

Supporting Information

Sulfurized Synthesis of a New Anode Material for Li-Ion Batteries: Understanding the Role of Sulfurization in Lithium Ion Conversion Reactions and Promoting Lithium Storage Performance

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1. SEM and TEM images of MnO@NC and NC

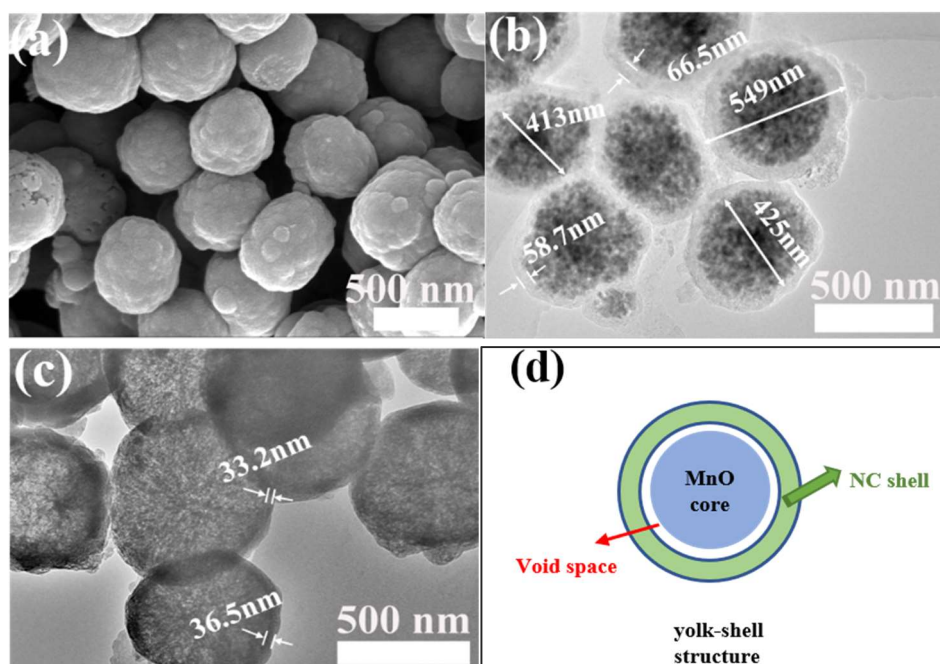


Figure S1. (a) SEM and (b) TEM images of MnO@NC. (c) TEM image of NC obtained from MnO@NC through the etching of MnO. (d) Schematic illustration of the yolk-shell structure of MnO@NC.

2. TGA curve of MnOS@NSC and XRD pattern after the TGA analysis

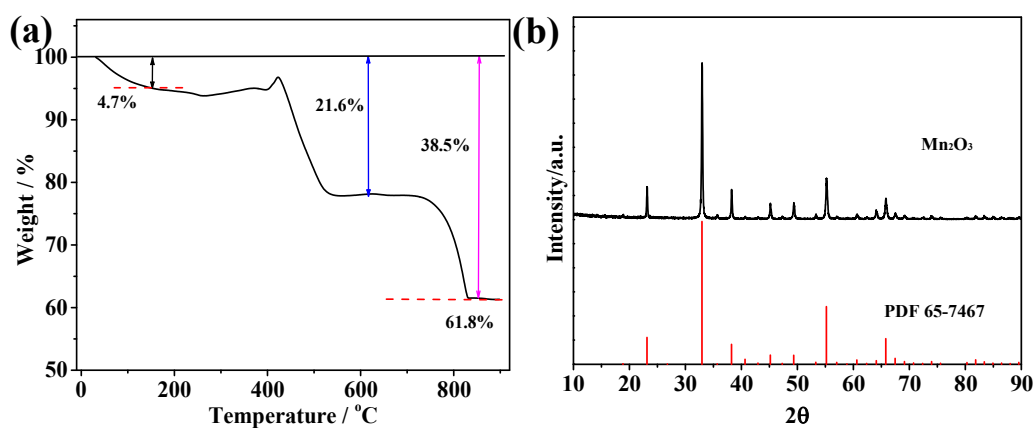


Figure S2. (a) TGA curve of MnOS@NSC, (b) XRD pattern of MnOS@NSC after the TGA analysis.

Calculation of the weight percentage of the NSC in the MnOS@NSC

The weight loss of the MnOS@NSC at the TGA curves in Figure S2a below 150 °C could be attributed to the removal of physically adsorbed water. The weight increment at 420 °C can be attributed to the formation of MnSO₄ and/or Mn₃O₄¹ and the subsequent weight loss is the decomposition of the NSC. The weight loss at 700 °C – 830 °C is the transformation of MnSO₄ and/or Mn₃O₄ to Mn₂O₃. The formation of Mn₂O₃ after the TGA analysis is demonstrated by the XRD pattern in Figure S2b. The content of NSC in the MnOS@NSC (M_{NSC}) can be estimated based on Eq. S2 (where M is the weight percentage, W is the molecular weight).

$$\frac{2 \times W_{MnOS}}{100 - M_{H_2O} - M_{NSC}} = \frac{W_{Mn_2O_3}}{M_{Mn_2O_3}} \quad (S1)$$

3. Raman spectra of MnOS@NSC

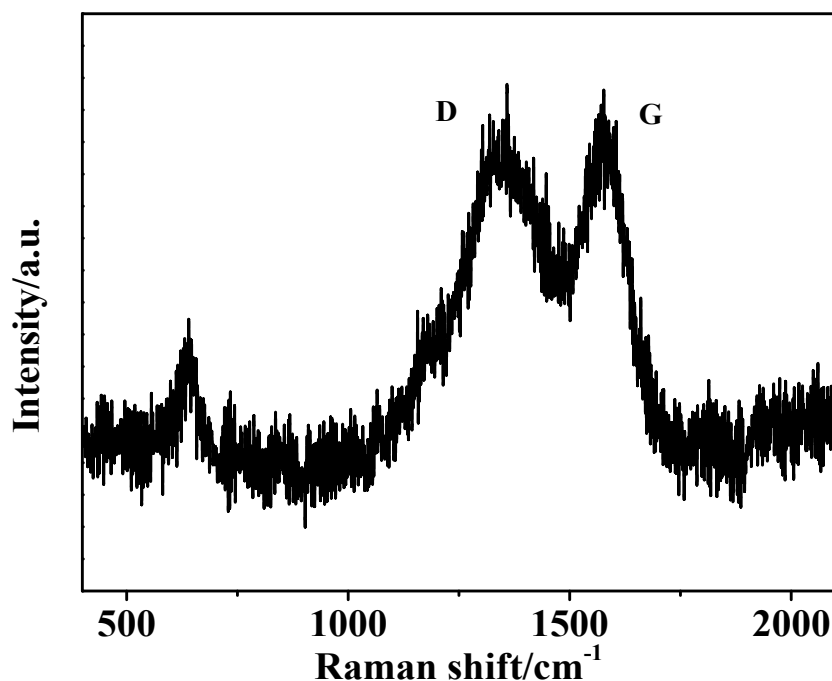


Figure S3. Raman spectra of MnOS@NSC.

4. Rate performance comparison of the MnOS@NSC with other TMO-based anode materials

Table S1. Rate performance comparison of the MnOS@NSC with other TMO-based anode materials.

Samples	mass loading mg cm ⁻²	0.1 A g ⁻¹	0.2 A g ⁻¹	0.5 A g ⁻¹	1.0 A g ⁻¹	2.0 A g ⁻¹	5.0 A g ⁻¹	10.0 A g ⁻¹	Reference
MnOS@NSC	1.5	1339.3	1204.1	1073	928.2	734.7	506.5	290.1	This work
HCF/Mn ₃ O ₄		880	827	750	665	528			2
Mn ₃ O ₄ -rGO	1.2	605	480	385	302	198			3
MnO ₂ @C@ MnO		867.6	709.6	597.1	483.5	387.9			4
m MnO ₂ -srGO		946.1	852	805	690	643			5
MnO ₂ /rGO		811	624	394.4	278.2	242.4	168.2		6
MnO ₂ @HCSO	1.2	792	699	582	495	411	328		7
Porous Mn ₂ O ₃		1012	809	625	509	411	185		8
G/MnO-800	1.5	1000	930	875	762	604			9
MnO@NC	1.0	762	707	643	570	512			10
MnO/RGO		948	817	575	489				11
p-MnO@N-C NTs	1-1.5	945.5	922	859.5	785.7				12
MnO@GS/CNT	1.0	677	600	620	580	530			13
MnO@CNFs	1.2-1.5	817	755	637	520	407			14
MnO@NC		780	650	520	410	335			15
Fe ₂ O ₃ /carbon			790	570	450	300		130	16
α- Fe ₂ O ₃ -CNFs	1.77	430	385	288					17
Fe ₃ O ₄ -C			750	585	518	435	198		18
Fe ₃ O ₄ -graphene	1.0	1045		600	410				19
Mesoporous NiO		712	656	607	582	515			20
Porous NiO			510	495	468				21
NiO/C		790		616	461				22
NiO-GNS		1053	1059	967	823				22
CoO-G-C		770	680	570	490	400			23
CoO/C		485	382						24
Co ₃ O ₄ /graphene		990	975	805	600				25
Co ₃ O ₄ @CNT		789	680	505	453		408		26

5. Electrochemical performance of NSC and NC

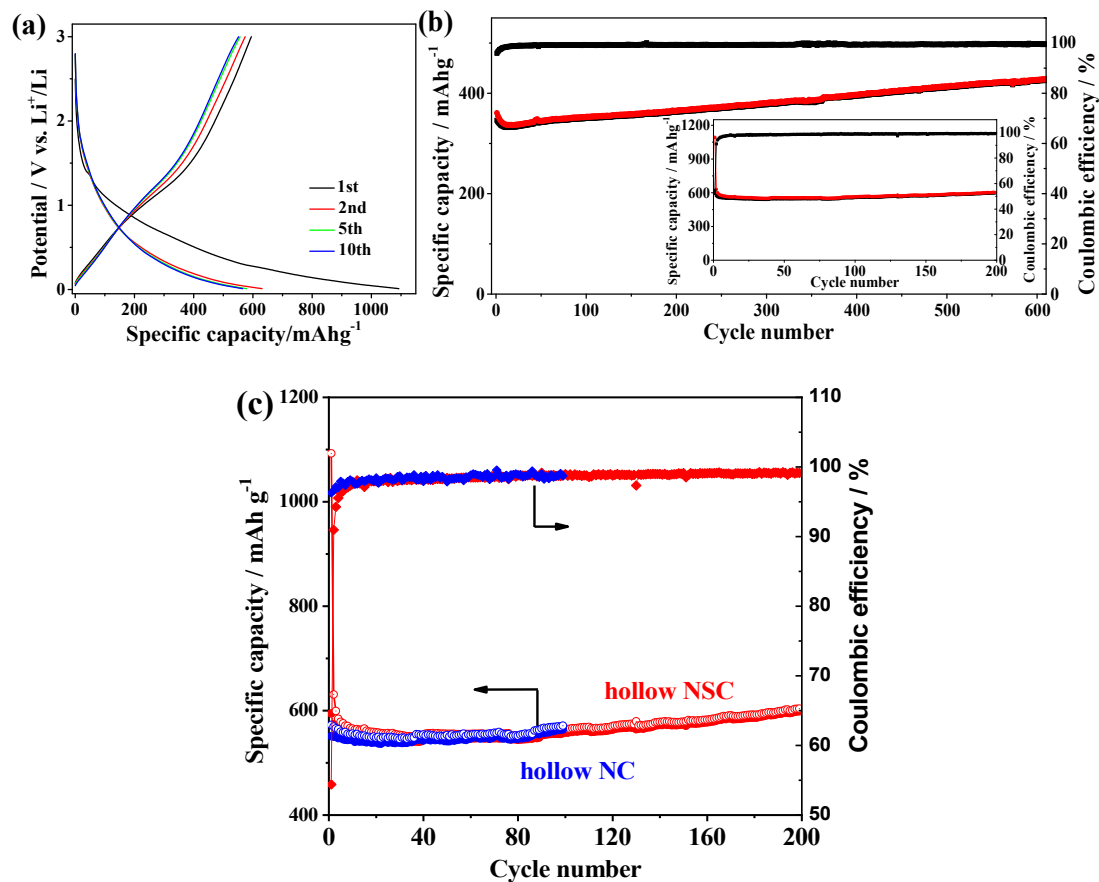


Figure S4. (a) Charge/discharge profiles of the NSC at 100 mA g⁻¹. (b) Cycling performance and Coulombic efficiency of the NSC at 1000 mA g⁻¹. The inset shows the cycling performance and Coulombic efficiency of the NSC at 100 mA g⁻¹. (c) The cycling performance and Coulombic efficiency of the hollow NSC and hollow NC at 100 mA g⁻¹.

6. High resolution XPS spectra of C 1s, O 1s, N 1s, and S 2p in NSC.

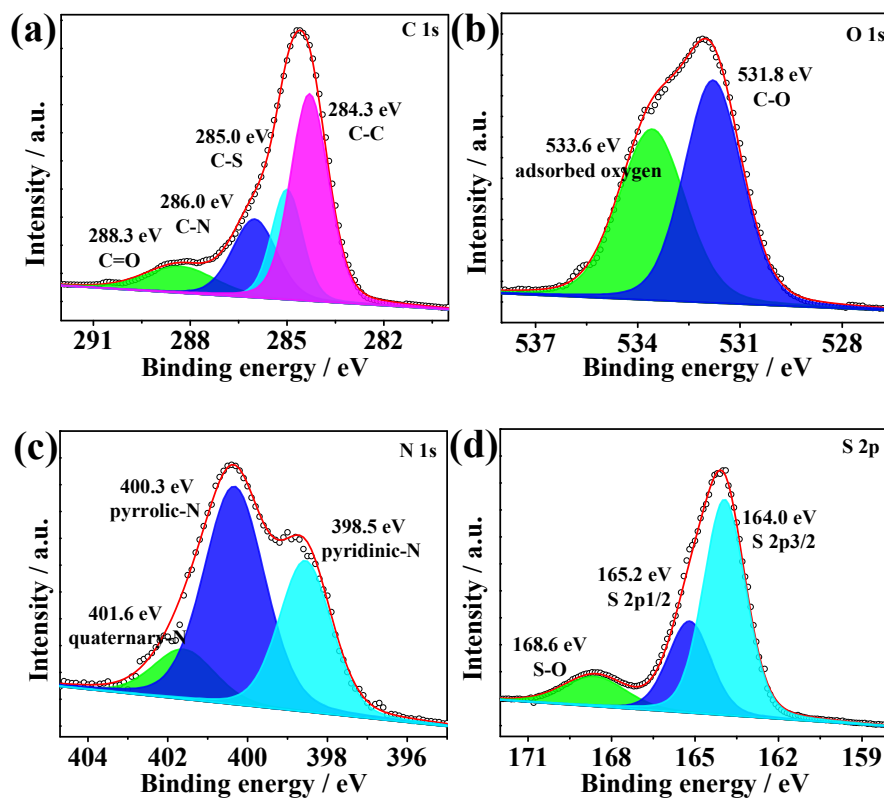


Figure S5. High resolution XPS spectra of (a) C 1s, (b) O 1s, (c) N 1s, and (d) S 2p in NSC.

Table S2. Atomic percentages of C, O, N and S in NSC.

Sample	C (%)	O (%)	N (%)	S (%)
NSC	79.53	11.99	6.89	1.59

7. Total and projected DOSs of MnO₂

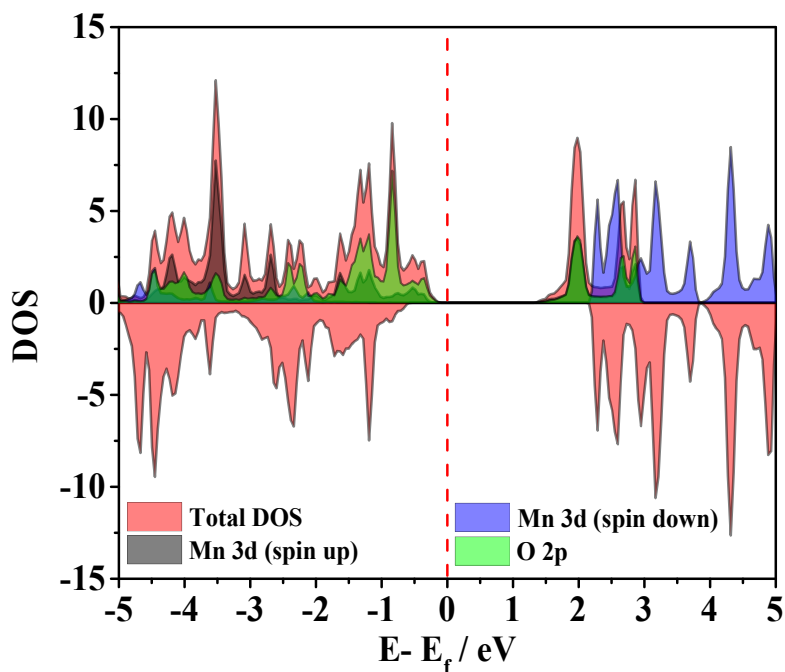


Figure S6. Total and projected DOS of Mn and O atoms.

8. Comparison of the charge transfer resistance of MnOS@NSC with other MnO₂-based electrodes

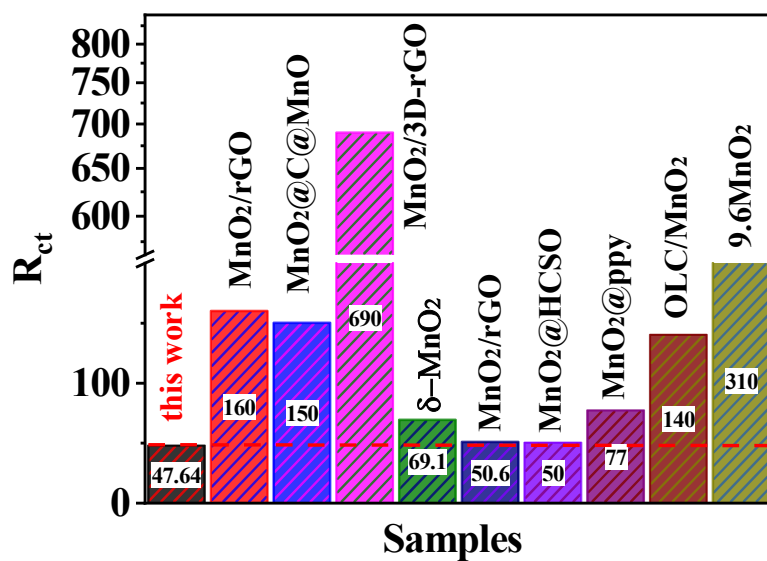


Figure S7. Comparison of the charge transfer resistance with MnO and other MnO₂-

based electrodes.

Table S3. Comparison of the charge transfer resistance with MnO and other MnO₂-based electrodes.

Samples	mass loading mg cm ⁻²	R _{ct}	Reference
MnOS@NC-1	1.5	47.64	This work
MnO ₂ /rGO	-	160	27
MnO ₂ @C@MnO	-	150	4
MnO ₂ /3D-rGO	-	690	28
δ-MnO ₂	1.1	69.1	29
MnO ₂ /rGO	-	50.6	6
MnO ₂ @HCSO	1.2	50	7
MnO ₂ @ppy	0.87	77	30
OLC/MnO ₂	3-4	140	31
9.6 MnO ₂	1.0	310	32
MnO@NC	1.4	100	33

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