

Supplementary information for

A novel surface-heterostructured $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2@\text{Ce}_{0.8}\text{Sn}_{0.2}\text{O}_{2-\sigma}$ cathode material for Li-ion batteries with improved initial irreversible capacity loss

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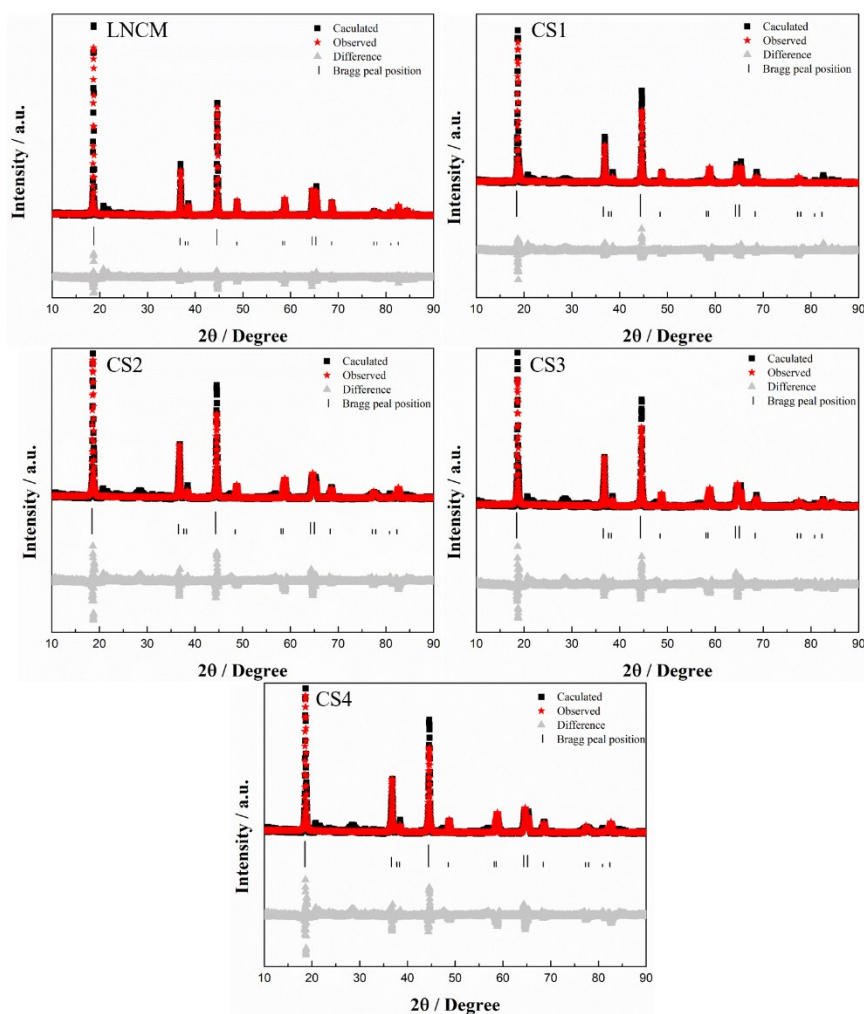


Fig. S1. Reitveld fitting of the XRD patterns of (a) as-prepared LNCM, (b) CS1, (c) CS2, (d) CS3

and (e) CS4 based on the hexagonal R-3m space group

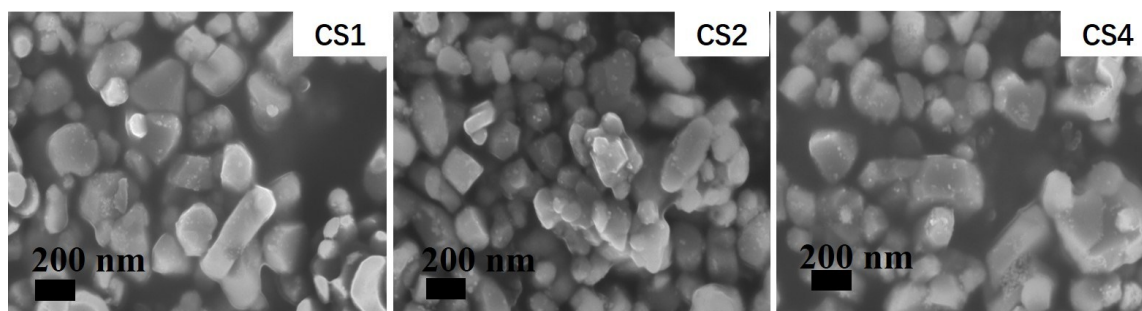


Fig. S2. SEM images of CS1, CS2 and CS4.

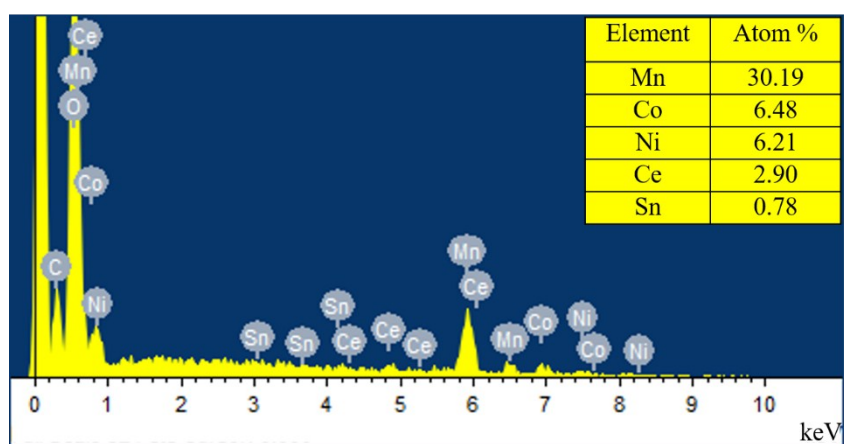


Fig. S3. EDX spectrum of CS3.

Table S1 Relative amounts of Li, Ni, Co, Mn, Ce and Sn in the material and in an acid-treated product.

sample	Li	Ni	Co	Mn	Ce	Sn
Theoretical value	1.200	0.130	0.130	0.540	-	-
LNCM	1.217	0.128	0.134	0.540	-	-
CS1	1.231	0.126	0.136	0.540	0.041	-
CS2	1.232	0.126	0.136	0.540	0.037	0.004
CS3	1.232	0.127	0.135	0.540	0.036	0.009
CS4	1.232	0.126	0.136	0.540	0.034	0.013

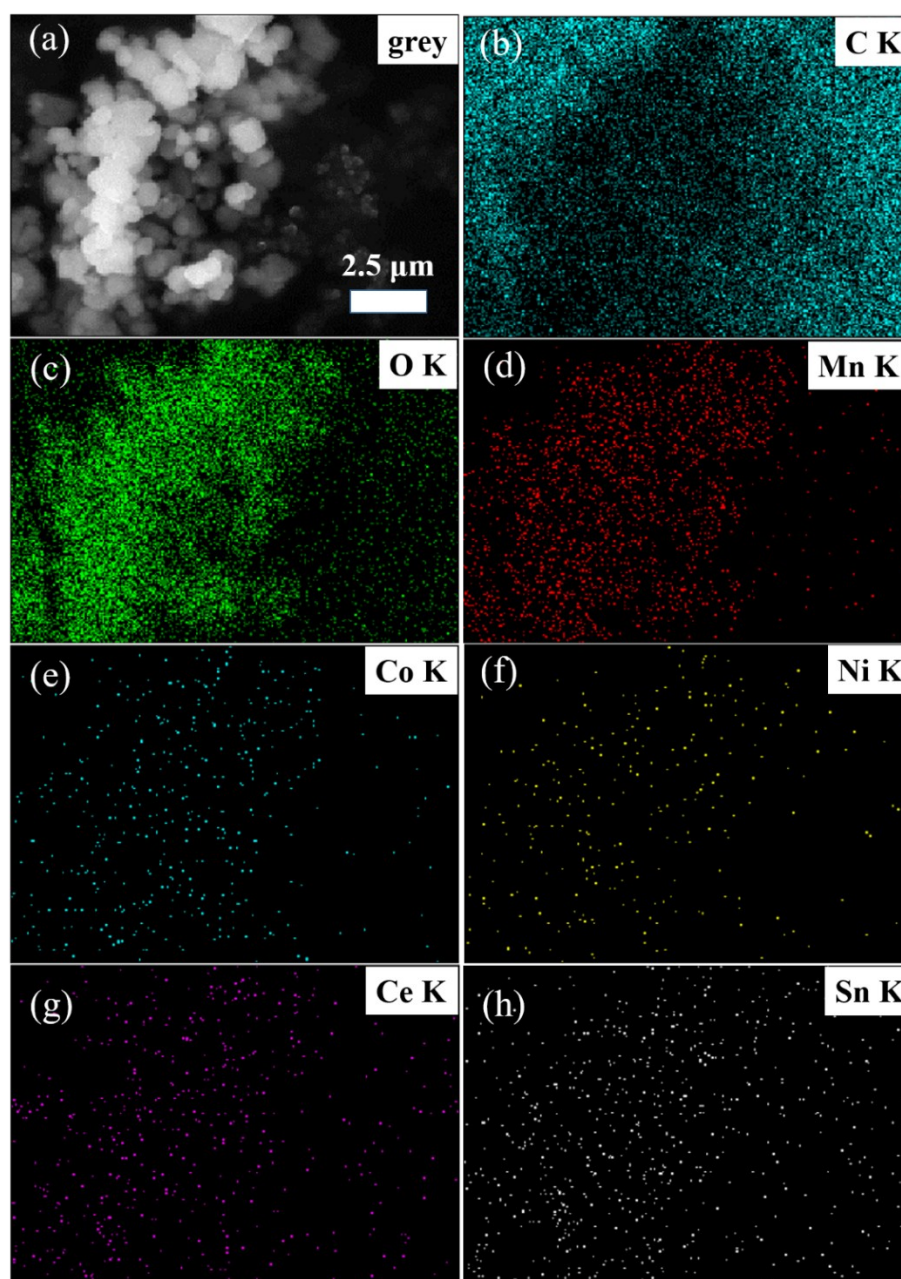


Fig. S4. Elemental mapping of CS3 sample.

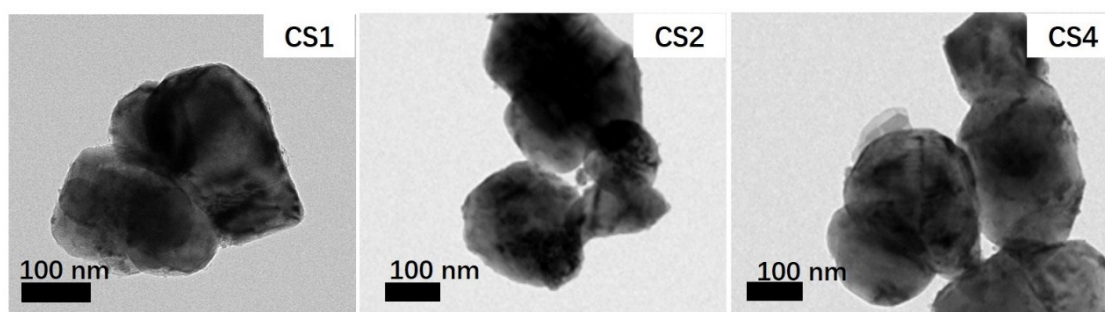


Fig. S5. TEM images of CS1, CS2 and CS4.

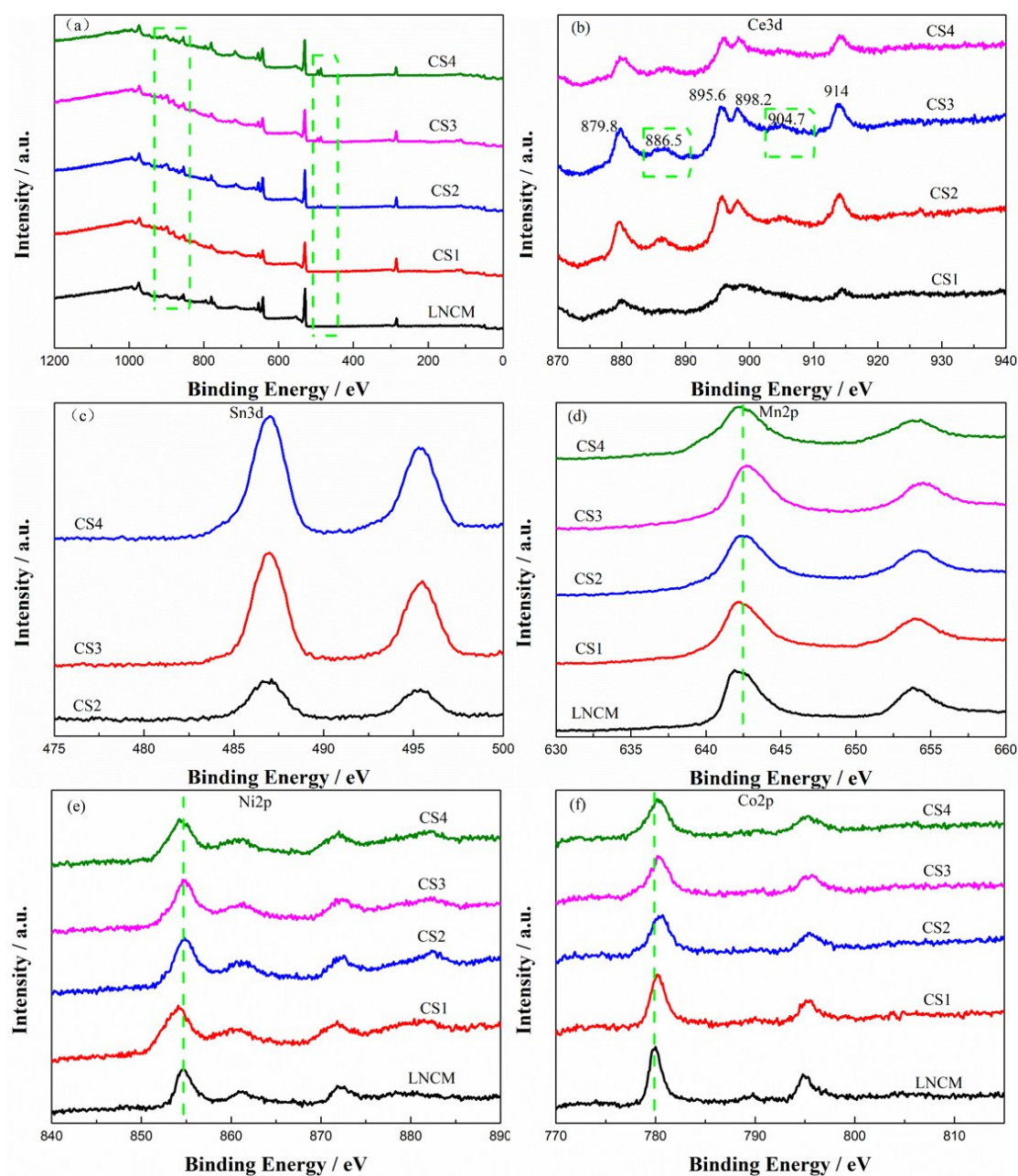


Fig. S6. XPS spectra of the prepared samples (a) full spectra, (b) Ce 3d, (c) Sn 3d, (d) Ni 2p, (e) Co 2p, (d) Mn 2p.

Table S2 Binding energies and surface compositions from deconvolution of XPS spectra for Ce 3d

Sample	CS1	CS2	CS3	CS4
Binding energy (eV)				
Species				

Ce(IV)	880.074	880.084	880.292	880.17
Ce(IV)	896.039	895.789	895.56	895.517
Ce(IV)	899.063	878.935	879.722	879.699
Ce(IV)	914.44	900.409	900.037	899.999
Ce(III)	876.651	878.935	879.722	879.699
Ce(III)	901.918	900.409	900.037	899.999
Ce(III)	—	886.624	886.287	886.276
Ce(III)	—	904.742	904.41	904.62

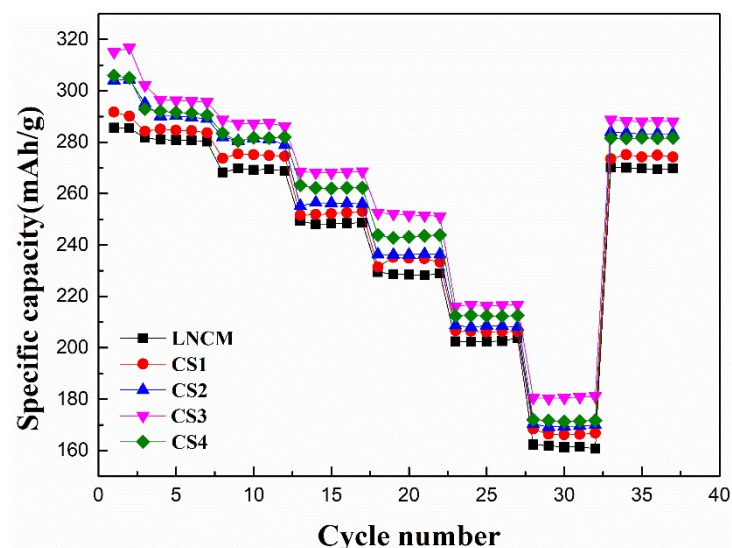


Fig. S7. Rate performance of the pristine LCMN and modified samples.

Table S3. Comparison on the electrochemical performance of Li-rich layered oxides

$\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$ with that of LMNC reported in the literatures.

Samples	Initial coulombic efficiency	discharge capacity (mAh g^{-1})	Irreversible capacity loss (mA h g^{-1})	Ref.
PrPO ₄ treated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	90.0%	286.9	31.9	23
NH ₄ BF ₄ treated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	84.83%	308.7	55.2	42
Ti doped	73.1%	320	118	43

$\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$				
V ₂ O ₅ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	87.8%	279.5	38.7	44
PPy coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	90.7%	273	28	45
FeF ₃ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	80%	280	70	46
LiVO ₃ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	92.6%	272	22	47
Mo doped $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	74.3%	260.8	90	48
LiAlO ₂ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	74.89%	237.1	79.5	49
Samaria Doped Ceria (SDC) coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	77.9%	261	74	50
Gadolinium doped ceria $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	83.3%	265.5	72.2	51
F doped $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	71.2%	240.2	97	52
P ₂ O ₅ surface modified $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	90%	269	30	53
Mg doped $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	72.8%	275.8	103	54
$\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	74.6%	277.3	94.4	55
In situ polyaniline modified $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	89.01%	313.5	38.7	24
LiNi _{0.5} Mn _{1.5} O ₄ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	69.2%	222.9	99	56
CeF ₃ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	80.8%	222.9	53	57
CaF ₂ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	89.6%	277.3	32.2	58
MgO coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	81%	282.2	66.2	59
ZrO ₂ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	80%	253.1	63.3	60
FePO ₄ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	86.6%	259.1	40	61
Na doped $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	87%	307	45.9	62
Y ₂ O ₃ coated $\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2$	82.3%	280.3	60	63

$\text{Li}_{1.2}\text{Mn}_{0.54}\text{Ni}_{0.13}\text{Co}_{0.13}\text{O}_2@\text{Ce}_{0.2}\text{Sn}$ $0.8\text{O}_{2-\sigma}$	92.77%	315.1	24.4	This work
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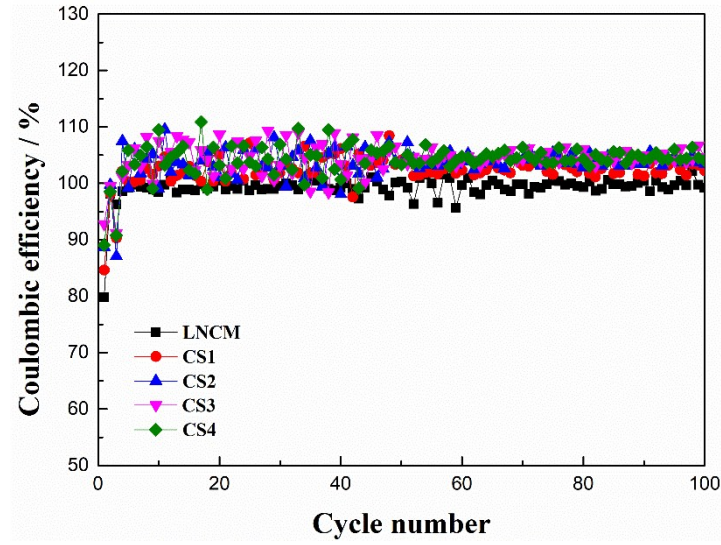


Fig. S8. Columbic efficiency of the pristine LNCM and modified samples at 0.1C.

Table S4. Fitted parameters of the prepared samples for the first cycle.

Samples	Pristine	CS1	CS2	CS3	CS4
	LNCM				
R_s/Ω	3.425	3.398	3.332	2.931	3.232
R_{sf}/Ω	152.6	148.5	134.6	79.2	110.0
R_{ct}/Ω	83.8	66.2	64.6	20.5	38.4
σ	20.626	18.337	16.079	10.721	12.230
$D_{\text{Li}^+}/\text{cm}^2\text{s}^{-1}$	3.99×10^{-16}	5.06×10^{-16}	6.57×10^{-16}	1.48×10^{-15}	1.14×10^{-15}

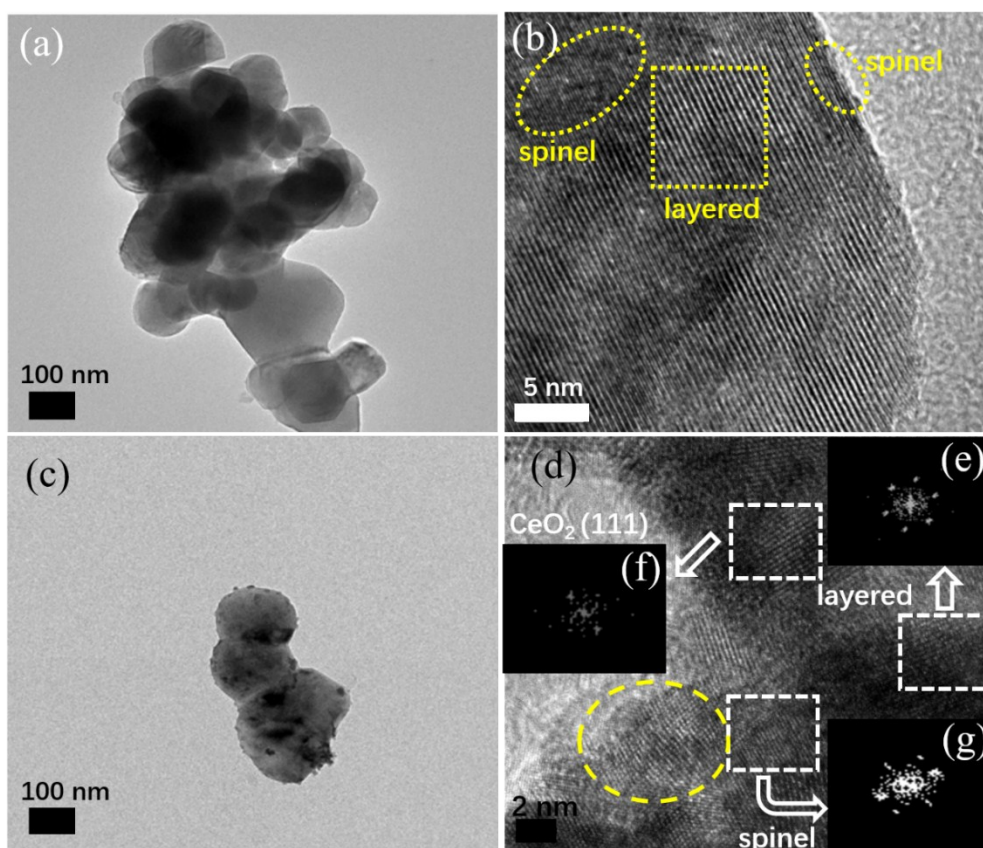


Fig. S9. (a) TEM and (b) HRTEM images of the pristine LNCM; (c) TEM and (d) HRTEM images of the CS3 samples after 100 cycles; Further FFT images for sections corresponding to the white boxes, as shown in panels (e), (f) and (g).

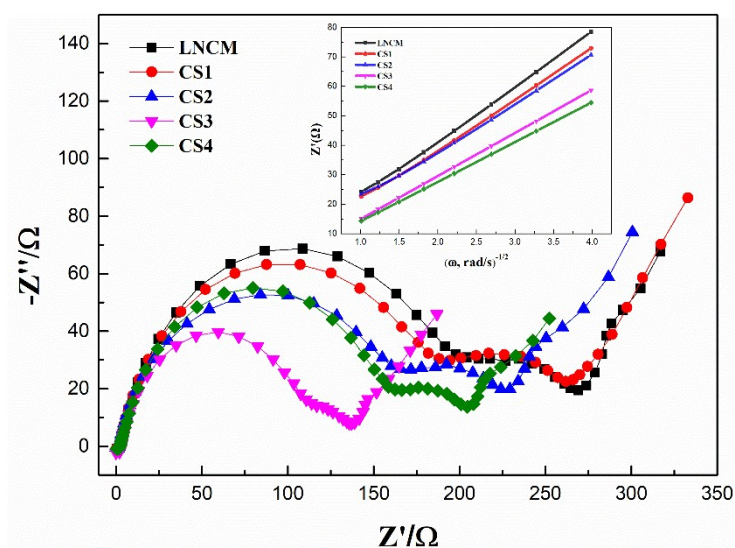


Fig. S10. Electrochemical impedance spectra (EIS) of the prepared samples and the inset is Randles plots of the prepared samples

Table S5. Fitted parameters of the prepared samples after the 100 th cycles.

Samples	Pristine	CS1	CS2	CS3	CS4
LNCM					
R_s/Ω	3.802	3.632	3.621	3.215	3.539
R_{sf}/Ω	204.1	194.5	165.0	110.2	158.1
R_{ct}/Ω	103.6	70.6	59.2	34.2	46.5
D_{Li^+}/cm^2s^{-1}	5.08×10^{-16}	5.88×10^{-16}	6.64×10^{-16}	1.34×10^{-15}	9.35×10^{-16}