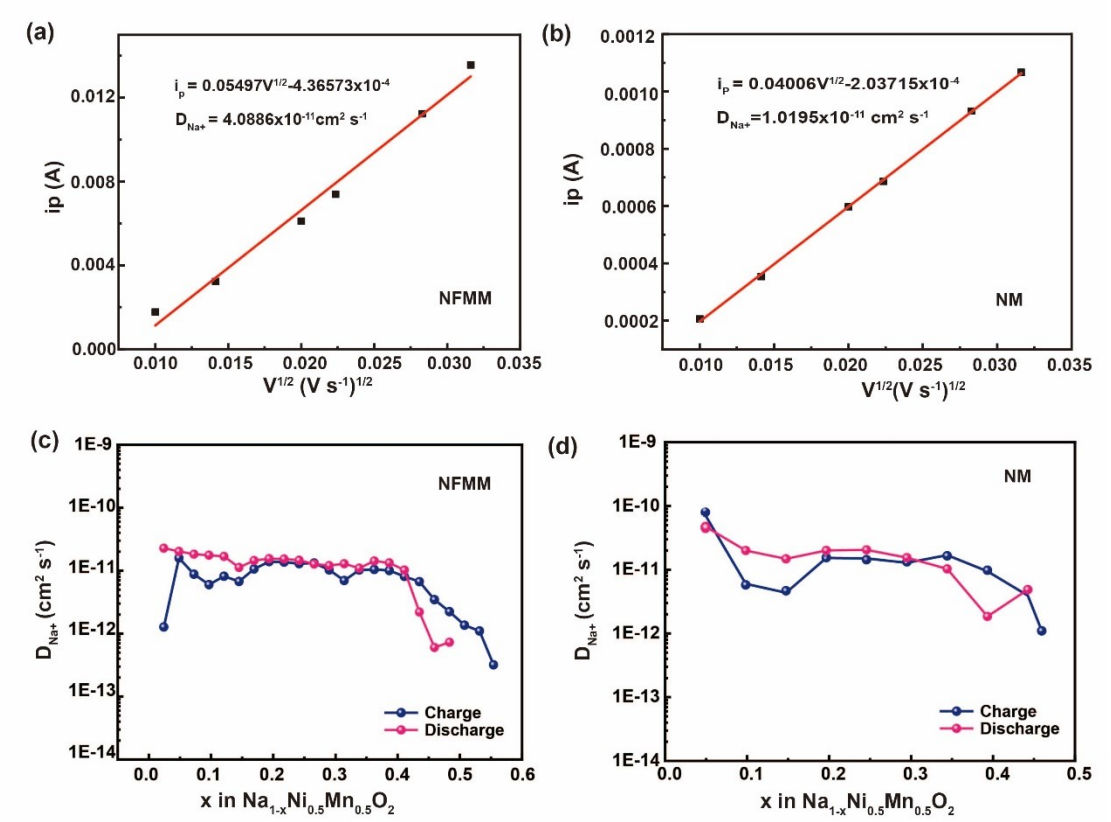

Figure S6. Peak current I_p as a function of the square root of scan rate $v^{1/2}$ of (a) O3-NFMM and (b) O3-NM based on variable CV test. Na^+ diffusion coefficients of (c) O3-NFMM and (d) O3-NM during charge/discharge process based on GITT test.

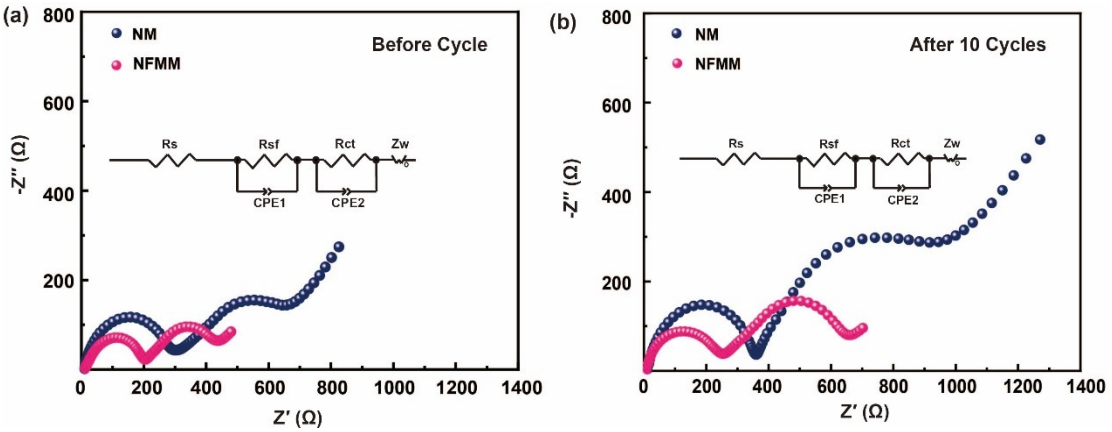

Figure S7. Comparison of EIS spectra between the O3-NM and O3-NFMM cathodes measured (a) before and (b) after 10 cycles .

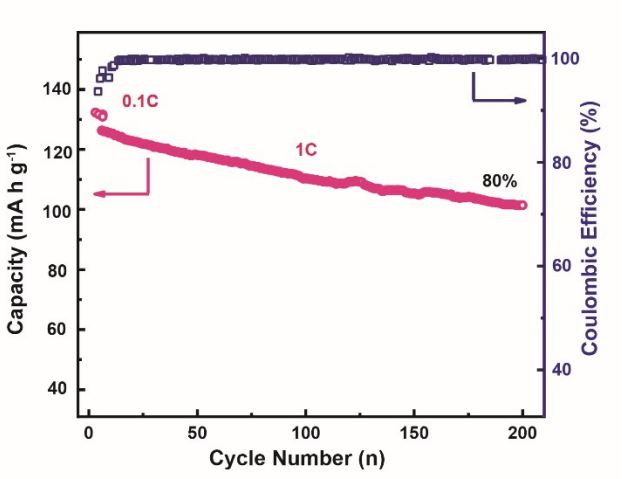

Figure S8. Capacity retention of O3-NFMM for sodium-ion full batteries during 200 cycles at 1 C rate (the first five cycles for the activation process at 0.1 C).

Table S1

Structural parameters and atomic positions of O3-NFMM from Rietveld refinement.

Atom	Site	x	y	z	Occ
Na	3a	0.00000	0.00000	0.00000	1
Ni	3b	0.00000	0.00000	0.50000	0.35
Fe	3b	0.00000	0.00000	0.50000	0.2
Mg	3b	0.00000	0.00000	0.50000	0.05
Mn	3b	0.00000	0.00000	0.50000	0.4
O	6c	0.00000	0.00000	0.23094	1
	a= 2.96937Å	c=16.03337Å	V=122.42897Å	Rwp=7.21%	Rp=5.64%

Table S2

Structural parameters and atomic position of O3-NM from Rietveld refinement.

Atom	Site	x	y	z	Occ
Na	3a	0.00000	0.00000	0.00000	1
Ni	3b	0.00000	0.00000	0.50000	0.5
Mn	3b	0.00000	0.00000	0.50000	0.5
O	6c	0.00000	0.00000	0.22792	1
	a=2.95261Å	c=16.00056Å	V=120.80337Å	Rwp=4.97%	Rp=3.50%

Table S3

Atomic distances, slab thickness (TMO_6), the d-spacings of the Na layer and the Inter-slab distance for as-prepared materials.

Samples	NM	NFMM
TM-O (Å)	1.96632	2.00019
TM-TM (Å)	2.95262	2.96937
TMO_2 (Å)	1.96017	2.06104
Interslab distance (Å)	5.33352	5.34445

Table S4

Impedance parameters derived from the equivalent circuit model for all the samples before cycle and after 10 cycles.

Sample	Before Cycling			After 10 Cycles		
	R_s/Ω	R_{sf}/Ω	R_{ct}/Ω	R_s/Ω	R_{sf}/Ω	R_{ct}/Ω
O3-NM	10.30	271.70	493.80	12.40	344.60	938.50
O3-NFMM	4.19	173.10	151.00	9.16	225.50	492.30