

Enabling High-voltage and Long Lifespan Sodium Batteries via Single-crystal Layer-structured Oxide Cathode Material

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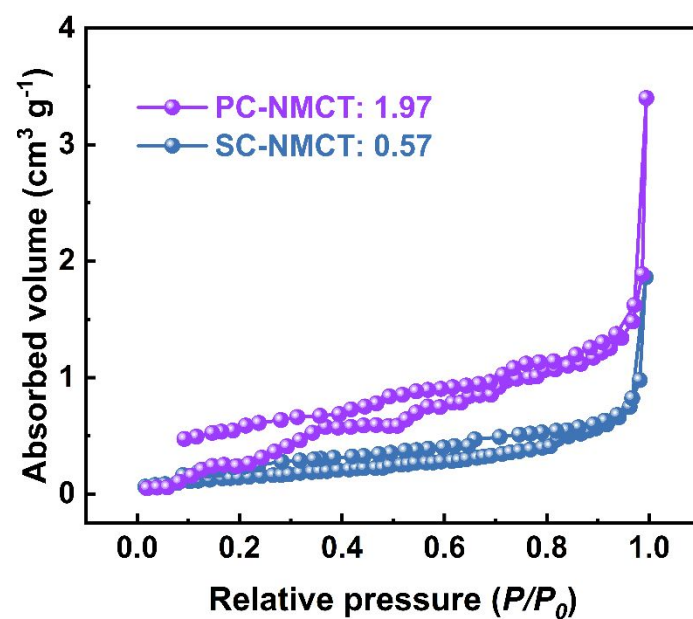


Figure S1. The N₂ adsorption and desorption isotherms for PC- and SC-NMCT materials.

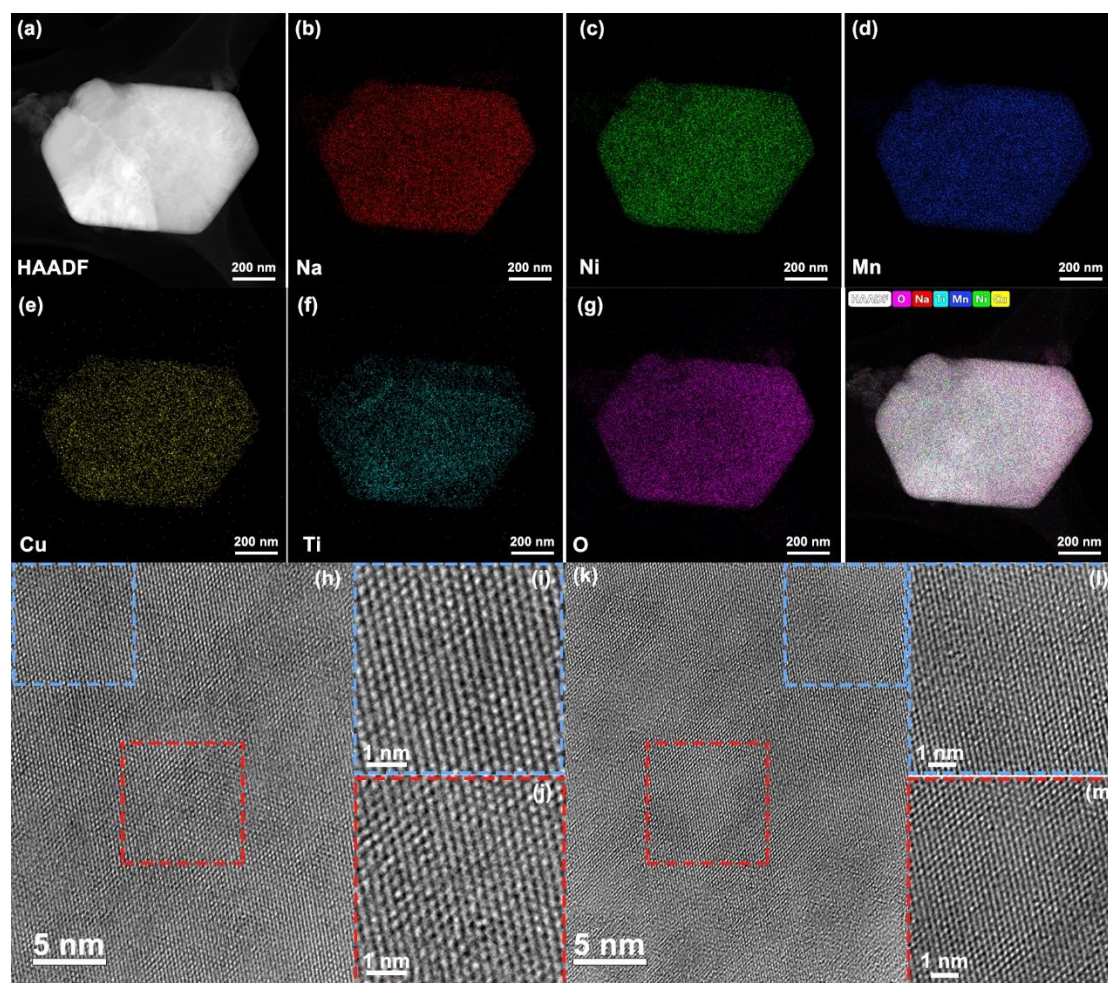


Figure S2. a-g) EDS mapping of remaining elements in SC-NMCT. h-m) HRTEM of SC-NMCT.

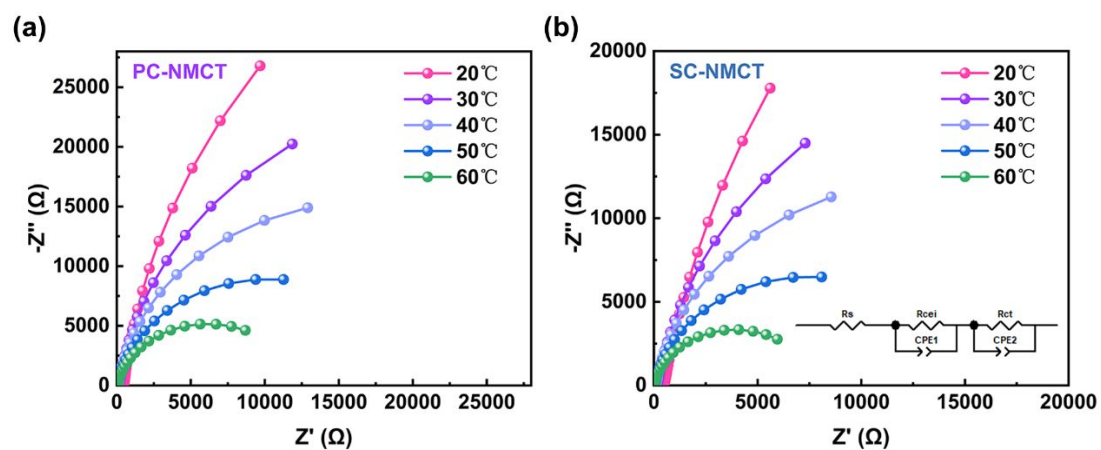


Figure S3. Nyquist plots of a) PC- and b) SC-NMCT at a cathodic potential of 2.3 V vs. Na/Na⁺ at different temperatures. The inset shows the equivalent circuit.

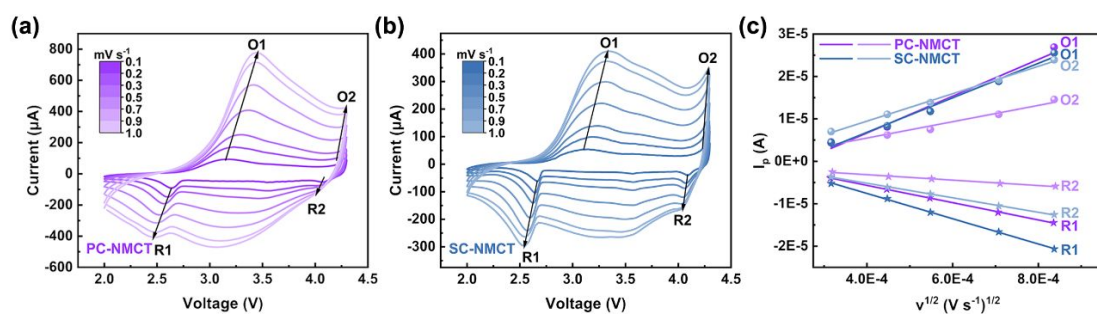


Figure S4. CV curves of a) PC- and b) SC-NMCT at different sweep speeds; c) Peak current I_p as a function of square root of scan rate $v^{1/2}$.

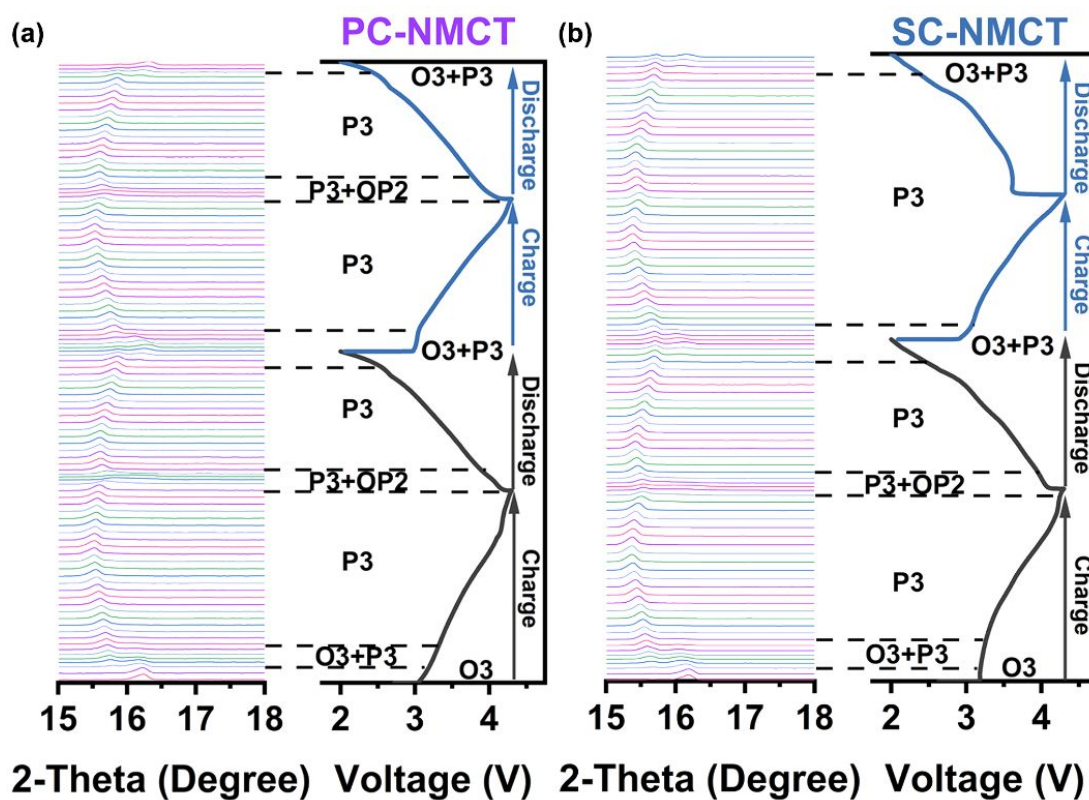


Figure S5. In situ XRD of the first two cycles of (a) PC- and (b) SC-NMCT.

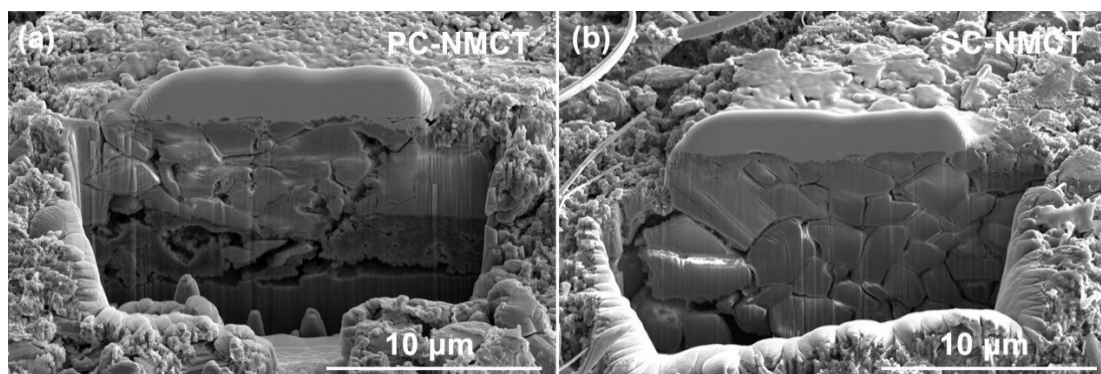


Figure S6. SEM image of a) PC- and b) SC-NMCT electrodes after localized FIB cutting.

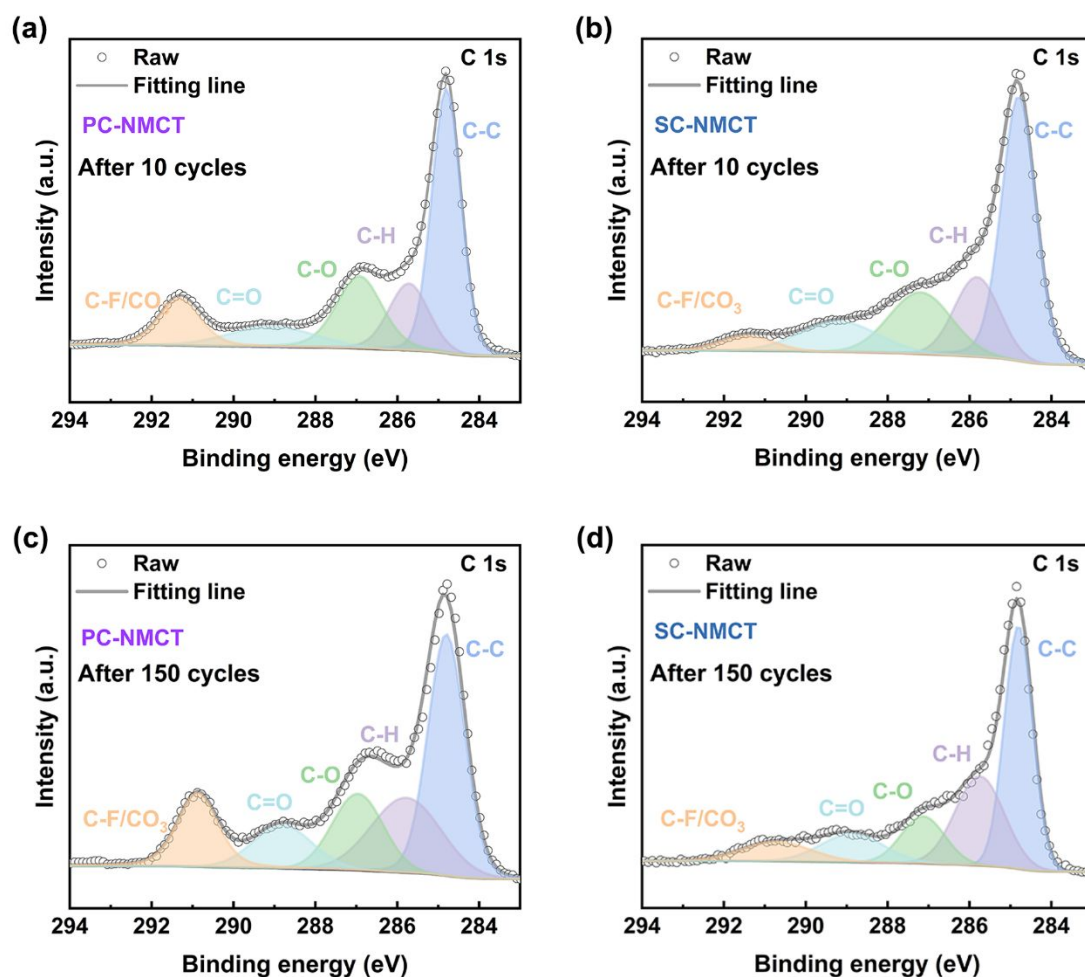


Figure S7. $\text{C } 1s$ XPS spectra of a) PC- and b) SC-NMCT electrodes before cycling; $\text{C } 1s$ XPS spectra of c) PC- and d) SC-NMCT electrodes after cycling.

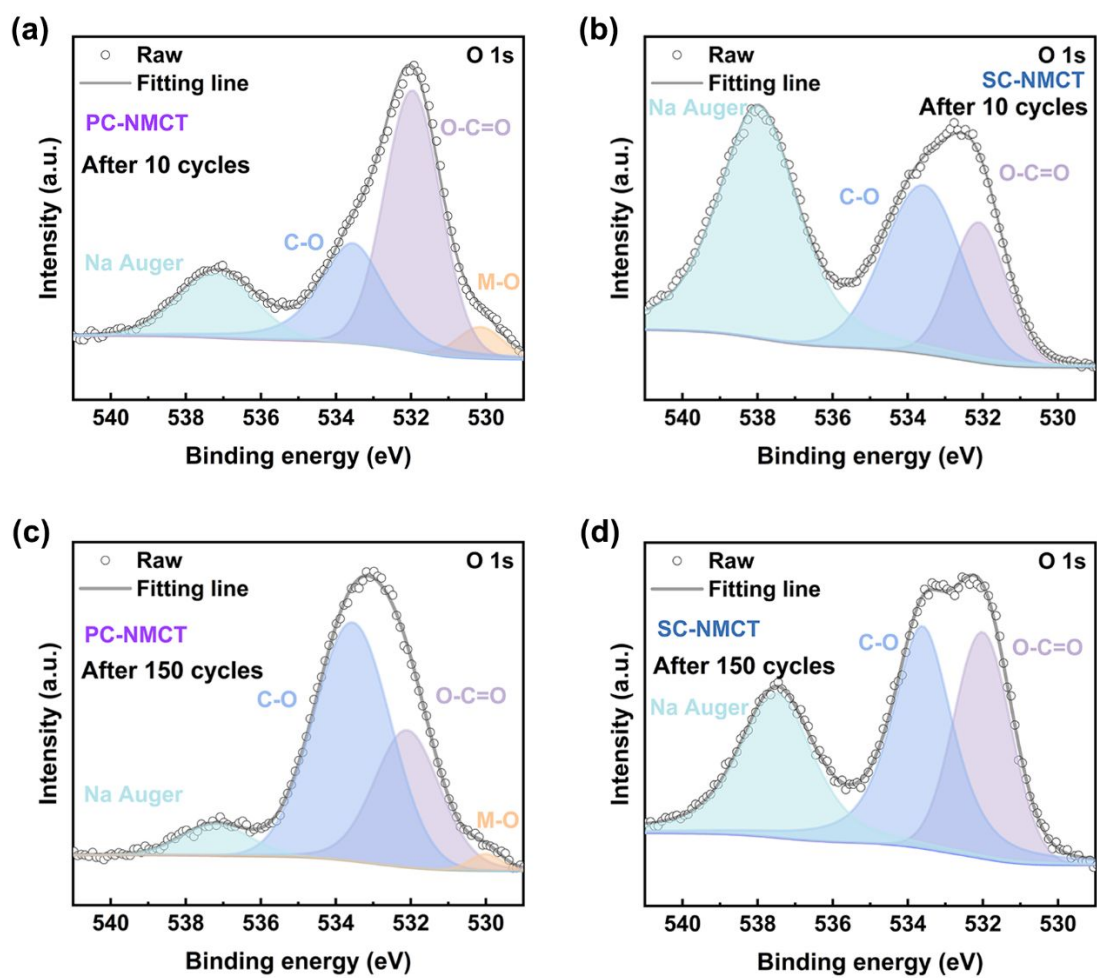


Figure S8. O 1s XPS spectra of a) PC- and b) SC-NMCT electrodes before cycling; O 1s XPS spectra of c) PC- and d) SC-NMCT electrodes after cycling.

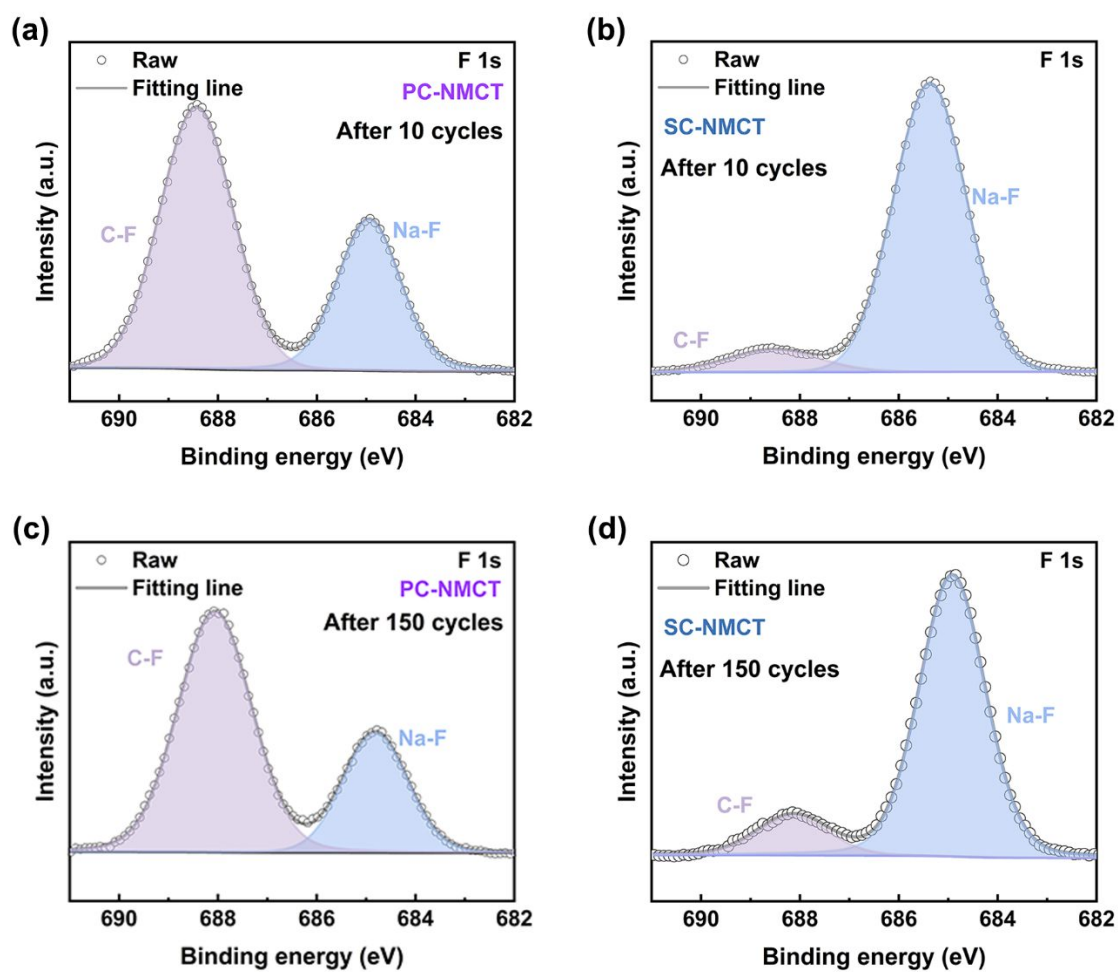


Figure S9. F $1s$ XPS spectra of a) PC- and b) SC-NMCT electrodes before cycling; F $1s$ XPS spectra of c) PC- and d) SC-NMCT electrodes after cycling.

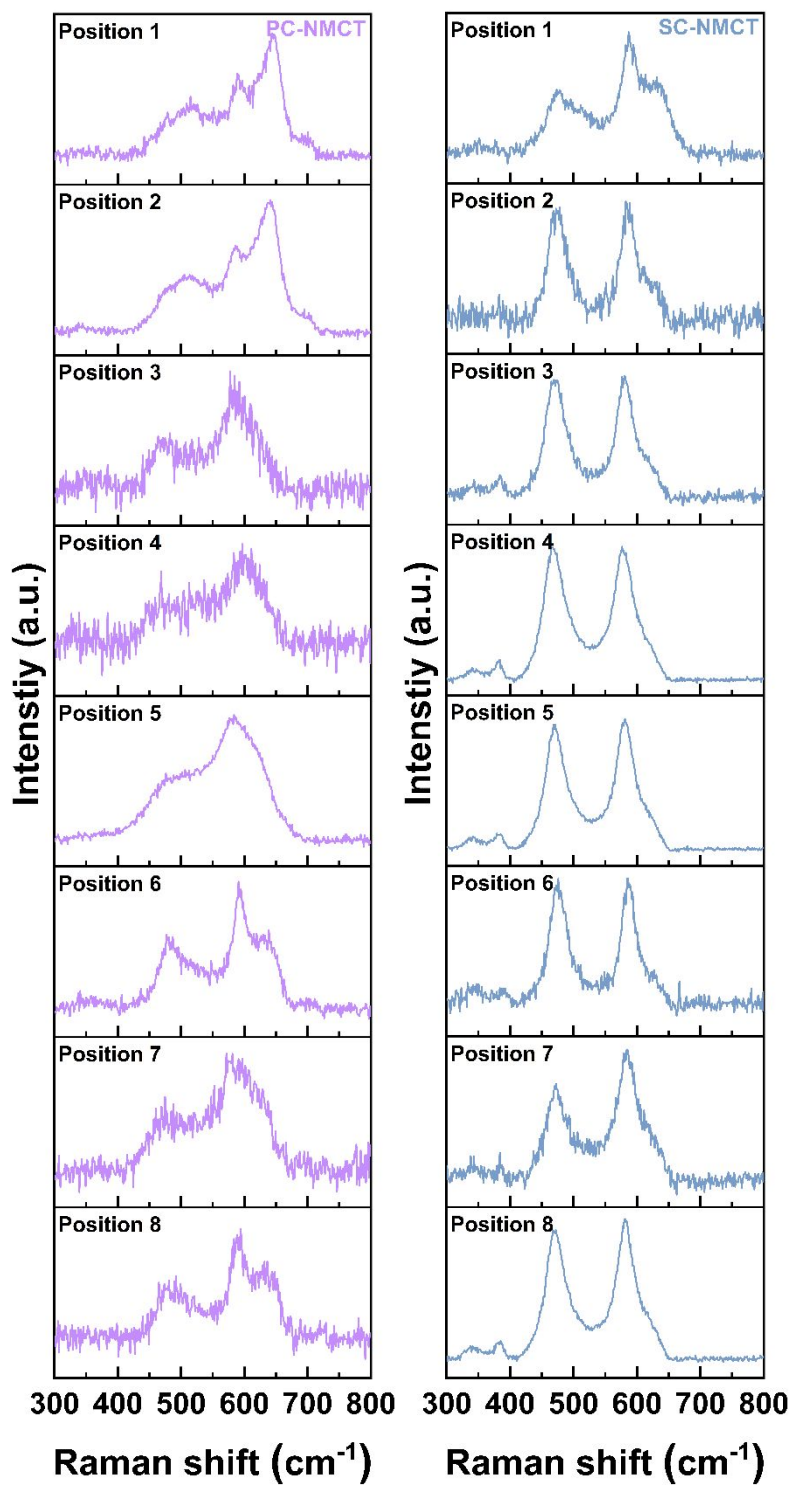


Figure S10. Raman spectra of the materials after cycling for (a) PC- and (b) SC-NMCT.

Table S1. Structural parameters and atomic positions of PC-NMCT deduced from Rietveld refinement of XRD data.

Atom	Wyckoff	x	y	z	Occupancy
Na	3a	0	0	0	0.083
Ni	3b	0	0	0.5	0.025
Mn	3b	0	0	0.5	0.042
Cu	3b	0	0	0.5	0.008
Ti	3b	0	0	0.5	0.008
O	6c	0	0	0.23149	0.167
a = b = 2.94067 Å, c = 16.20494 Å R _p = 1.57% R _{wp} = 2.11% Chi2 = 2.41					

Table S2. Structural parameters and atomic positions of SC-NMCT deduced from Rietveld refinement of XRD data.

Atom	Wyckoff	x	y	z	Occupancy
Na	3a	0	0	0	0.972
Ni	3b	0	0	0.5	0.025
Mn	3b	0	0	0.5	0.042
Cu	3b	0	0	0.5	0.01
Ti	3b	0	0	0.5	0.01
O	6c	0	0	0.22902	0.171
a = b = 2.93044 Å, c = 16.32533 Å R _p = 1.46% R _{wp} = 2.07% Chi2 = 2.74					