

Supporting Information

Nano-TiO₂ coated single-crystal LiNi_{0.65}Co_{0.15}Mn_{0.2}O₂ for lithium-ion batteries with stable structure and excellent cycling performance at a high cut-off voltage

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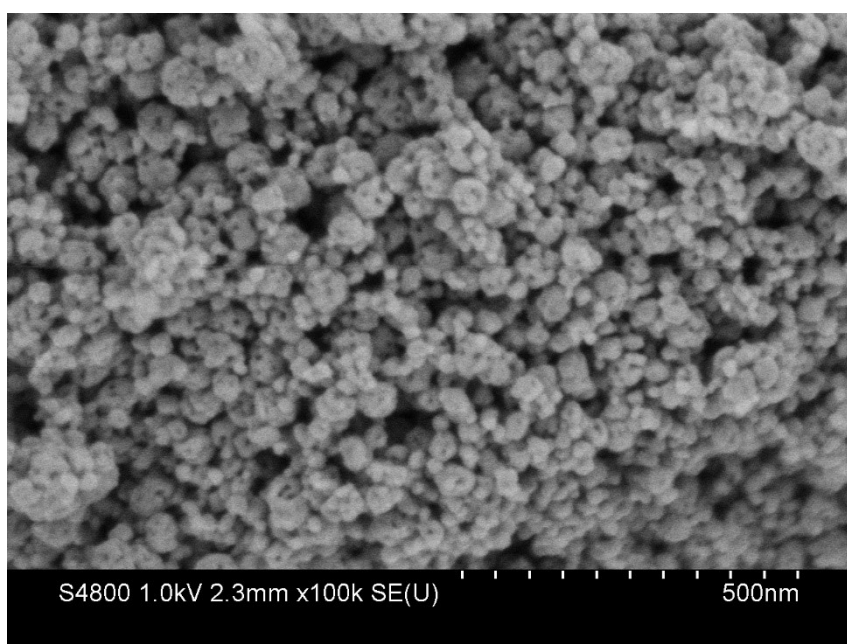


Fig. S1 SEM images of nano-TiO₂

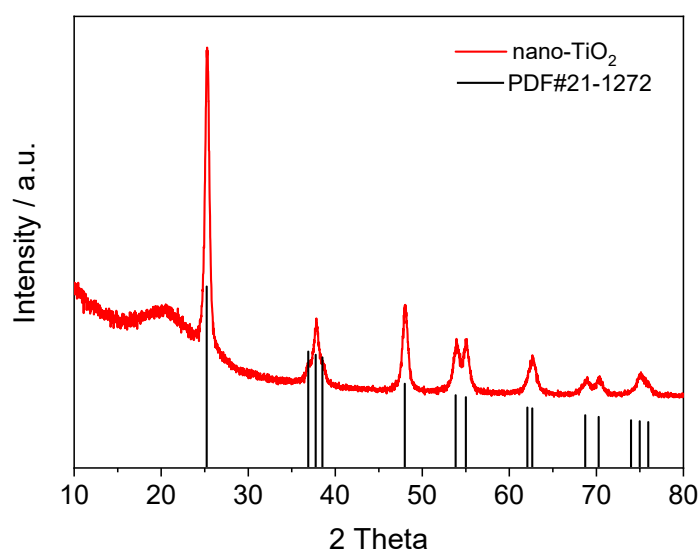


Fig. S2 XRD patterns of nano-TiO₂ and anatase TiO₂ (JCPDS no. 21-1272)

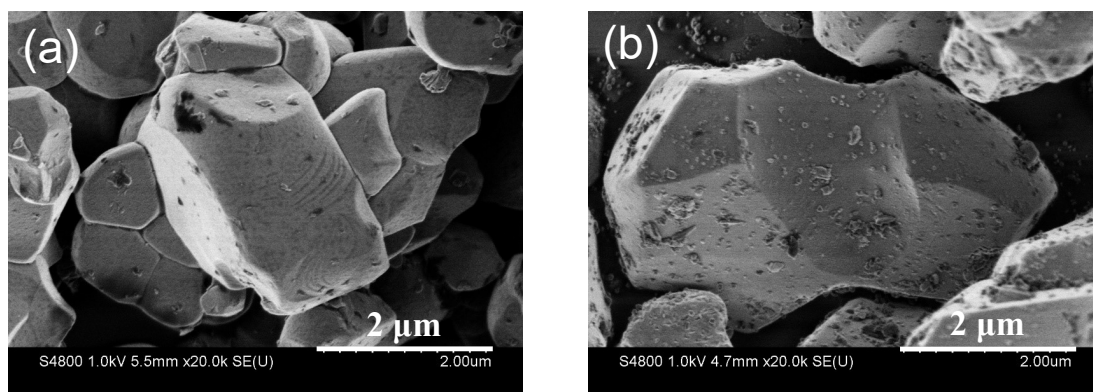


Fig. S3 The magnified SEM images of S-NCM65 and 5TS-NCM65

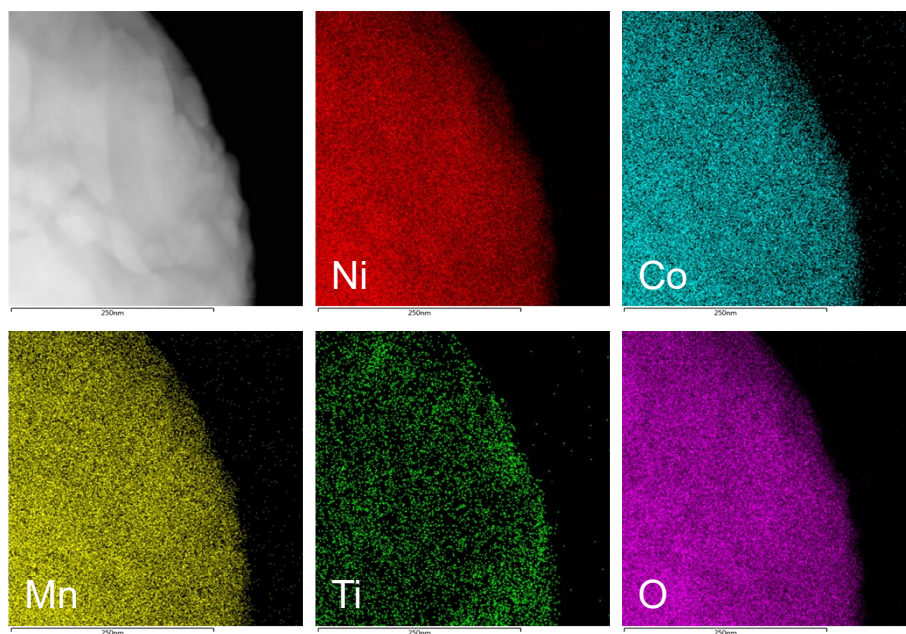


Fig. S4 EDS elemental mapping of selected area of 5TS-NCM65

Table S1 Content of selected elements and residual lithium

Element	Line Type	k Factor	Absorption Correction	Wt%	Atomic %
O	K series	1.260	1.00	42.03	71.6
Ti	K series	0.687	1.00	0.29	0.28
Mn	K series	0.732	1.00	11.37	5.64
Co	K series	0.762	1.00	9.19	4.25
Ni	K series	0.753	1.00	39.25	18.23
Total:				100.00	100.00
Samples			Residual lithium (Li_2CO_3 , ppm)		
S-NCM65			5695		
5T-NCM65			3992		

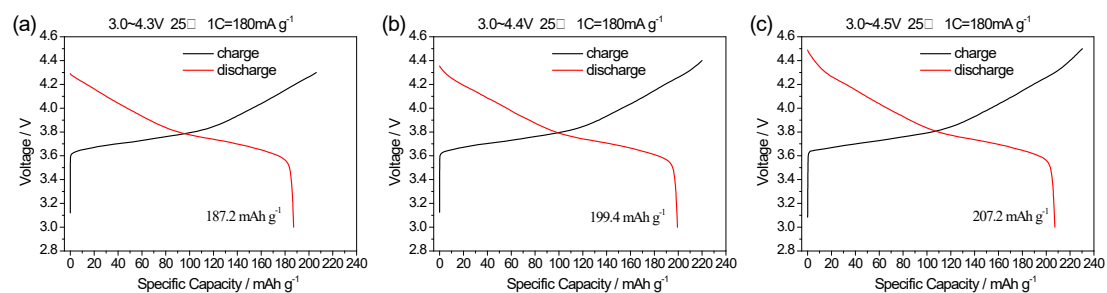


Fig. S5 Initial charge-discharge curves of P-NCM65 at 0.1C and 25°C in the voltage range of (a) 3.0-4.3 V, (b) 3.0-4.4 V and (c) 3.0-4.5 V, respectively

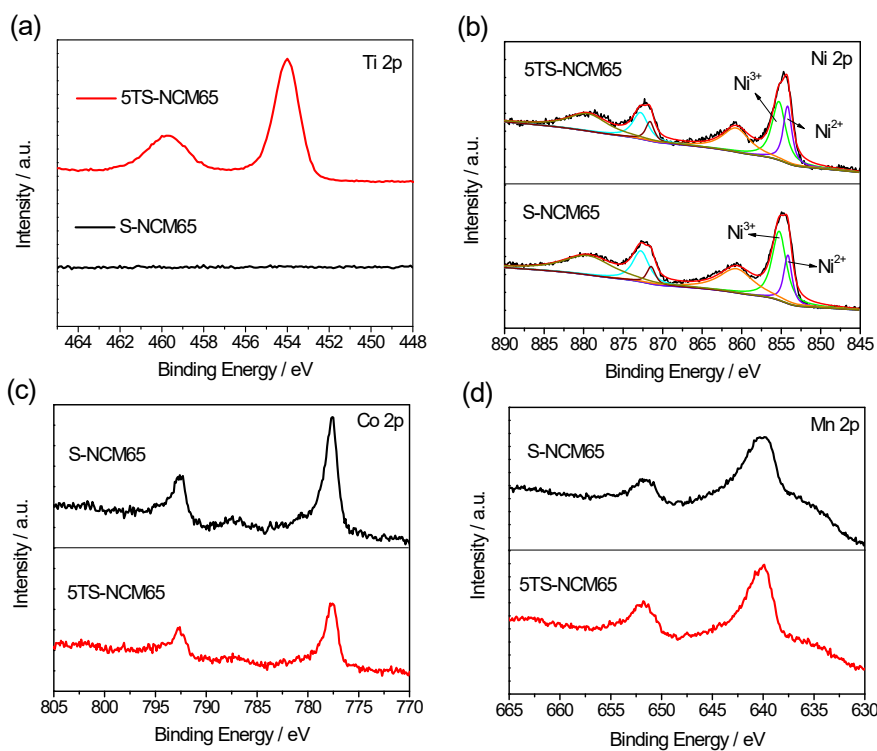


Fig. S6 XPS spectra of (a) Ti 2p, (b) Ni 2p, (c) Co 2p and (d) Mn 2p for S-NCM65 and 5TS-NCM65 cathode. XPS, X-ray photoelectron spectroscopy.

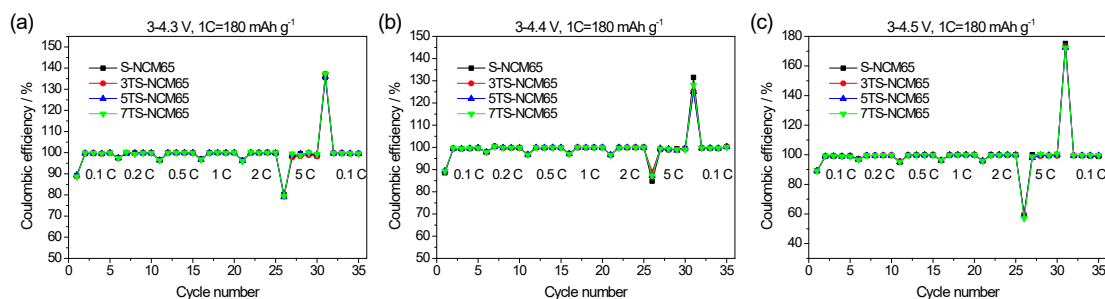


Fig. S7 Coulombic efficiencies of each sample at 25°C in the voltage range of (a) 3.0-4.3 V, (b) 3.0-4.4 V and (c) 3.0-4.5 V, respectively

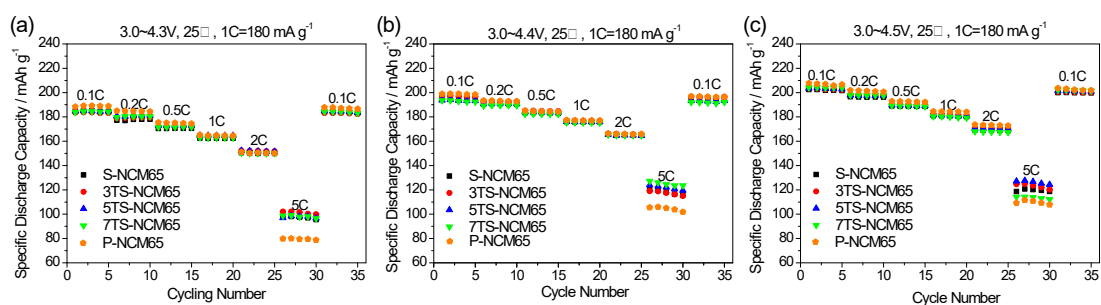


Figure. S8 Rate-performance of single-crystal samples and P-NCM65 at 25°C in the

voltage range of (a) 3.0-4.3 V, (b) 3.0-4.4 V and (c) 3.0-4.5 V, respectively

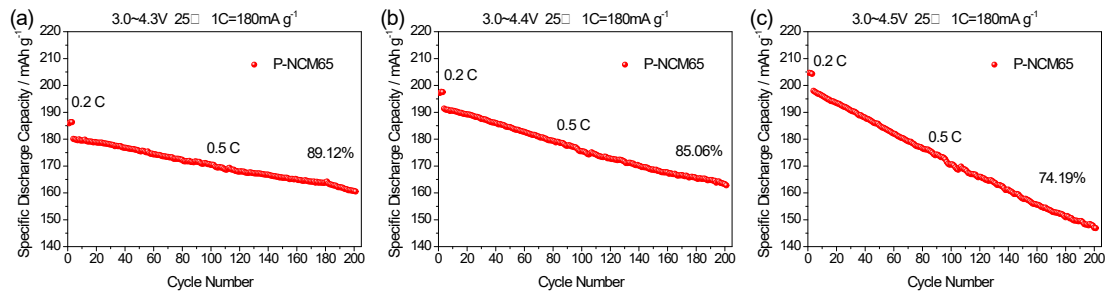


Fig. S9 Cycling performance of P-NCM65 at 25°C in the voltage range of (a) 3.0-4.3 V, (b) 3.0-4.4 V and (c) 3.0-4.5 V, respectively

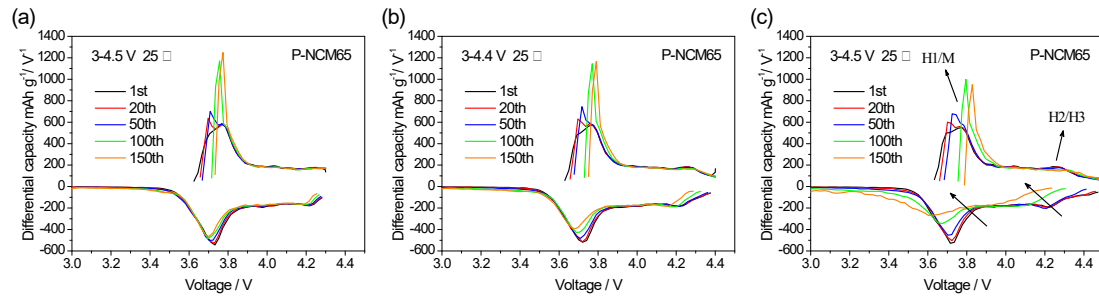


Fig. S10 dQ/dV curves of P-NCM65 at 25°C at 0.5C in the voltage range of (a) 3.0-4.3 V, (b) 3.0-4.4 V and (c) 3.0-4.5 V, respectively

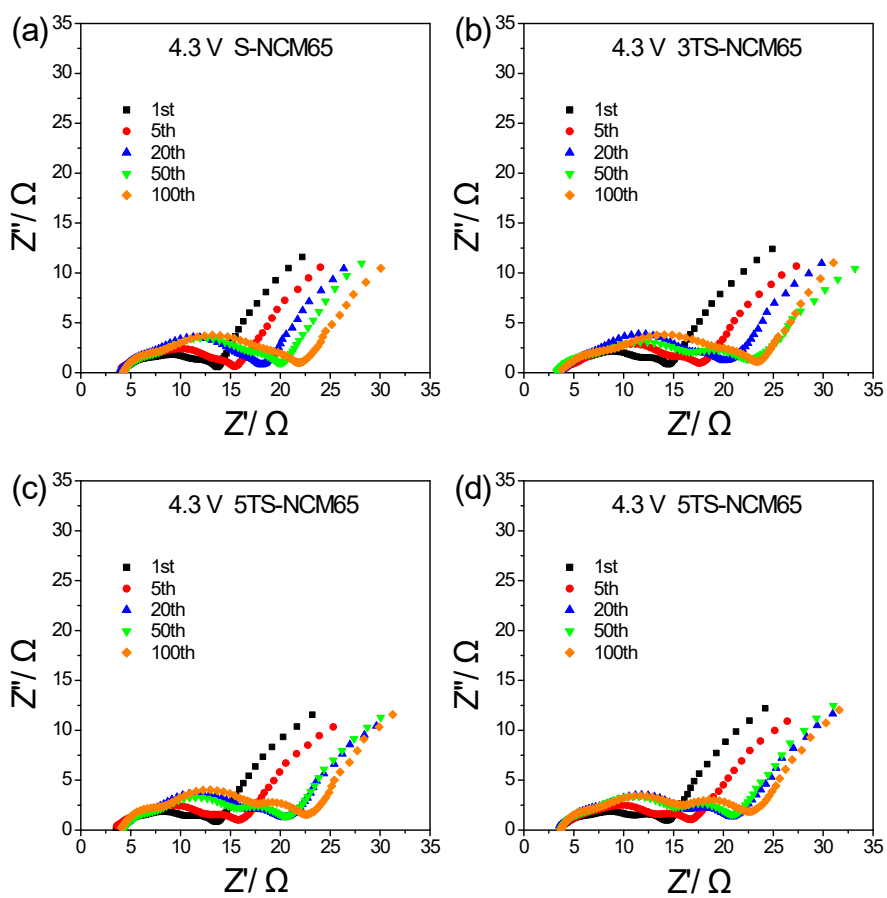


Fig. S11 Nyquist diagram of the sample at 4.3 V cut-off voltage with different cycle numbers

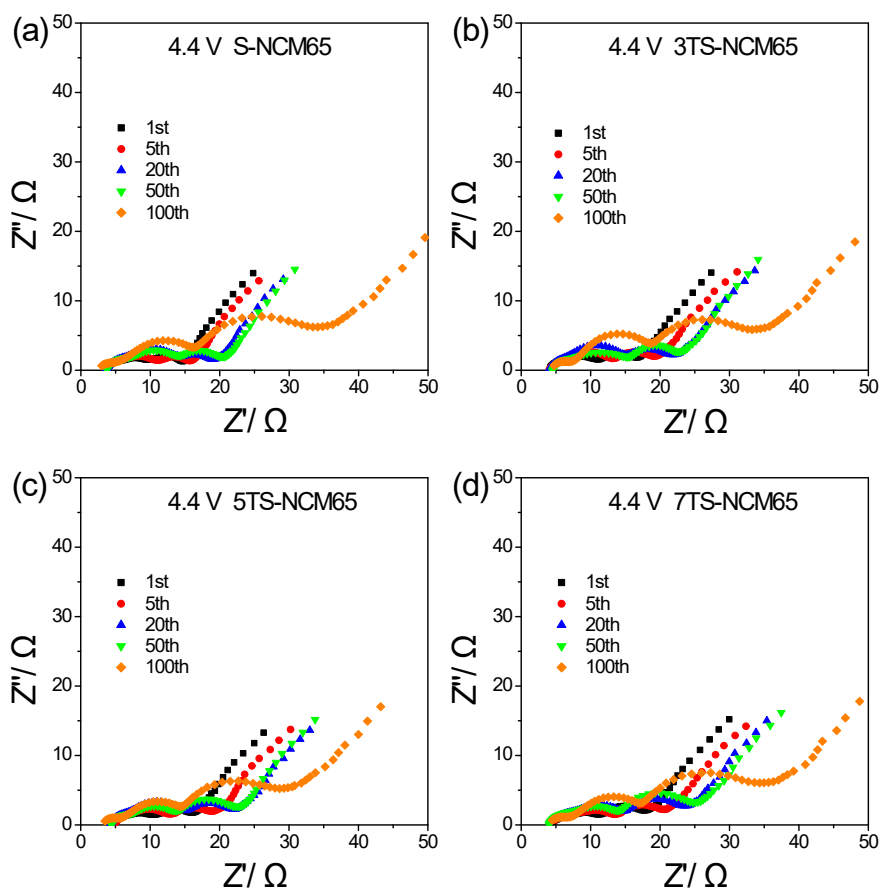


Fig. S12 Nyquist diagram of the sample at 4.3 V cut-off voltage with different cycle numbers

Table S2 EIS fitting data of S-NCM65 and 5TS-NCM65 cycling at different cut-off voltages.

3.0-4.3 V								
Samples	S-NCM65				5TS-NCM65			
	$R_s(\Omega)$	$R_f(\Omega)$	$R_e(\Omega)$	$R_{ct}(\Omega)$	$R_s(\Omega)$	$R_f(\Omega)$	$R_e(\Omega)$	$R_{ct}(\Omega)$
1 st	4.67	3.28	3.83	2.93	3.53	3.20	3.98	3.61
5 th	4.05	3.68	5.63	3.00	3.65	3.83	5.34	3.98
20 th	4.11	3.92	8.56	3.16	3.87	3.91	9.69	4.51
50 th	4.49	3.99	9.46	4.35	4.32	3.76	8.19	5.40
100 th	4.27	4.51	10.23	5.16	4.05	4.57	9.08	5.82

3.0-4.4 V								
Samples	S-NCM65				5TS-NCM65			
	$R_s(\Omega)$	$R_f(\Omega)$	$R_e(\Omega)$	$R_{ct}(\Omega)$	$R_s(\Omega)$	$R_f(\Omega)$	$R_e(\Omega)$	$R_{ct}(\Omega)$
1 st	3.44	3.39	3.99	5.25	4.62	2.02	4.21	5.74
5 th	3.51	3.32	4.88	5.10	4.96	2.50	5.67	7.21
20 th	3.89	4.21	7.21	6.55	4.70	2.58	8.41	7.64
50 th	3.67	3.90	7.21	6.83	4.37	3.43	6.78	8.52
100 th	2.96	3.16	10.66	19.67	3.59	2.84	8.42	14.87

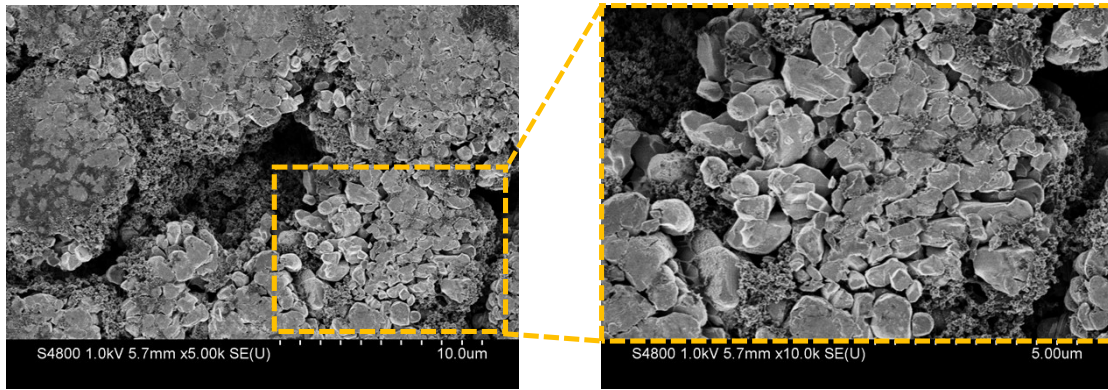


Figure. S13 SEM images of P-NCM65 after 200 cycles at different magnification

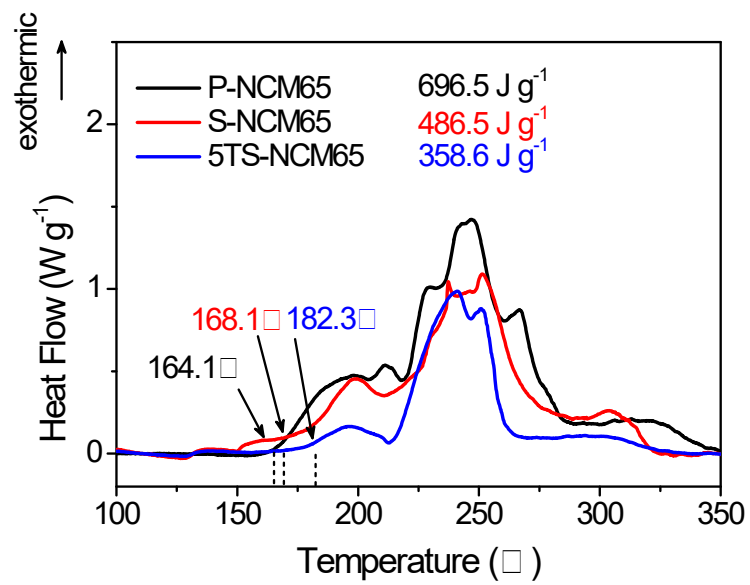


Fig. S14 DSC curves of S-NCM65, 5TS-NCM65 and P-NCM65