Supporting information

Subnanometric CoSn clusters Embedded N-doped Carbon Nanobox (SN-CoSn@C NBs) Realizes High Efficiency Adsorption-Conversion of Polysulfide

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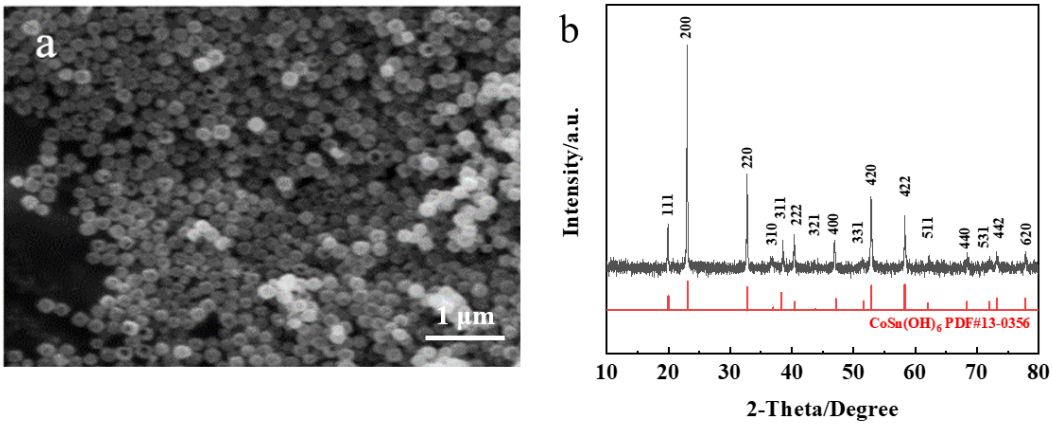

Fig. S1. SEM image and XRD pattern of the $CoSn(OH)_6$ sample.

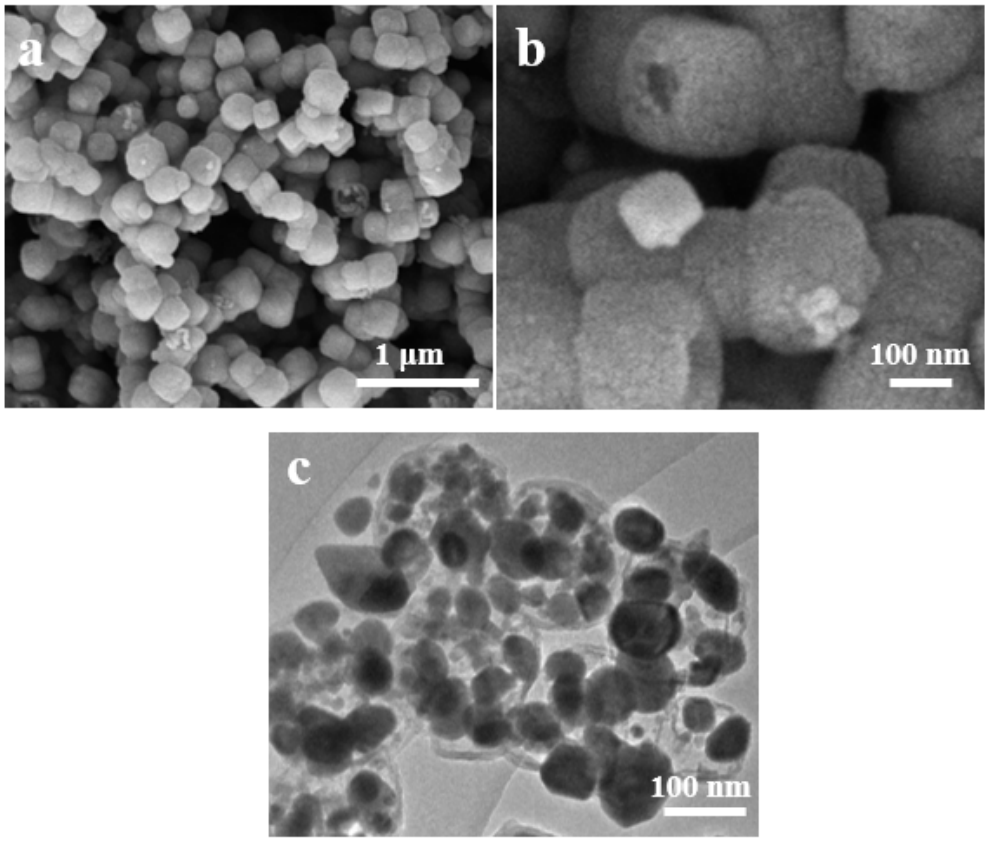

Fig. S2. (a, b) SEM and (c) TEM images of the $CoSnO_x$@C NBs sample.

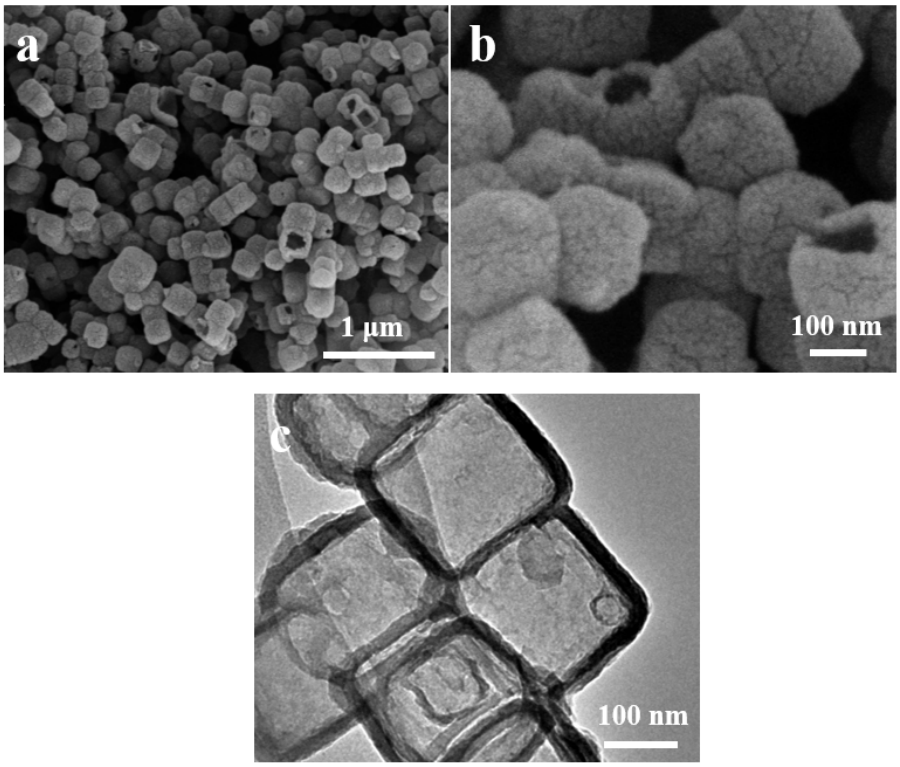

Fig. S3. (a, b) SEM and (c) TEM images of the CoSn@C NBs sample.

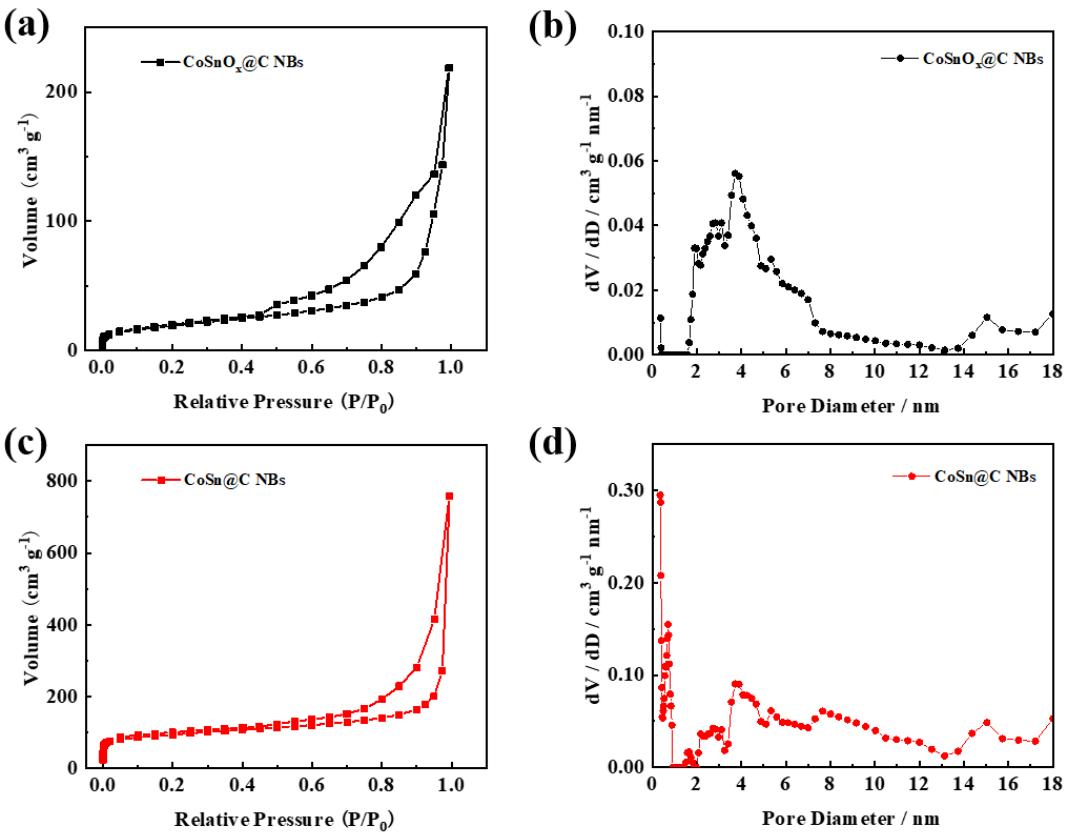

Fig. S4. (a) N_2 sorption isotherm and (b) pore-size distribution (PSD) of the $CoSnO_x$@C NBs sample. (c) N_2 sorption isotherm and (d) pore-size distribution (PSD) of the CoSn@C NBs sample.

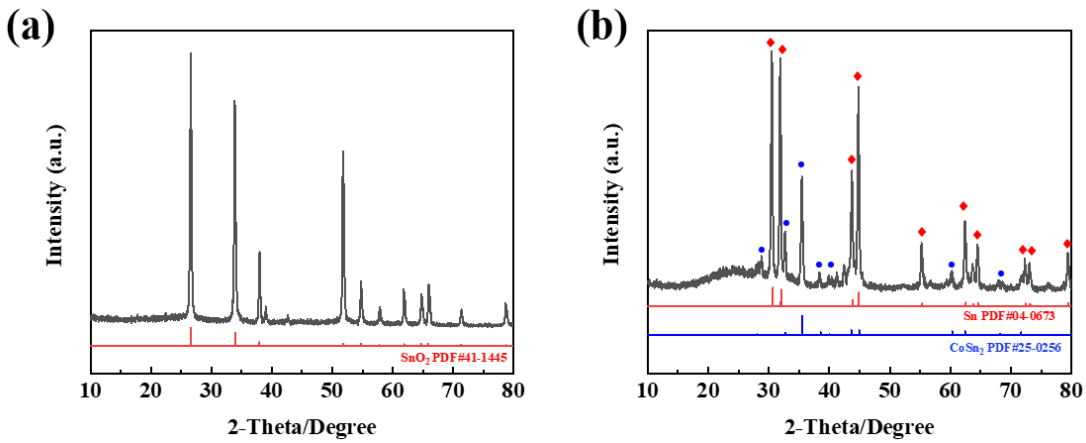

Fig. S5. XRD patterns of (a) after 6 M H_2SO_4 etching, and (b) after H_2 reduction.

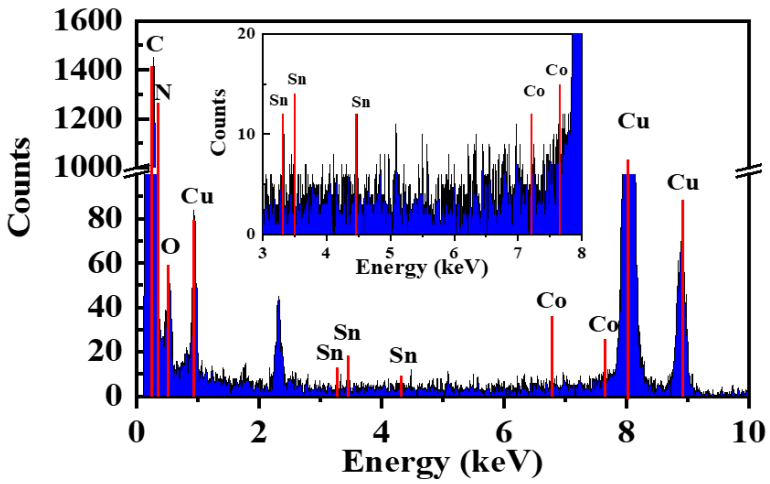

Fig. S6 EDS spectra of the SN-CoSn@C NBs sample.

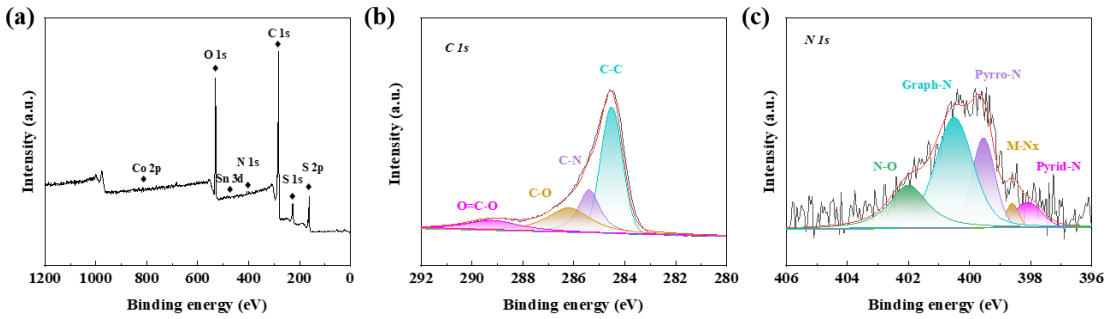

Fig. S7. (a) XPS spectrum, (b) high-resolution C *1s* and (c) N *1s* XPS spectrum of the SN-CoSn@C NBs sample.

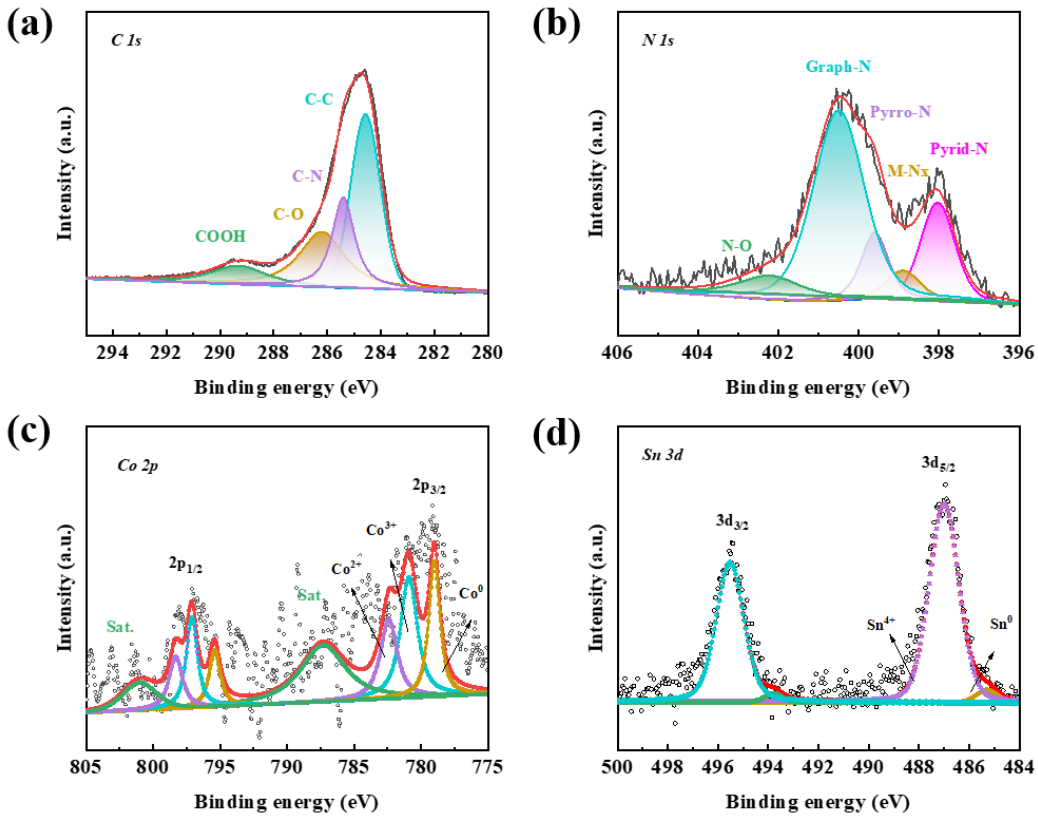

Fig. S8. High-resolution XPS spectra of the CoSn@C NBs sample: (a) C *1s,* (b) N *1s* (c) Co *2p* and (d) Sn *3d.*

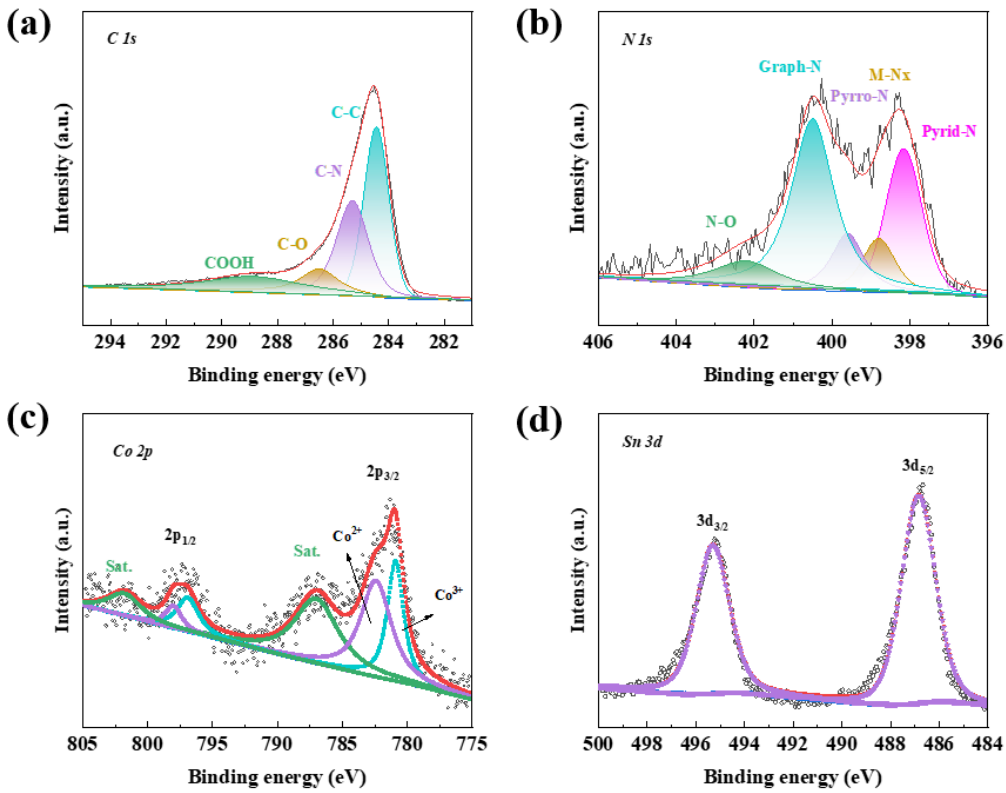

Fig. S9. High-resolution XPS spectra of the $CoSnO_x$@C NBs sample: (a) C *1s*, (b) N

1s (c) Co *2p* and (d) Sn *3d*.

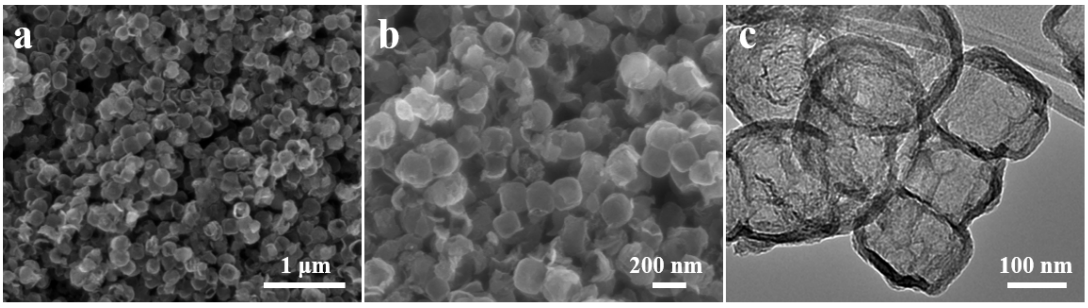

Fig. S10. (a, b) SEM and (c)TEM images of the CoSn@C NBs/S sample.

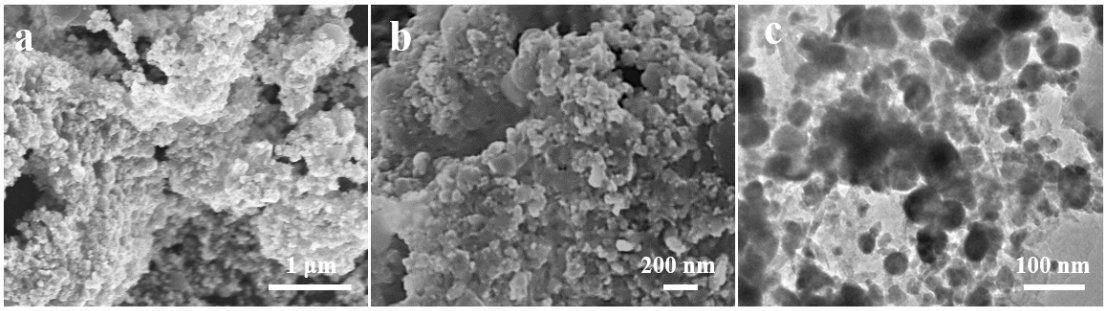

Fig. S11. (a, b) SEM and (c) TEM images of the $CoSnO_x$@C NBs/S sample.

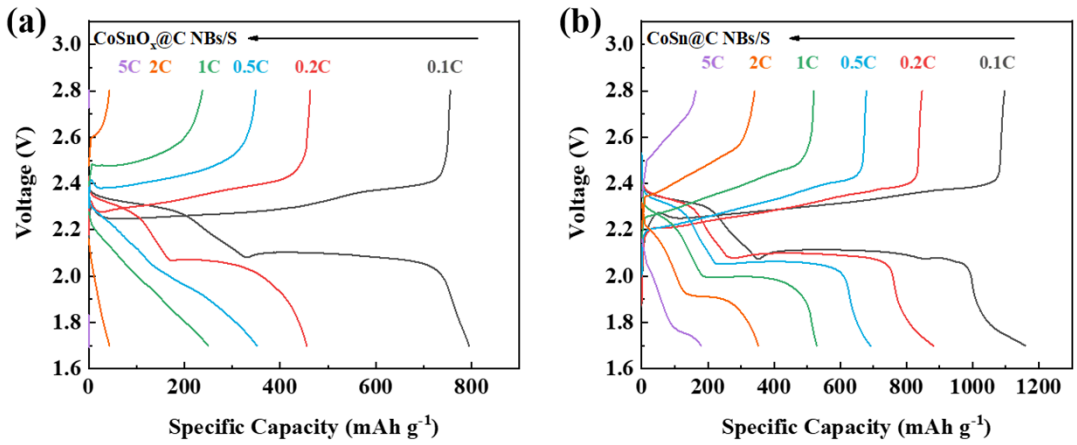

Fig. S12. The charge-discharge curves of (a) $CoSnO_x$@C NBs/S and (b) CoSn@C NBs/S electrodes at different current densities.

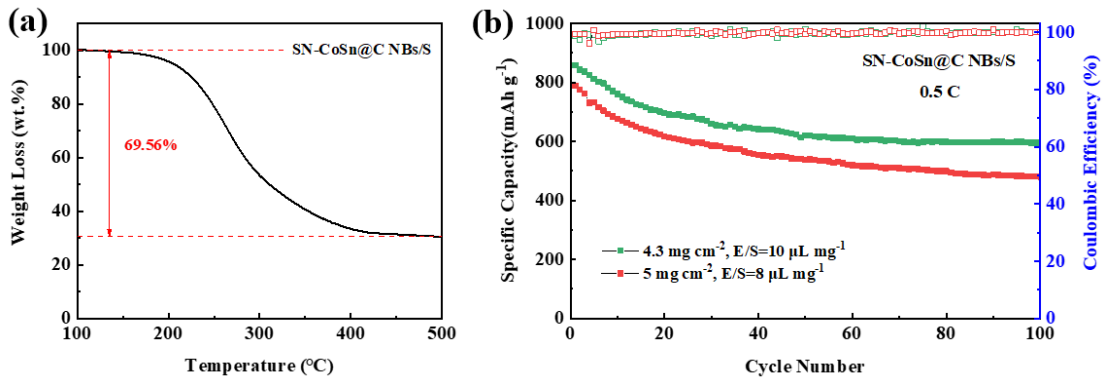

Fig. S13. (a) TGA analysis of the SN-CoSn@C NBs sample with 70% S-loading. (b) Cycling stability of SN-CoSn@C NBs/S electrode at 0.5 C: sulfur loading of 4.3 mg cm^{-2}, E/S=10 μL mg^{-1} and 5 mg cm^{-2}, E/S=8 μL mg^{-1}。

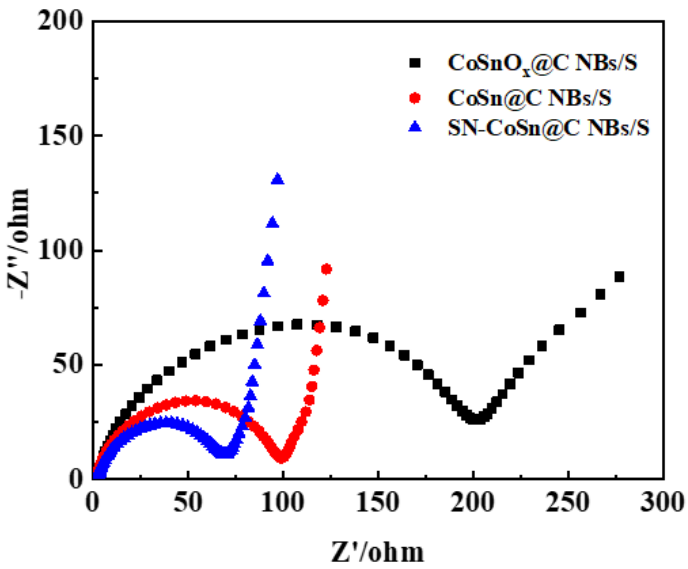

Fig. S14. EIS curves of the $CoSnO_x$@C NBs/S, CoSn@C NBs/S and SN-CoSn@C NBs/S samples.

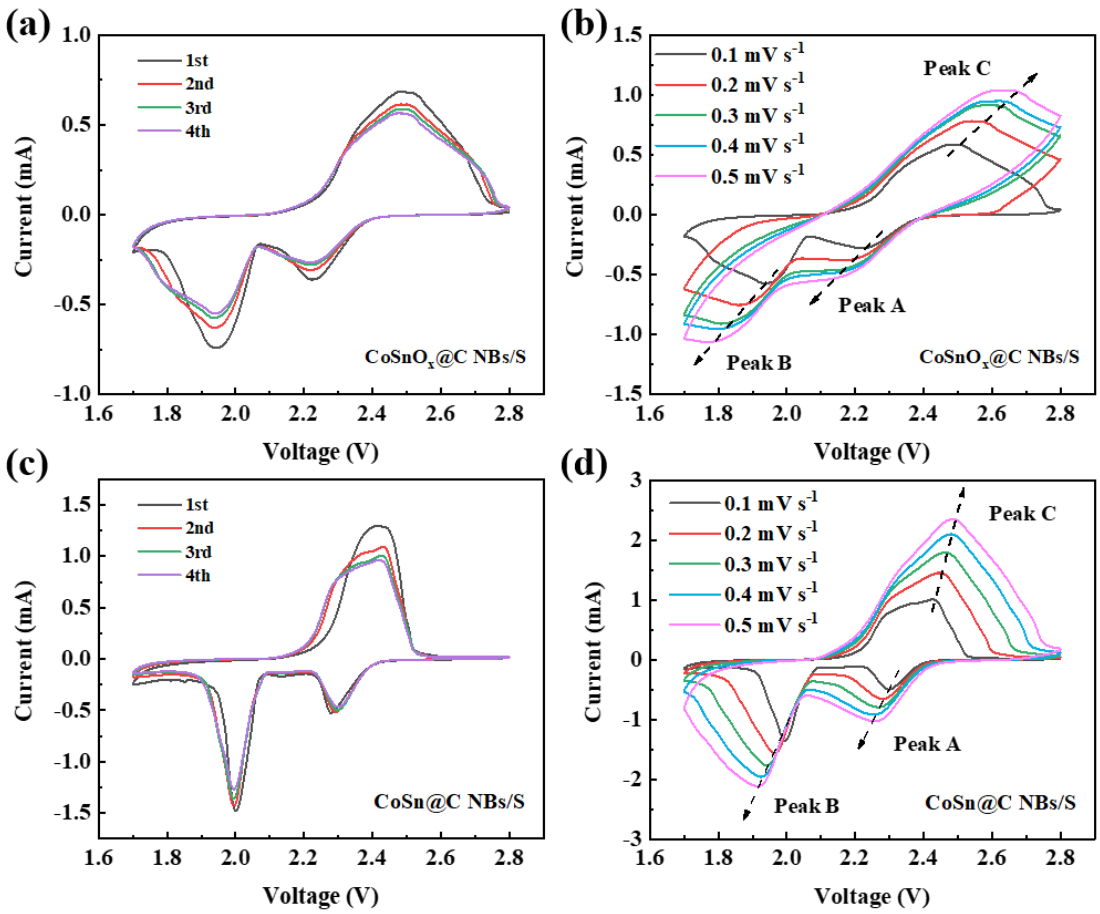

Fig. S15. CV curves of the $CoSnO_x$@C NBs/S sample: (a) 0.1 mV s^{-1} and (b) 0.1-0.5 mV s^{-1}. CV curves of the CoSn@C NBs/S sample: (c) 0.1 mV s^{-1} and (d) 0.1-0.5 mV s^{-1}.

Table S1. Li^+ diffusion coefficients of the $CoSnO_x$@C NBs/S, CoSn@C NBs/S and SN-CoSn@C NBs/S three samples.

D_{Li^+}(cm^2 s^{-1})	A(cathodic peak)	B(cathodic peak)	C(anodic peak)
	$S_8 \rightarrow LiPS(Li_2S_n, 4 \leq n \leq 8)$	LiPS (Li_2S_n,$2 \leq n < 4$)$\rightarrow Li_2S_2/Li_2S$	$Li_2S_2/Li_2S \rightarrow$ LiPS$\rightarrow S_8$
$CoSnO_x$@C NBs/S	$5.03*10^{-10}$	$1.62*10^{-9}$	$1.43*10^{-9}$
CoSn@C NBs/S	$2.04*10^{-9}$	$4.31*10^{-9}$	$1.33*10^{-8}$
SN-CoSn@C NBs/S	$7.02*10^{-9}$	$1.88*10^{-8}$	$4.33*10^{-8}$

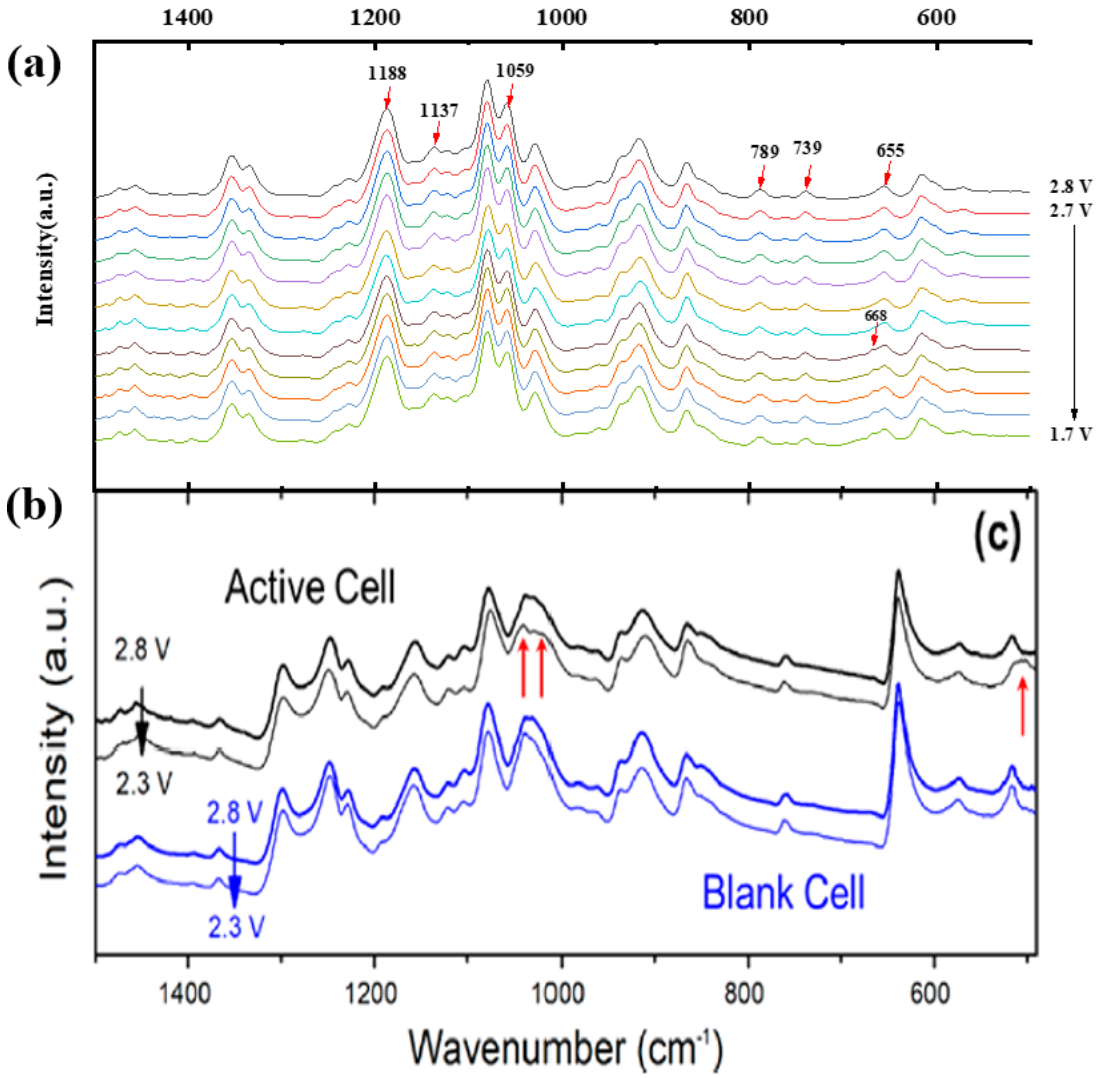

Fig. S16. (a) The discharging FTIR spectra of the SN-CoSn@C NBs-assembled LSBs at 500-1500 cm^{-1}. (b) FTIR spectra from the blank cell in literature [1]. The adsorption peaks are pointed by the red arrows.

Table S2. FT-IR peak assignments in literature [1].

Peak (cm^{-1})	Assignment	Species	Ref.
1298	$\upsilon_s(SO_3)$	ion pairs	1
1248	$\upsilon_{as}(SO_3)$	ion pairs	
1228	υ_s (CF3)	free triflate ion	
1188	υ_{as} (SO_2)	triflate ion	2
1167	$\upsilon_{as}(CF_3)$	ion pairs	1
1158	$\upsilon_{as}(CF_3)$	free triflate ion	1

1137	υ (C-N)	ion pairs	3
1121	υ (C-O)	DOL, DME, and/or ROLi	1
1104	C-O	DME	
1080	C-O/CH_2 rocking	DOL	
1059	$\upsilon_s(SO_3)$	ion aggregates	
1050		ion aggregates	
1040		ion pairs	
1030		free ions	
1015	C-O	DME, DOL	
936		DOL ring vibration	
913		CH_2 rocking/C-O stretch	
868	δ (Li-O)	R-OLi edge groups	
789	υ_s(Co-N)	ion pairs	4
762	δ (CF_3)	R-OLi edge groups	1
		ion pairs	
		free ions	
739	υ(Sn-N)	ion pairs	5
668	υ_{as} (Sn-N)	ion pairs	
655	δ(Sn-N)	bending mode	
616	δ_s(S=O)	sulfone, $S_2O_3^{2-}$	1
572	δ (SO_3)	bending mode	
517	δ (CF_3)	bending mode	
504	(S-S)	$S_x^{2-}(2 \leq x \leq 8)$	

Table S3. Performance comparison with other electrodes reported in literature.

Material type	Initial capacity (mAh g^{-1})	High rate capacity (mAh g^{-1})	Capacity decay rate per cycle	Ref.
Co-NCNT@CF/S	1259/0.1 C	627/3 C	0.038%/3 C/500	6
S@CNTs/Co_3S_4@NC	1570/0.1 C	850/5 C	0.014%/5 C/1000	7
E-Co_xSn_y/NC/S-3	1264/0.1 C	778/2 C	0.0377%/1 C/500	8
S-FeCoNi@C-CNB/S	1238 /0.1 C	676/1 C	0.049%/1 C/200	9
S/FeCo-C	1251.9/0.2 C	791.9/1 C	0.073%/1 C/500	10
E-CoFeCN@C/S	1226/0.1 C	899.5/1 C	0.048%/1 C/300	11
S/$CoFe_2O_4$@C	1191/0.2 C	816/2 C	0.063%/2 C/500	12
$NiCo_2S_4$@MoS_2-S	1118/0.1 C	1200/5 C	0.12%/5 C/500	13
SN-CoSn@C NBs	1291/0.1 C	557.3/5 C	0.056%/5 C/800	This work

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