

Electronic supplementary information (ESI)

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

Xiaoqing Chen, Xianlong Zhou, Meng Hu, Jing Liang, Dihua Wu, Jinping Wei,* Zhen Zhou*

Key Laboratory of Advanced Energy Materials Chemistry (Ministry of Education), Institute of New Energy Material Chemistry, Collaborative Innovation Center of Chemical Science and Engineering (Tianjin), School of Materials Science and Engineering, National Institute of Advanced Materials, Nankai University, Tianjin 300071, P.R. China

Email: jpwei@nankai.edu.cn; zhouzhen@nankai.edu.cn

Table S1. Structural parameters and atomic position of P2/P3 biphase $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ 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

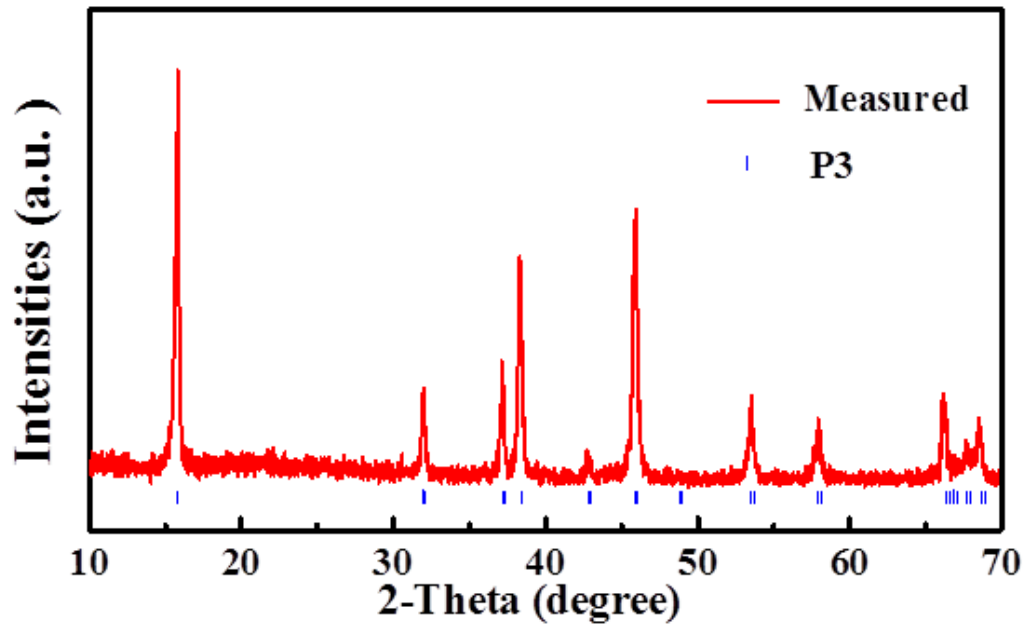


Fig. S1. XRD pattern of pure P3 phase $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ indexed with R3m space group.

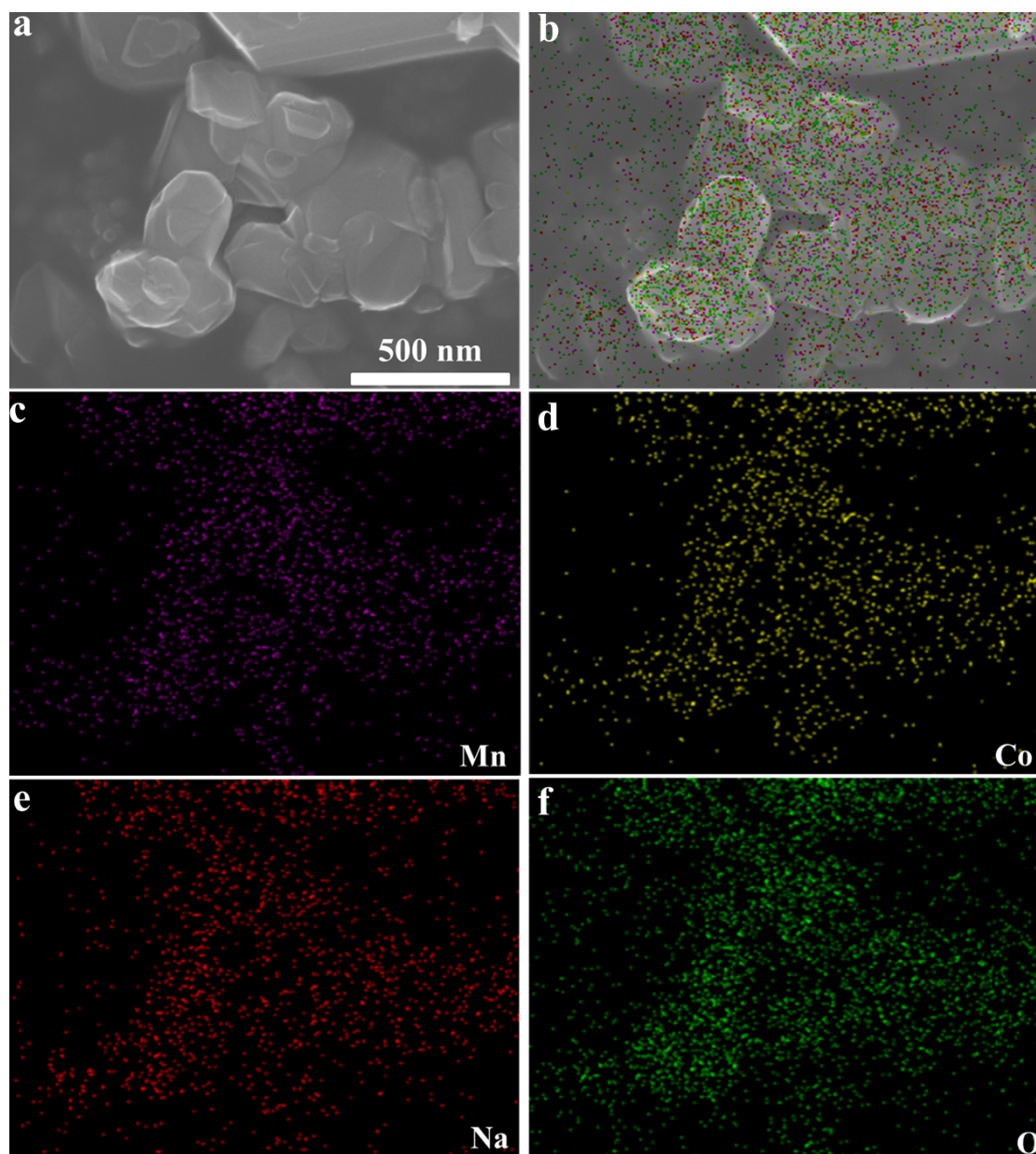


Fig. S2. EDS mapping patterns of P2/P3 biphas $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ composite.

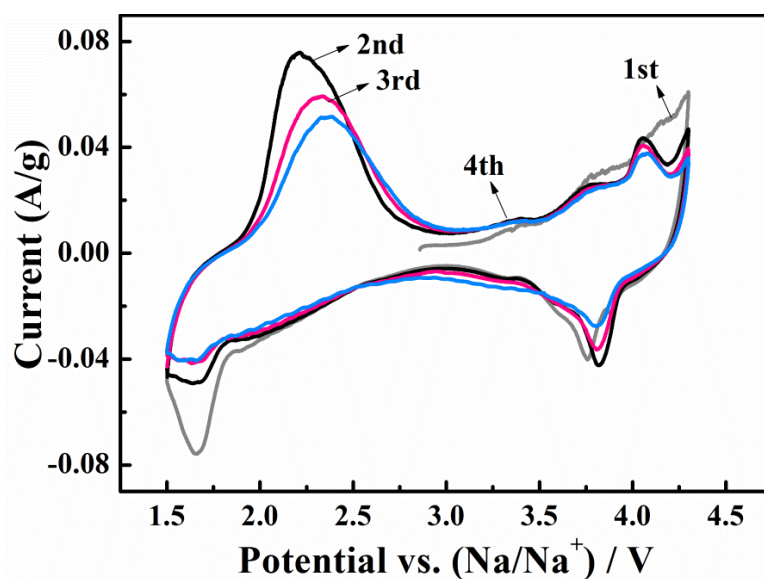


Fig. S3. CV curves of the P2/P3 biphasic electrode at 0.1 mVs^{-1} .

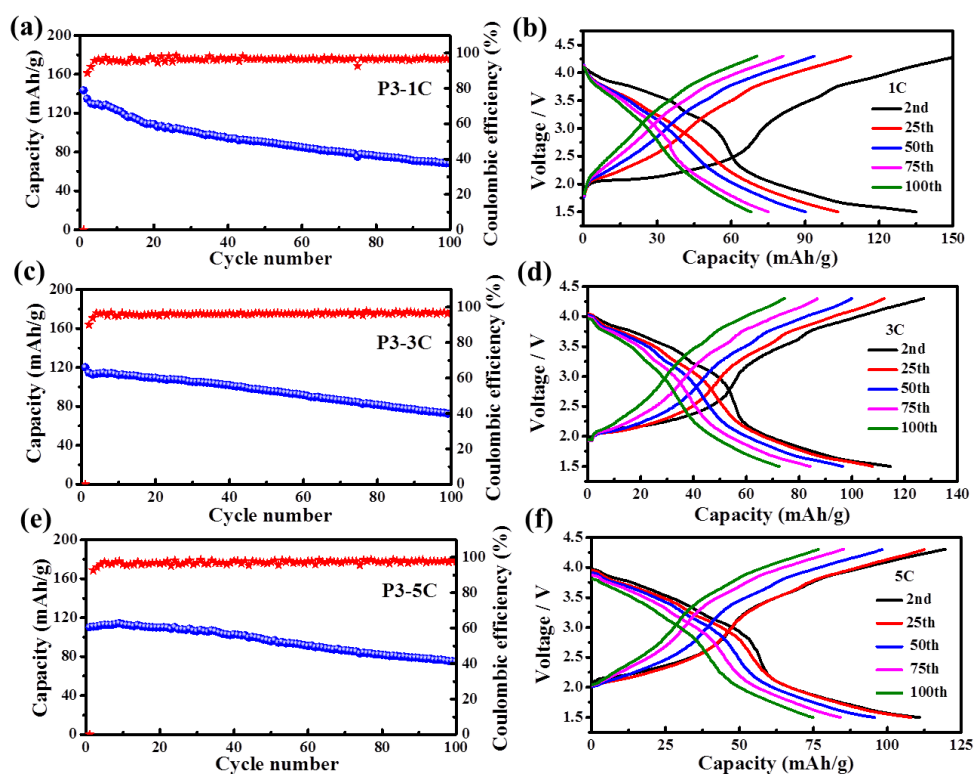


Fig. S4. Electrochemical performances of coin cells with P3 type $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ cathodes upon galvanostatic charge-discharge cycles in the range of 1.5-4.3 V. (a,c,e) Cycling performances and (b,d,f) charge/discharge curves at 1 C, 3 C and 5 C, respectively.

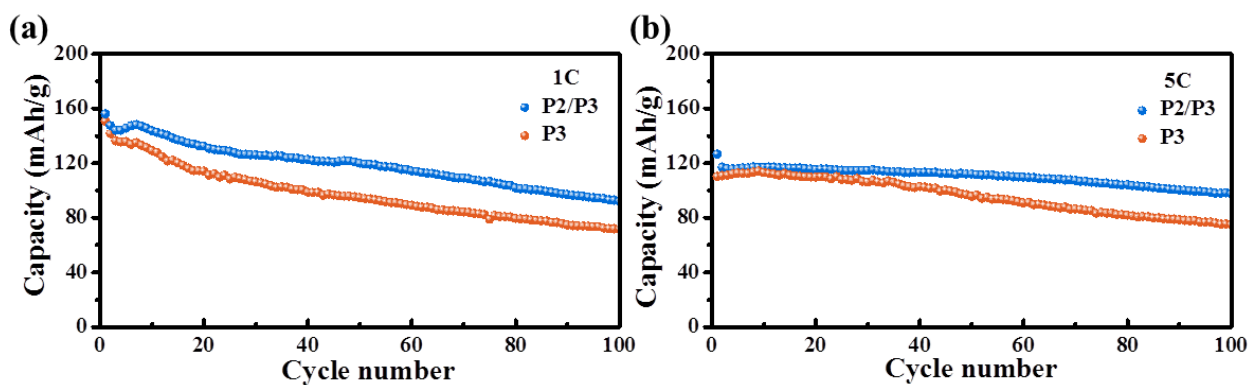


Fig. S5. Cycle performances of the P3 phase and P2/P3 biphasic of the $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ cathodes tested at 1C and 5 C, respectively.

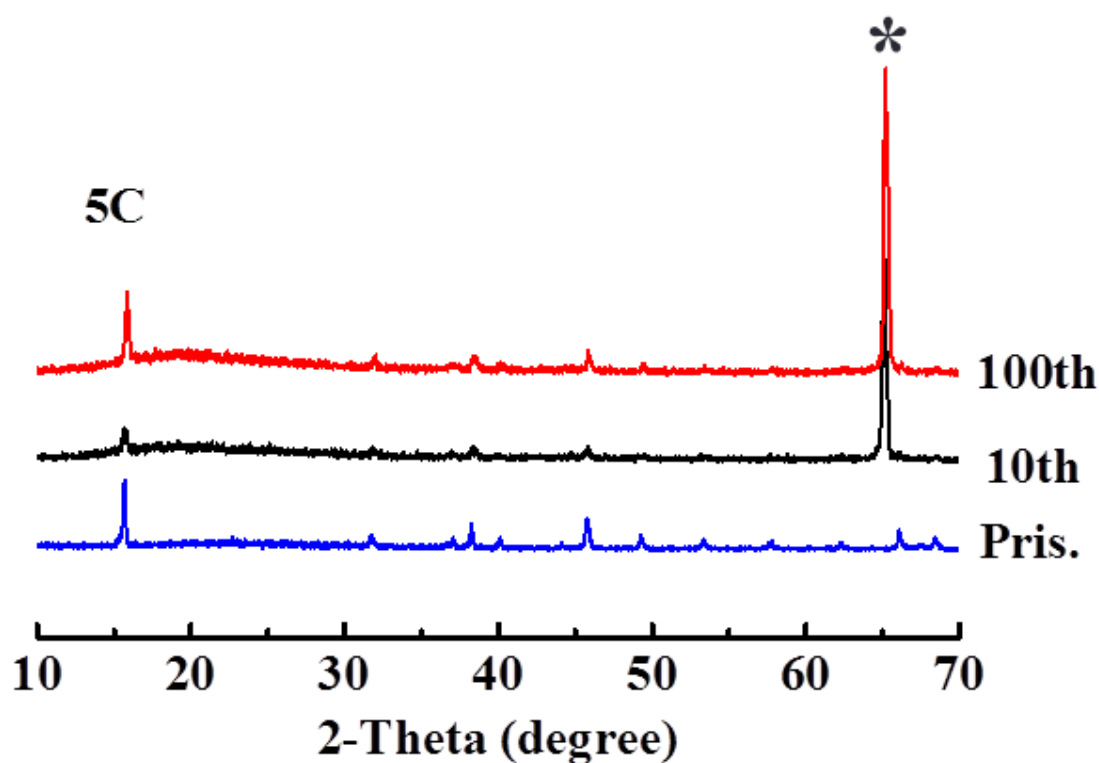


Fig. S6. XRD patterns of the pristine material and the P2/P3 biphasic $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrodes before and after cycling at 5 C in the potential range of 1.5-4.3 V. The asterisk is the characteristic diffraction peaks of intrinsic Al foils.

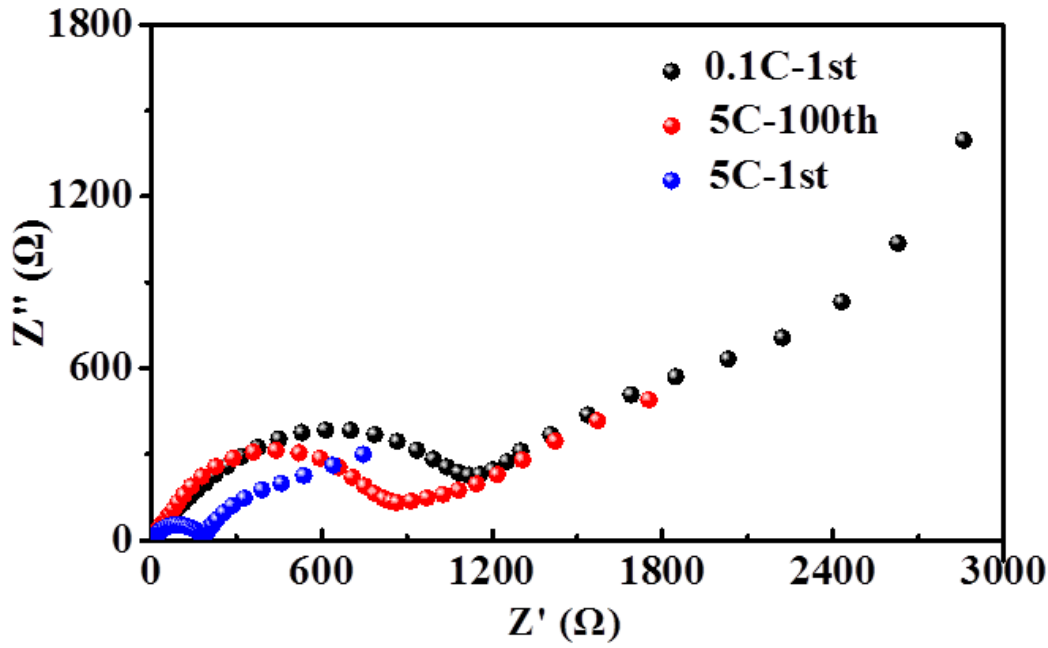


Fig S7. Evolution of impedance spectra of the P2/P3 biphased $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrode tested under various rates (0.1 C, or 5 C) at about the same stage.

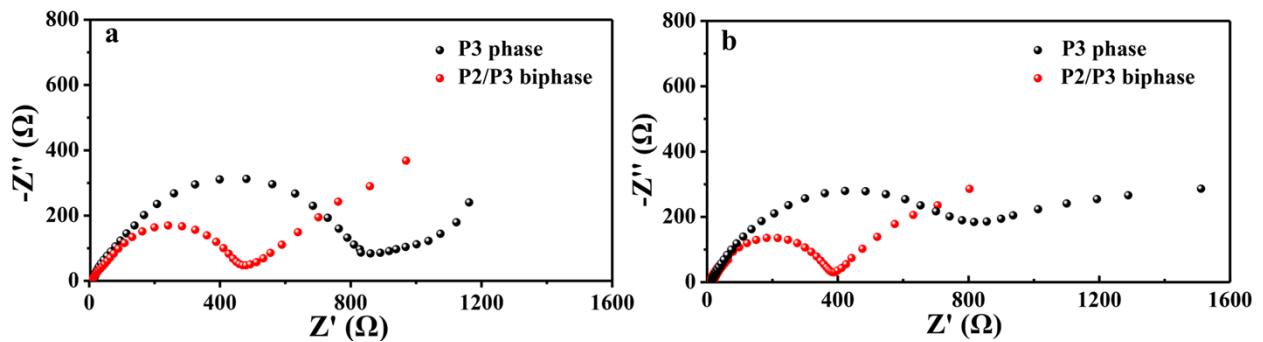


Fig S8. EIS of pure P3 and P2/P3 biphased $\text{Na}_{0.66}\text{Mn}_{0.5}\text{Co}_{0.5}\text{O}_2$ electrodes at different testing conditions: (a) after 100 charge/discharge cycles at 5 C; (b) after 20 charge/discharge cycles at 1 C and then 20 charge/discharge cycles at 5 C.