Suppressed P2-Z phase transition and Fe-migration in Na layered of Fe/Mn-based layered oxide cathode for advanced sodium-ion batteries

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Supplementary Figures and Tables

Na-ion diffusion coefficient (D_{Na}) calculation based on GITT results:

The Na-ion diffusion coefficient D_{Na} is calculated from the simplified equation: $D_{Na} = \frac{4}{\pi\tau}\left(\frac{m_B V_M}{M_B A}\right)^2\left(\frac{\Delta E_S}{\Delta E_\tau}\right)^2$,where the ΔE_τ is the transient voltage change caused by applying a constant current i during a constant current pulse τ, ΔE_S is the steady state voltage variation, τ duration time of the current pulse, M_B is the molar mass (g mol^{-1}), A is the total contact area of the electrode with the electrolyte, m_B is the mass of active material, V_M is the molar volume of electrode materical (cm^3 mol^{-1})[1,2].

Na-Ion Diffusion Coefficients Calculation Based on CV results:

The D_{Na} values can also be analysed by the following Randles-Sevcik equation: $i_p = 2.69 \times 10^5 n^{3/2} A {D_{Na}}^{1/2} C_{Na} v^{1/2}$, where i_p (A) is the peak current, A (cm^2) is the direct contact area between electrode and electrolyte, C_{Na} is the Na-ion concentration in the electrode, v (V s^{-1}) is the scan rate, and n is the number of transferred electrons. Figure 3c shows the linear relationship between the peak current (i_p) and the scan rate ($v^{1/2}$), Based on the linear relationships between i_p and $v^{1/2}$ of the redox peaks (Figure 4d)[3,4].

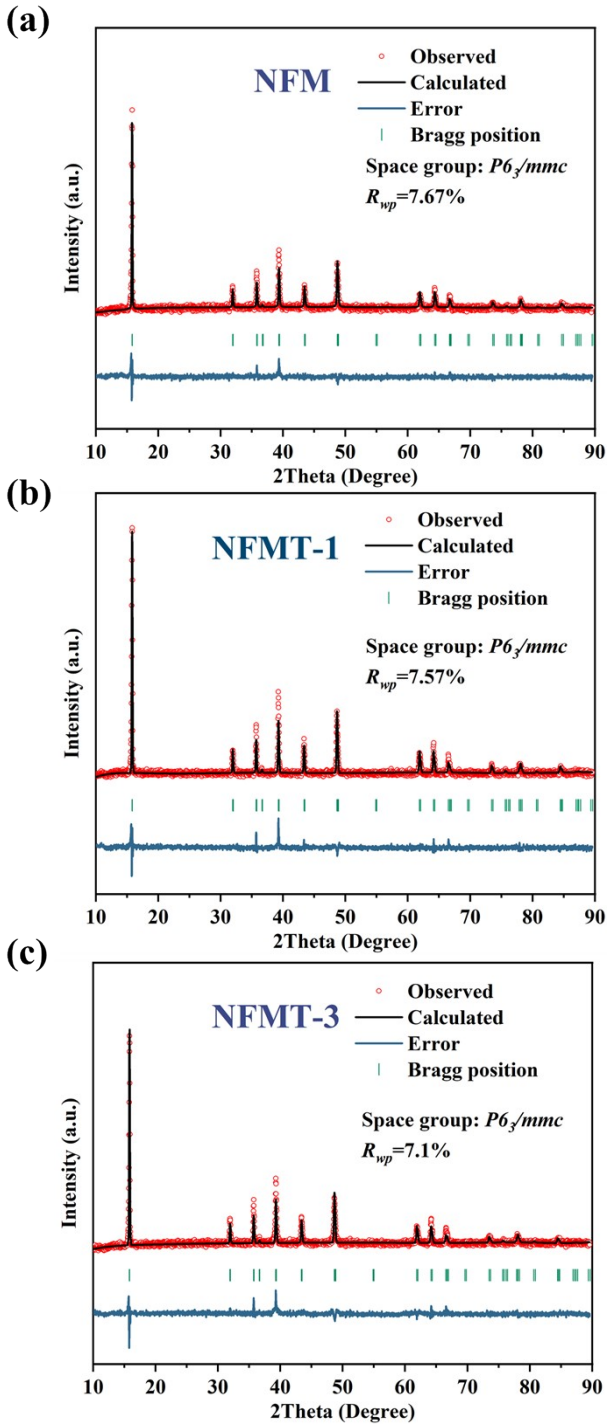

Figure S1 Rietveld refinements of the XRD patterns for a) NFM, b) NFMT-1 and (c) NFMT-3 cathode materials.

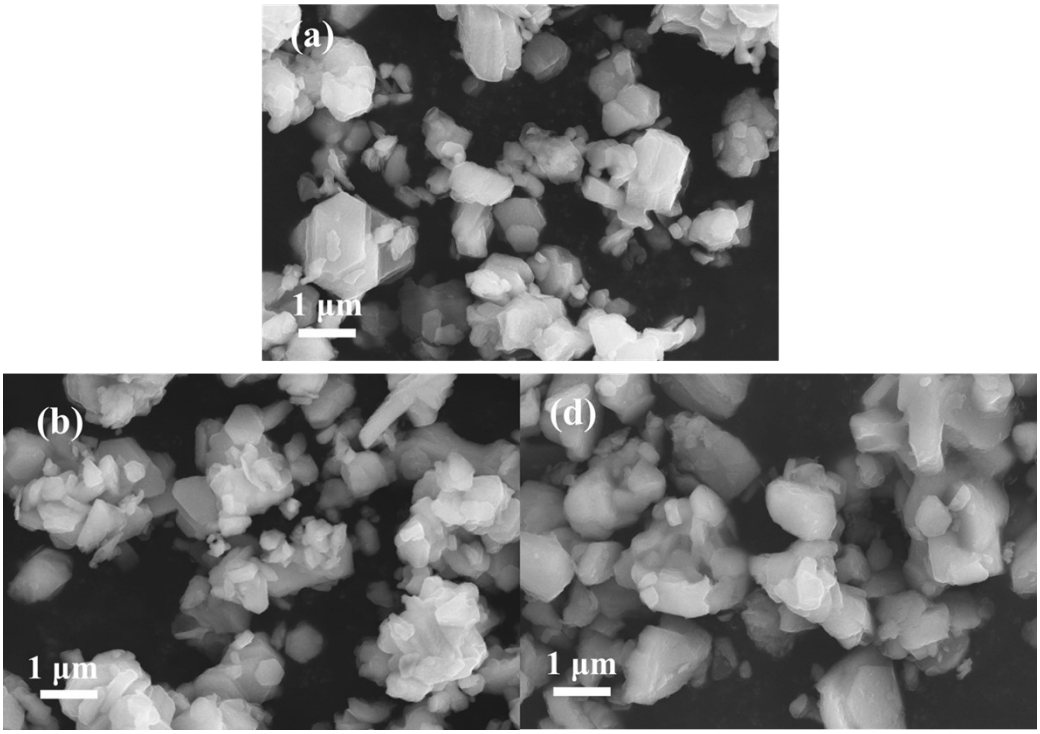

Figure S2. SEM images of (a) NFM, (b) NFMT-1, (c) NFMT-3.

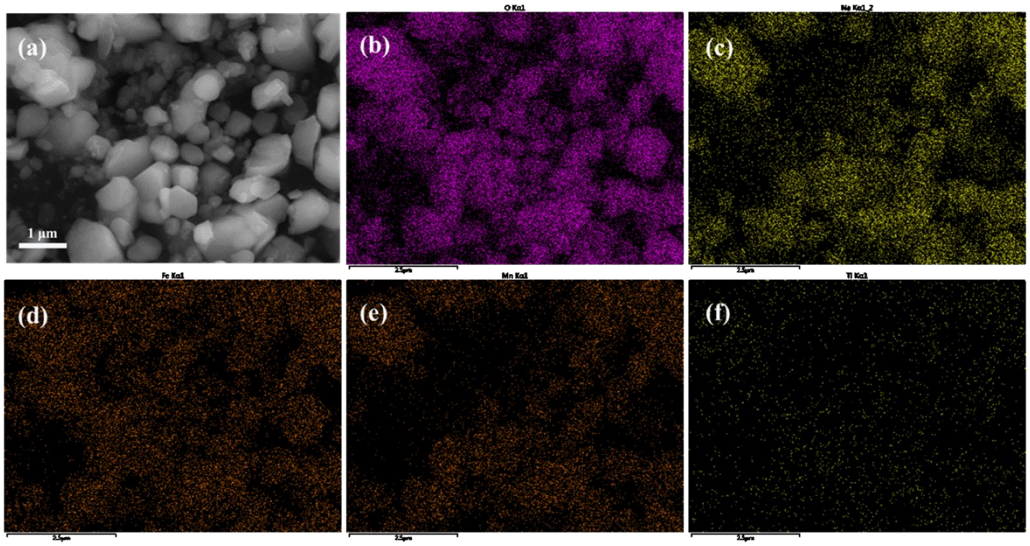

Figure S3 SEM-EDS images of (a-f) NFMT-2.

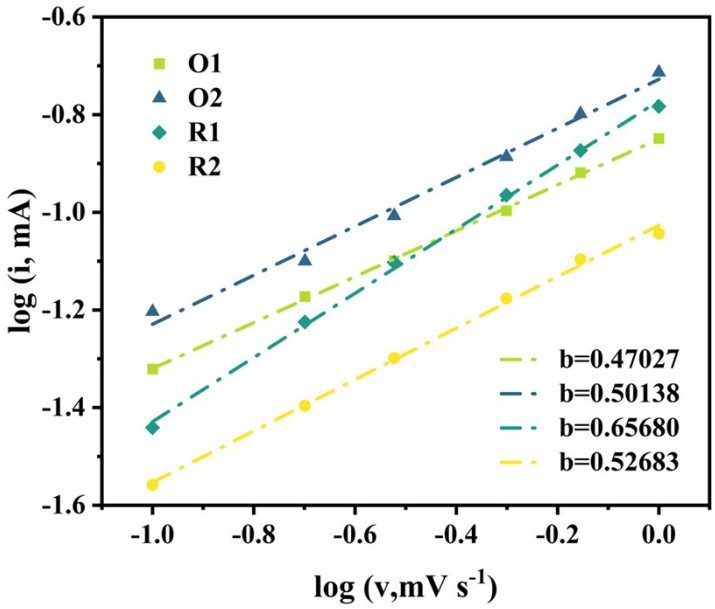

Figure S4. Linear relationships of logi_p versus log$v$.

Table S1. Detailed structural information of NFM, NFMT-1,2,3 determined from the Rietveld refined XRD pattern.

Samples	**NFM**	**MFMT-1**	**MFMT-2**	**MFMT-3**
Lattice	Hexagonal	Hexagonal	Hexagonal	Hexagonal
Space group	*P*63/*mmc*	*P*63/*mmc*	*P*63/*mmc*	*P*63/*mmc*
***a*=*b* (Å)**	2.9321	2.9384	2.9403	2.9412
***C* (Å)**	11.2043	11.2057	11.2081	11.2087
***V* (Å^3)**	83.3579	83.7898	83.91622	83.9721
R_p (%)	4.41	4.52	4.28	4.21
R_{wp} (%)	7.67	7.57	6.92	7.10

Table S2. ^{57}Fe-Mössbauer spectroscopy parameters of NFM and NFMT-2 charged to 4.3 V.

Sample	**IS/mm s^{-1}**	**QS/mm s^{-1}**	**FWHM/mm s^{-1}**	**Relative intensity**
NFMT-2	0.32622	0.68388	0.31703	(72.8%) Fe^{3+}
	0.42373	0.73671	0.31871	(27.42%) Fe^{4+}
NFM	0.37776	0.86196	0.32486	(68.85%) Fe^{3+}
	0.33976	0.62058	0.33501	(31.15%) Fe^{4+}

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