Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Electronic Supporting Information for

Construction of Co@N-CNTs grown on N-Mo_xC nanosheets for separator modification to enhance adsorption and catalytic conversion of polysulfides in Li-S batteries

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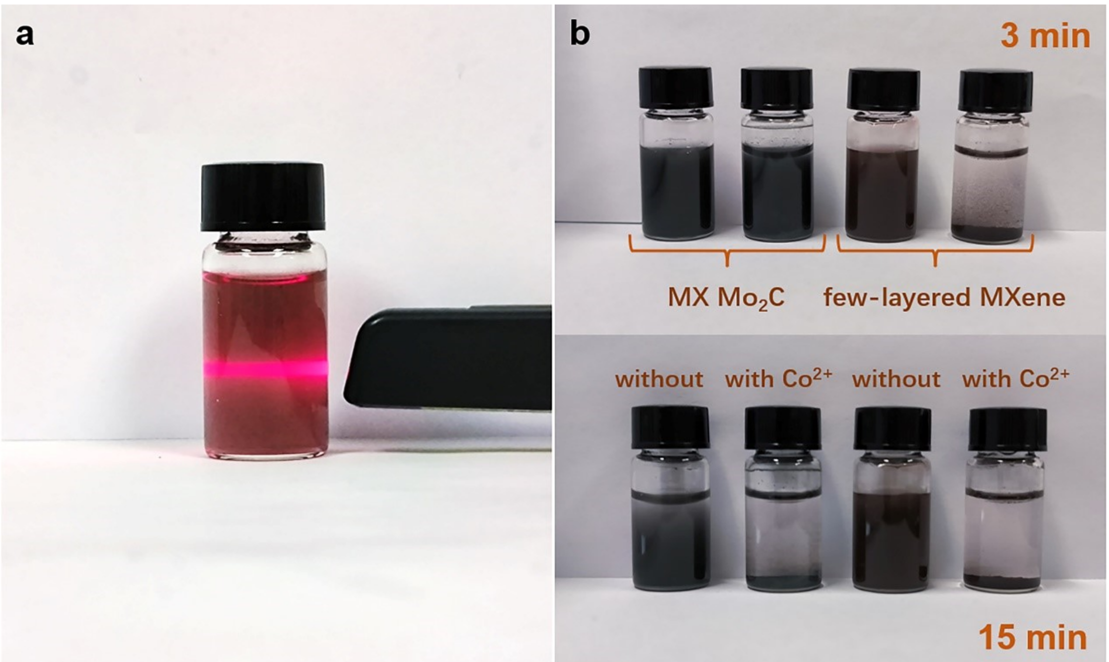

Fig. S1 (a) Tyndall effect in dispersive solution of few-layered MXene, (b) The cobalt ions closely attached to the negatively charged few-layered MXene nanosheets by electrostatic force.

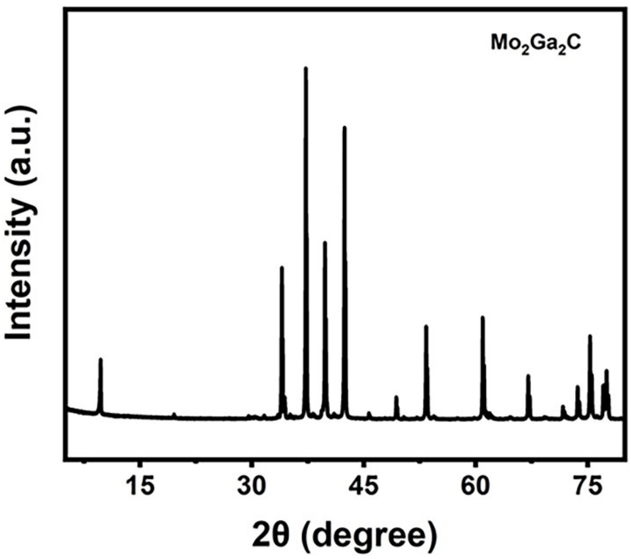

Fig. S2 XRD patterns of Mo_2Ga_2C MAX.

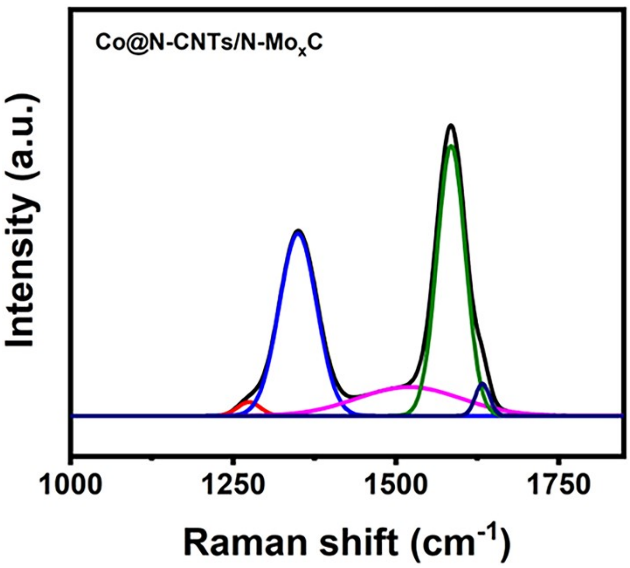

Fig. S3 Raman spectrum and corresponding fitted profiles of Co@N-CNTs/N-Mo_xC.

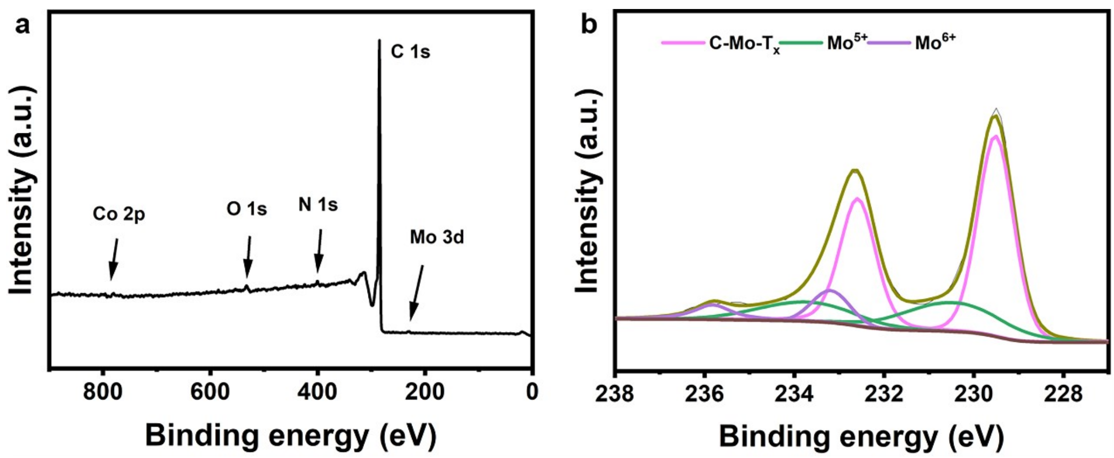

Fig. S4 (a) XPS survey spectrum of Co@N-CNTs/N-Mo_xC, and (b)Mo 3d spectra of MX Mo_2C.

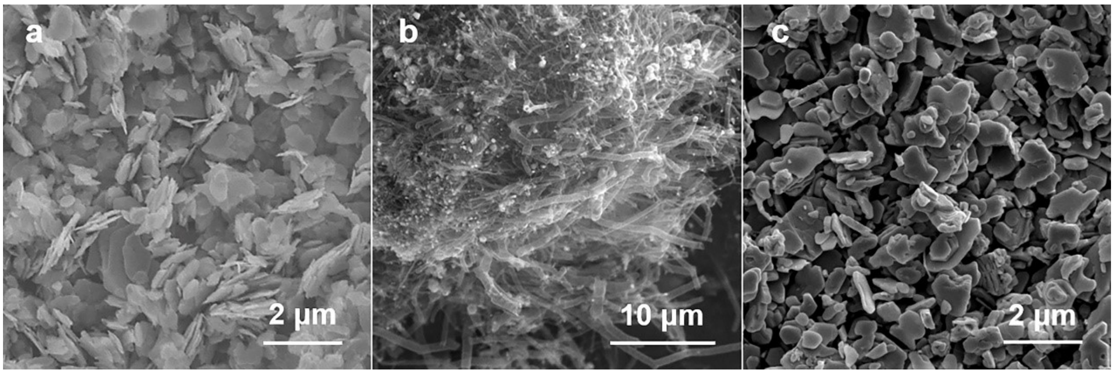

Fig. S5 SEM images of (a) N-Mo_xC, (b) Co@N-CNTs and (c) MX Mo_2C.

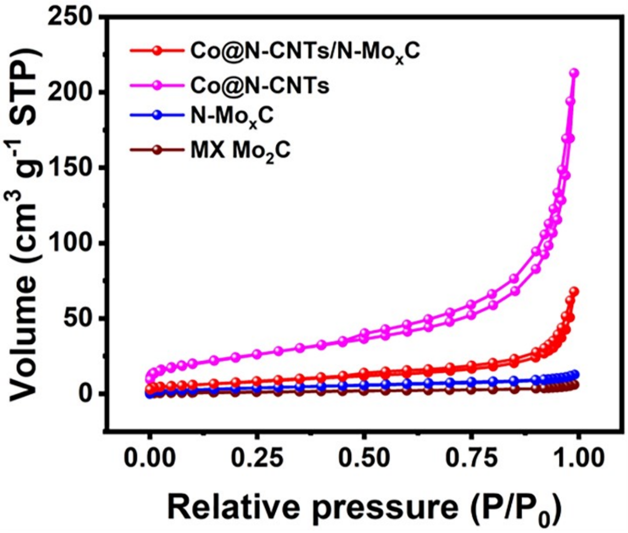

Fig. S6 N_2 adsorption-desorption curves of Co@N-CNTs/N-Mo_xC, Co@N-CNTs, N-Mo_xC and MX Mo_2C as indicated.

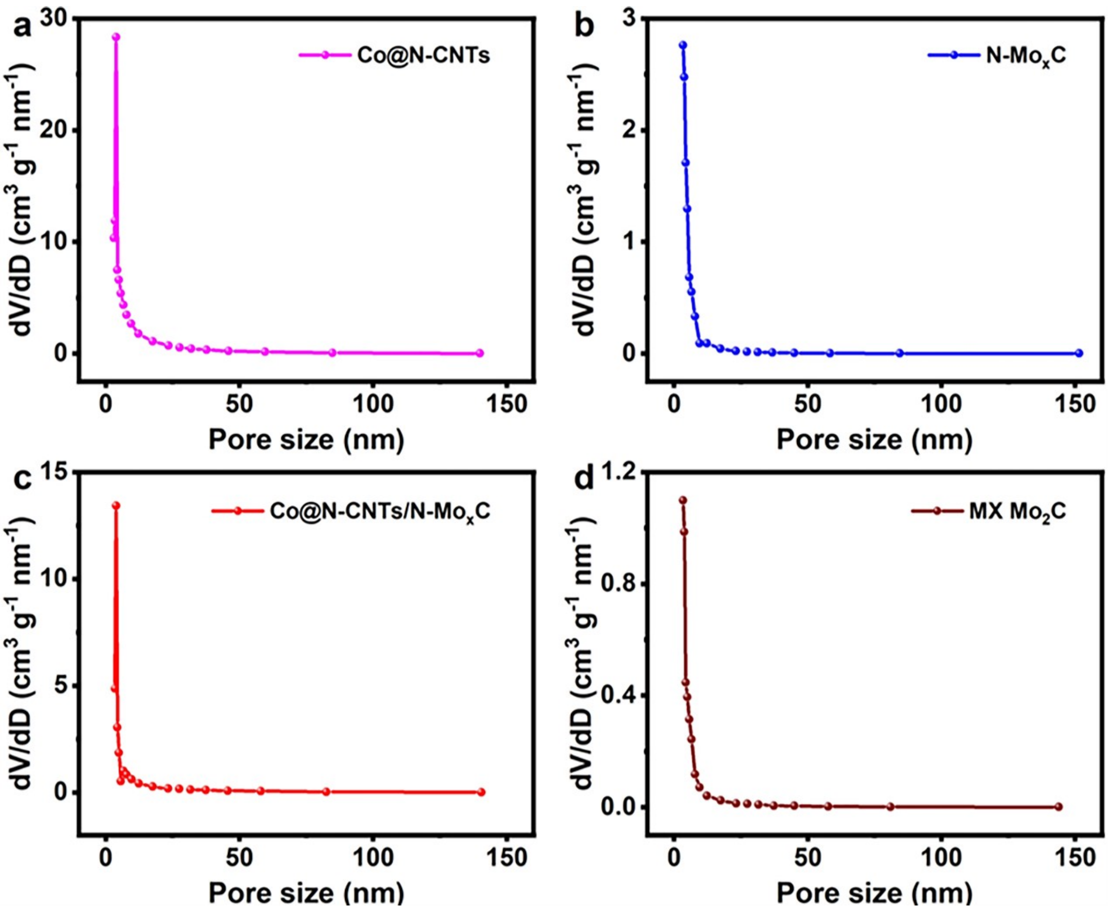

Fig. S7 Pore size distribution of (a) Co@N-CNTs, (b) N-Mo_xC, (c) Co@N-CNTs/N-Mo_xC and (d) MX Mo_2C.

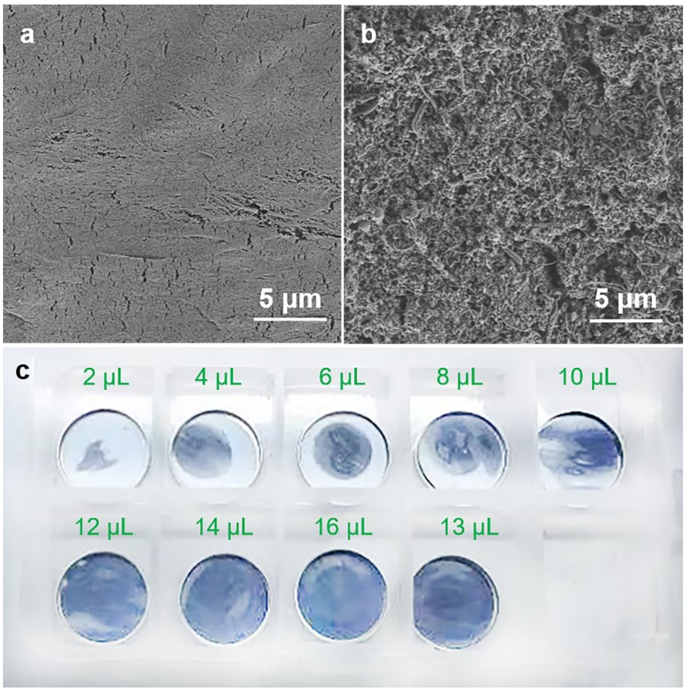

Fig. S8 SEM images of (a) PP separator and (b) coating surface for Co@N-CNTs/N-Mo_xC. (c) Digital photographs for the amount of electrolyte required to moisten the modified separator.

Gradient analysis (2, 4, 6, 8, 10, 12, 14, and 16 μL) was carried out to explore the amount of electrolyte necessary for the moisten the modified separator. With the increase in the amount of electrolyte, the wetting area of the modified separator expands. When the amount of electrolyte reached 12 μL, only two points of the modified separator were not completely wetted. When the electrolyte dosage reached 14 and 16 μL, it was fully wetted. For a more accurate reaction, the wetting condition was verified when the electrolyte dosage was 13 μL. The results showed that the necessary electrolyte dosage to wet modified separator was 13 μL. However, to achieve a good Li-sulfur battery performance test, we used the electrolyte dosage of 20 μL mg^{-1} (the amount of electrolyte used per milligram of sulfur) for relevant characterization.

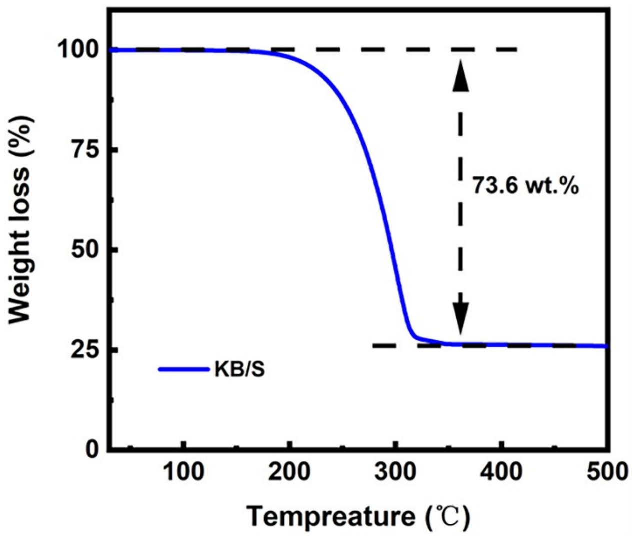

Fig. S9 TG diagram of KB/S for checking the sulfur loading.

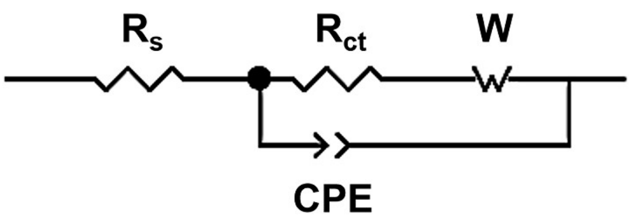

Fig. S10 Equivalent circuit diagram for EIS fitting.

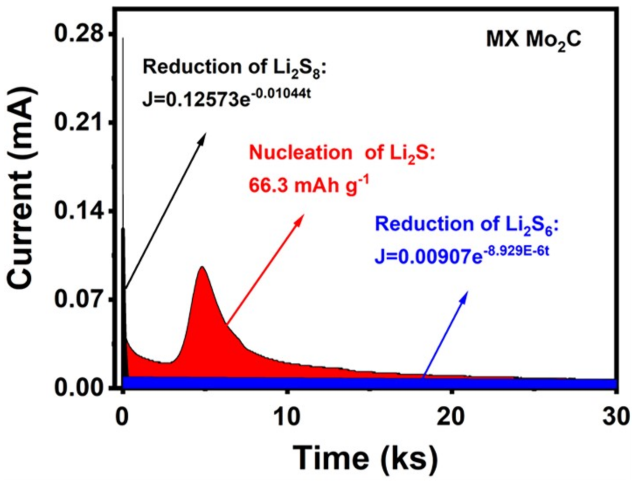

Fig. S11 Li_2S nucleation test of MX Mo_2C electrode.

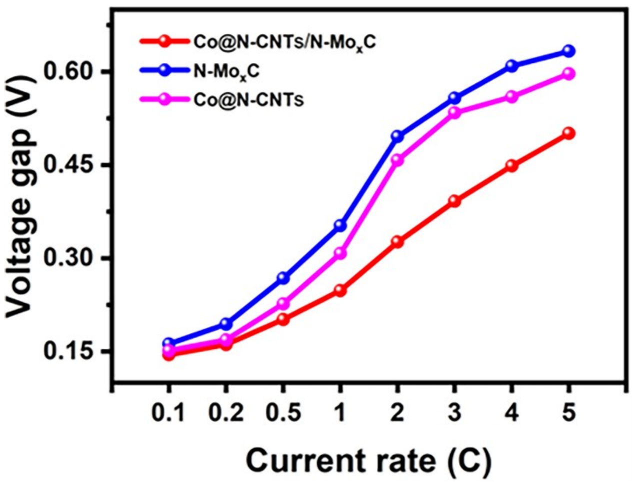

Fig. S12 The charge-discharge platform voltage gaps of cells with different separators under different current densities.

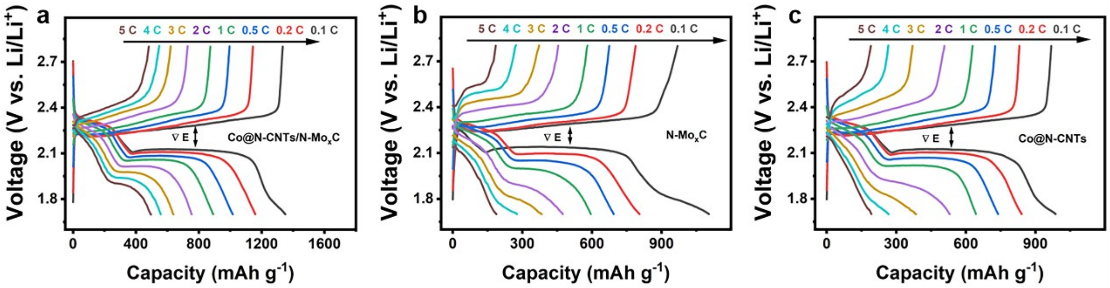

Fig. S13 Charge-discharge curve under a different current density of (a) Co@N-CNTs/N-Mo_xC, (b) N-Mo_xC and (c) Co@N-CNTs separators.

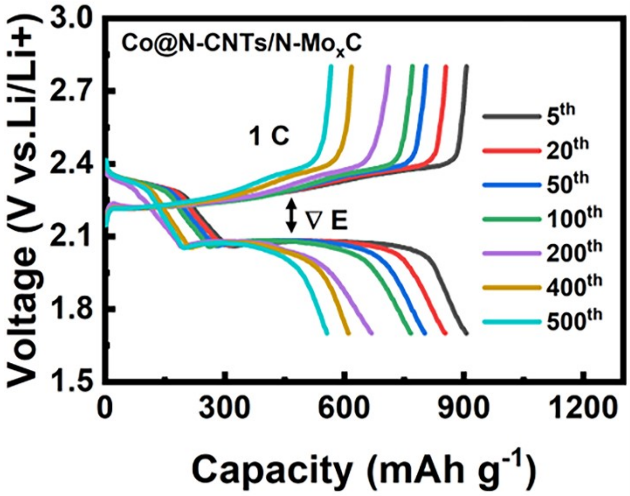

Fig. S14 Charge-discharge curve of Co@N-CNTs/N-Mo_xC separator under different cycles as indicated at 1 C.

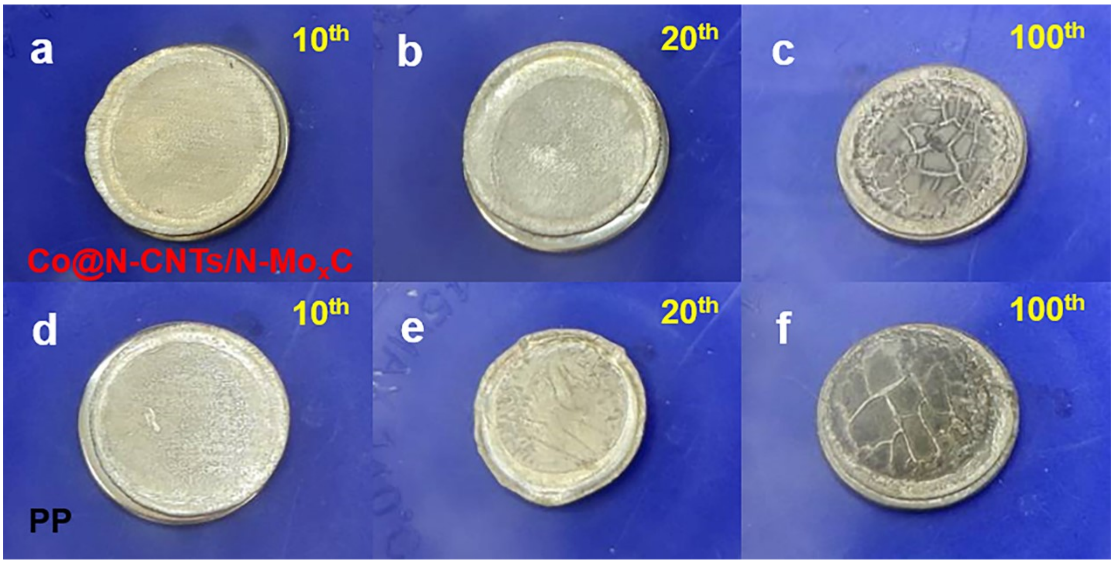

Fig. S15 Digital photos of lithium anodes after different times of charge and discharge cycles.

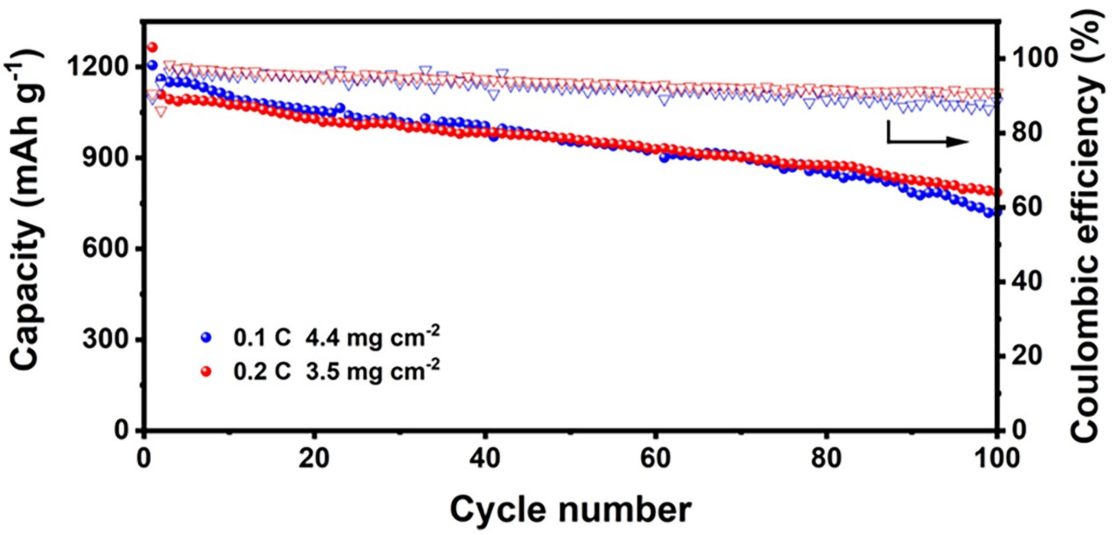

Fig. S16 Cycling stability of the cells with Co@N-CNTs/N-Mo_xC separator under high sulfur loading: 4.4 mg cm^{-2} at 0.1 C, 3.5 mg cm^{-2} at 0.2 C.

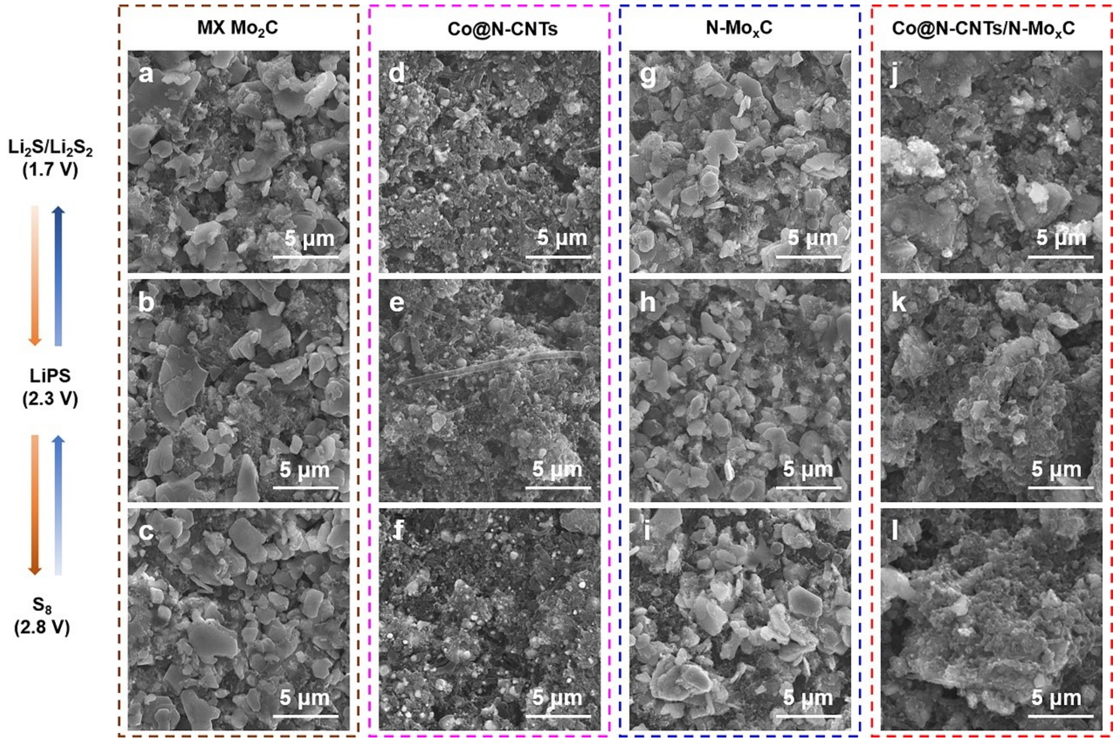

Fig. S17 SEM images of various modified layers after 10 cycles under different voltages as indicated.

To further clarify the role of Co@N-CNTs/N-Mo_xC in the aggregation of polysulfide and inhibition of sulfur aggregation, the cells were disassembled after 10 charge-discharge cycles at 1 C. SEM images of different modified layers at different voltages (1.7, 2.3, 2.8 V) are shown in **Fig. S17**. Taking Co@N-CNTs/N-Mo_xC as an example, at 2.8 V, S8 (solid) deposited on the surface of Co@N-CNTs/N-Mo_xC layer and encapsulated it. Upon discharge to 2.3 V, S8 is transformed into Li_2S_n (soluble, n = 4 or 6) and Co@N-CNTs/N-Mo_xC exposes its 3D structure. When discharged to 1.7 V, Li_2S_n are further transformed into Li_2S_2/Li_2S (solid) and deposited on the Co@N-CNTs/N-Mo_xC layer.

Table S1 Atomic information of Co@N-CNTs/N-Mo_xC

Name	Atomic (%)
Mo 3d	0.1
C 1s	95.7
N 1s	2.4
O 1s	1.5
Co 2P	0.3

Table S2 Specific surface area obtained in the BET test

Sample	Specific surface area (m^2 g^{-1})
Co@N-CNTs/N-Mo_xC	28
Co@N-CNTs	89
N-Mo_xC	13
MX Mo_2C	5

Table S3 The information obtained by fitting the electrochemical impedance

Modified separators	R_s (Ω)	R_{ct} (Ω)
Co@N-CNTs/N-Mo_xC	1.08	49.31
Co@N-CNTs	1.13	64.02
N-Mo_xC	1.35	74.19
MX Mo_2C	2.14	86.95
PP	2.21	104.80