

Electronic supplementary information (ESI)

Stable Layered P3/P2 Na_{0.66}Co_{0.5}Mn_{0.5}O₂ Cathode Materials for Sodium Ion Batteries

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Table S1. Structural parameters and atomic position of P2/P3 biphase Na_{0.66}Mn_{0.5}Co_{0.5}O₂ from Rietveld refinement.

Phase 1: P3

Atom	Site	x	y	z	Occ	U
Na	3	0.00000	0.00000	0.82790(48)	0.66	0
Mn	3	0.00000	0.00000	-0.00251(38)	0.50	0
Co	3	0.00000	0.00000	-0.00251(38)	0.50	0
O	3	0.00000	0.00000	0.39308(46)	1.00	0
O	3	0.00000	0.00000	0.61479(49)	1.00	0

Space group	R3m
a (Å)	2.81466(4)
c (Å)	16.78169 (49)
Cell weight	312.321
Cell Volume (Å ³)	115.138(5)
wt%-Rietveld	76.047

Phase 2: P2

Atom	Site	x	y	z	Occ	U
Na	2	0.00000	0.00000	0.25000	0.33	0
Na	2	0.33333	0.66667	0.75000	0.33	0
Mn	2	0.00000	0.00000	0.00000	0.50	0
Co	2	0.00000	0.00000	0.00000	0.50	0
O	4	0.33333	0.66667	0.08398(93)	1.00	0

Space group	P63/mmc
a (Å)	2.82319(4)
c (Å)	11.25026(4)
Cell weight	208.517
Cell Volume (Å ³)	77.656(3)
wt%-Rietveld	23.953

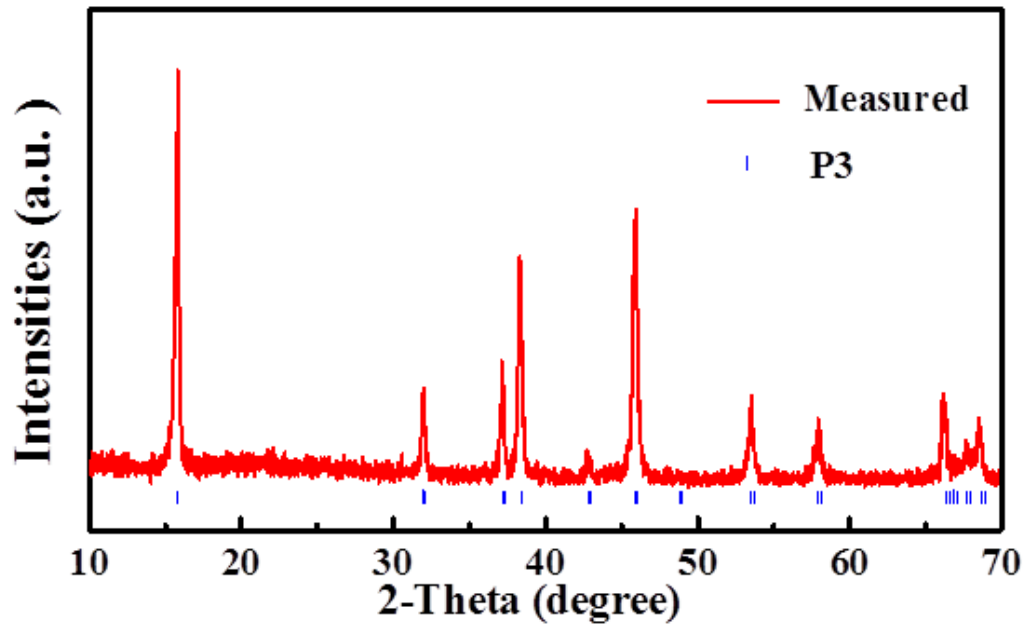


Fig. S1. XRD pattern of pure P3 phase $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ indexed with R3m space group.

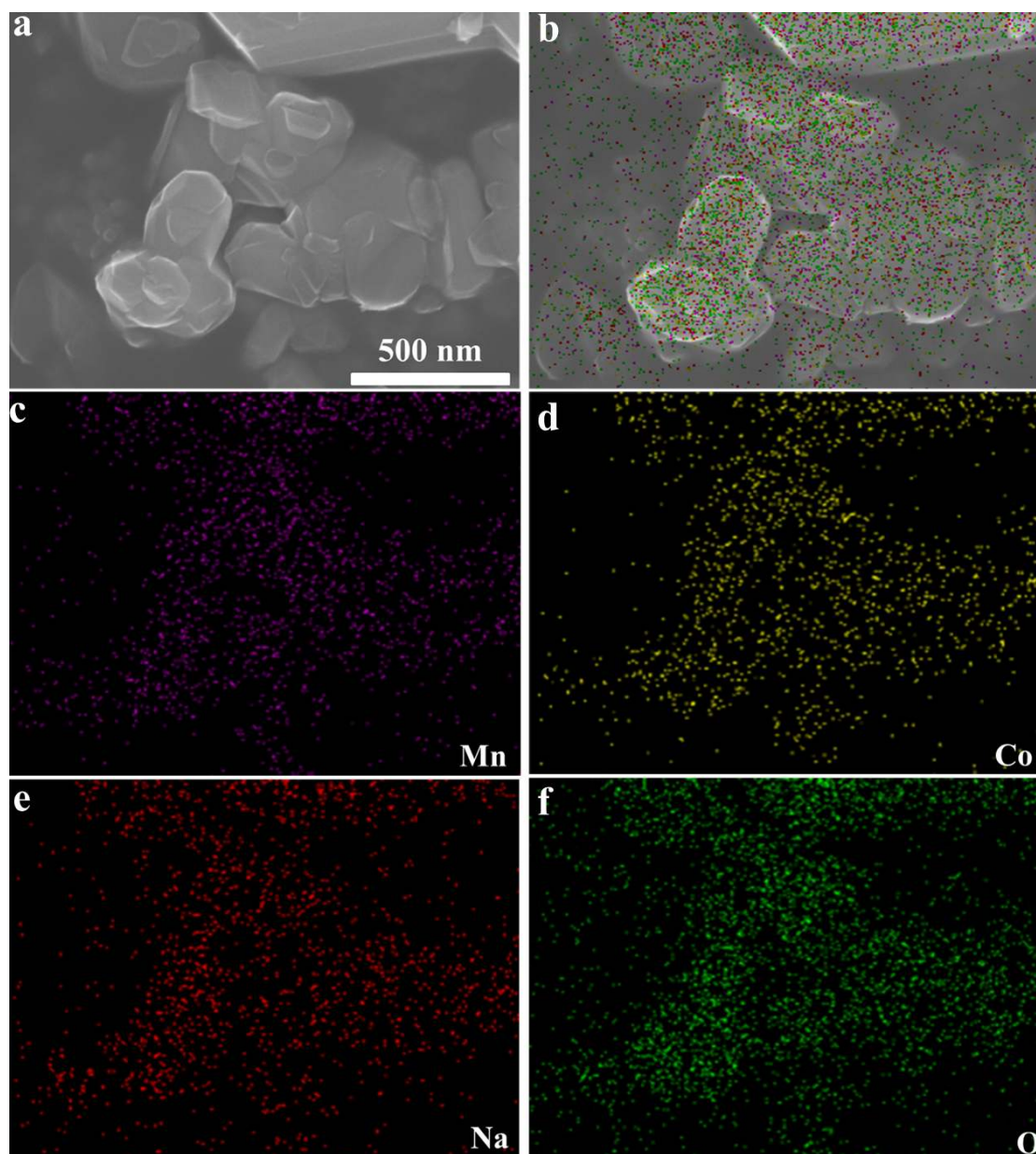


Fig. S2. EDS mapping patterns of P2/P3 biphas $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ composite.

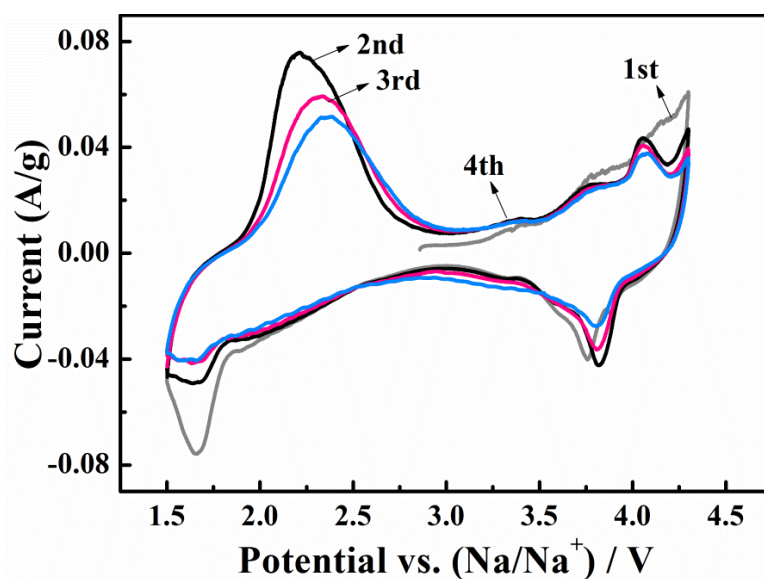


Fig. S3. CV curves of the P2/P3 biphas electrode at 0.1 mVs^{-1} .

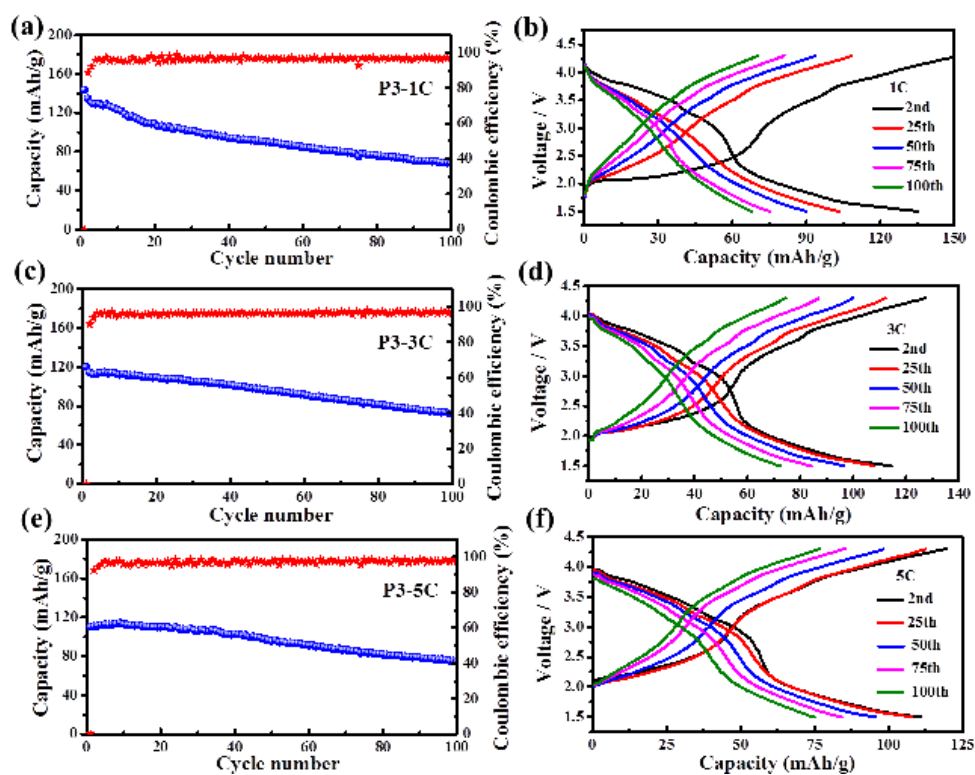


Fig. S4. Electrochemical performances of coin cells with P3 type $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ cathodes upon galvanostatic charge-discharge cycles in the range of 1.5-4.3 V. (a,c,e) Cycling performances and (b,d,f) charge/discharge curves at 1 C, 3 C and 5 C, respectively.

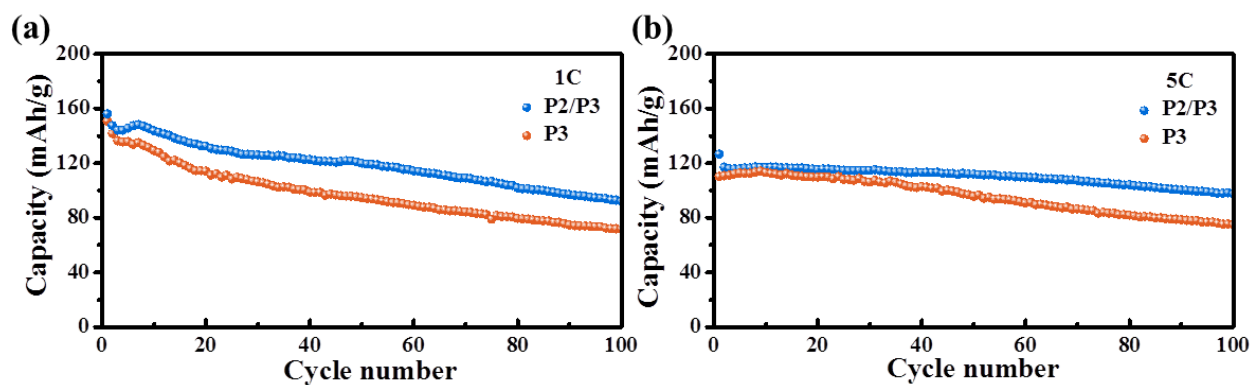


Fig. S5. Cycle performances of the P3 phase and P2/P3 biphasic of the $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ cathodes tested at 1C and 5 C, respectively.

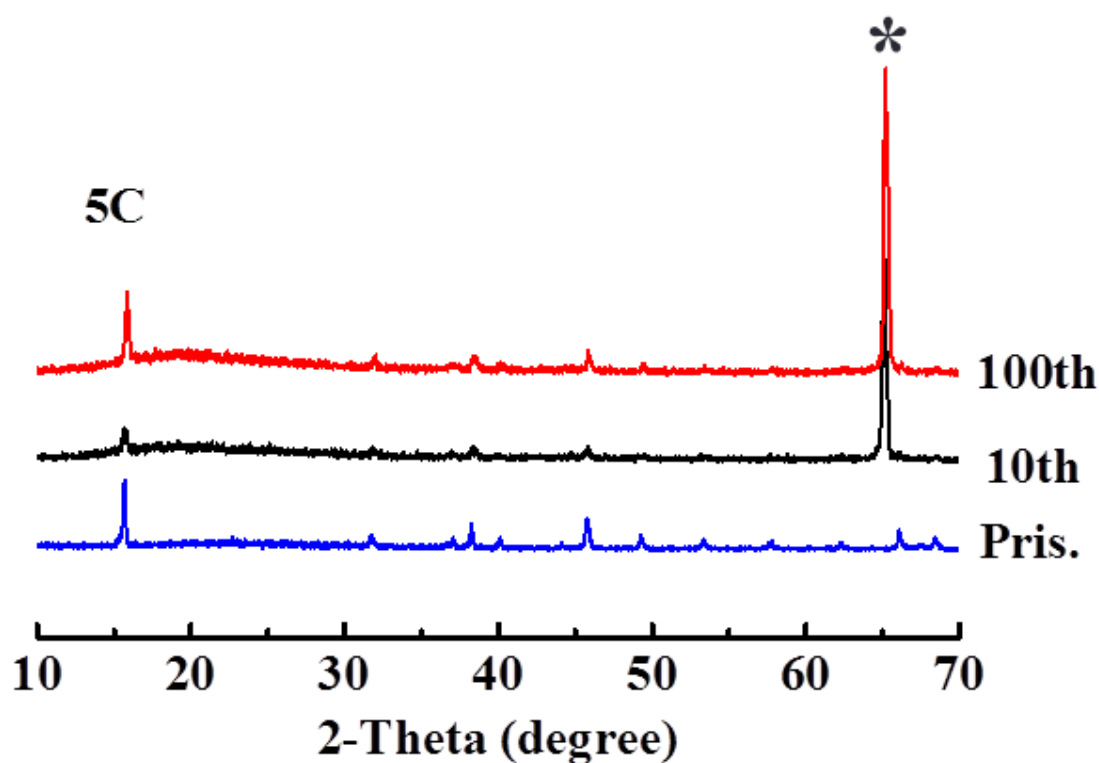


Fig. S6. XRD patterns of the pristine material and the P2/P3 biphasic $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrodes before and after cycling at 5 C in the potential range of 1.5-4.3 V. The asterisk is the characteristic diffraction peaks of intrinsic Al foils.

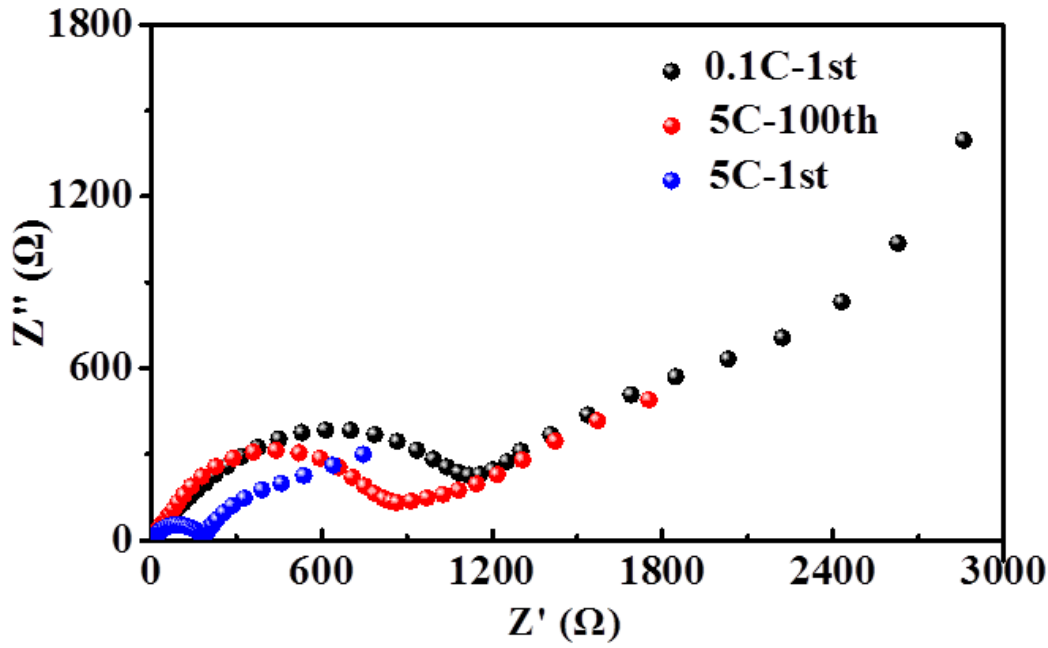


Fig S7. Evolution of impedance spectra of the P2/P3 biphased $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrode tested under various rates (0.1 C, or 5 C) at about the same stage.

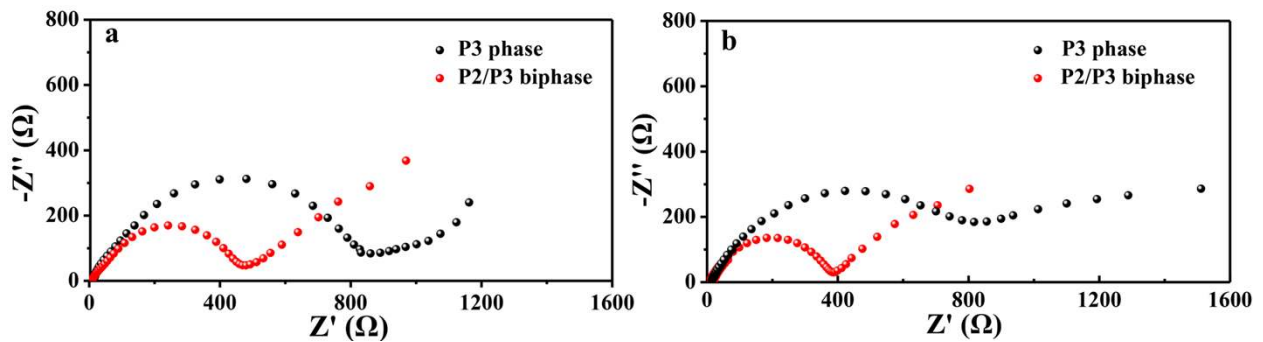


Fig S8. EIS of pure P3 and P2/P3 biphased $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrodes at different testing conditions: (a) after 100 charge/discharge cycles at 5 C; (b) after 20 charge/discharge cycles at 1 C and then 20 charge/discharge cycles at 5 C.