Electronic Supplementary Material (ESI) for Nanoscale.

Balanced capture and catalytic ability toward polysulfides by designing $MoO_2-Co_2Mo_3O_8$ heterostructure for lithium-sulfur batteries

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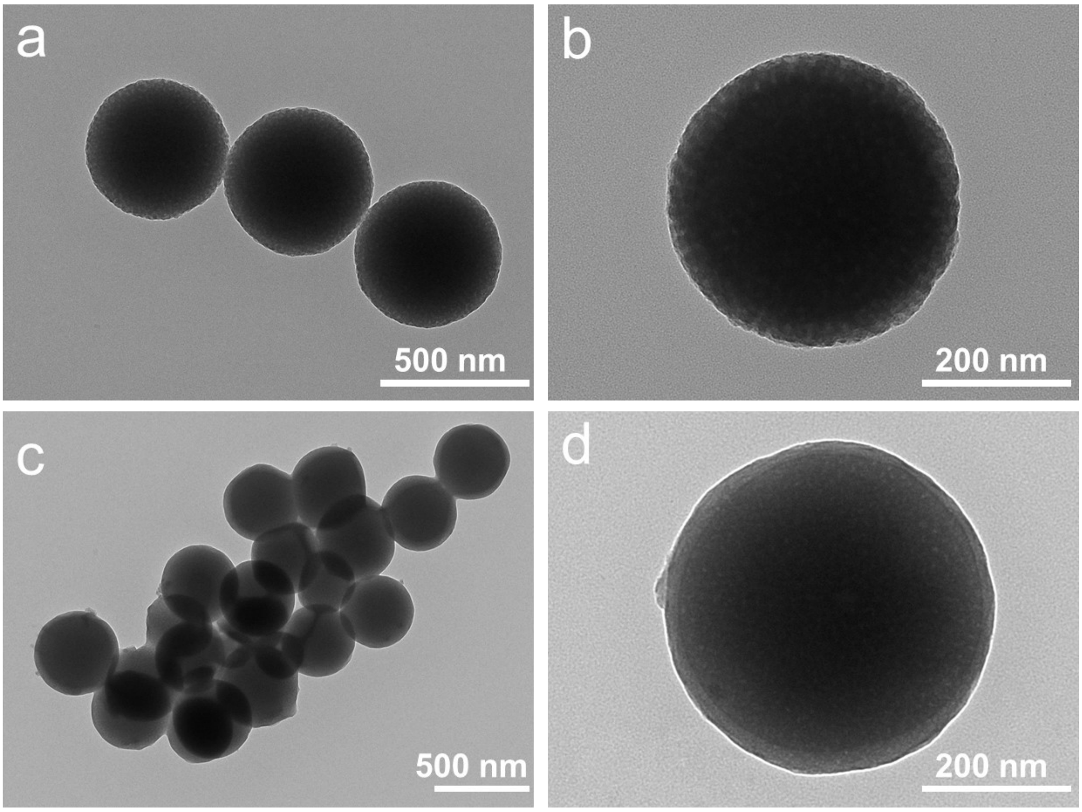

Figure S1.TEM images of (a, b) polymer nanospheres and (c, d) NMCSs.

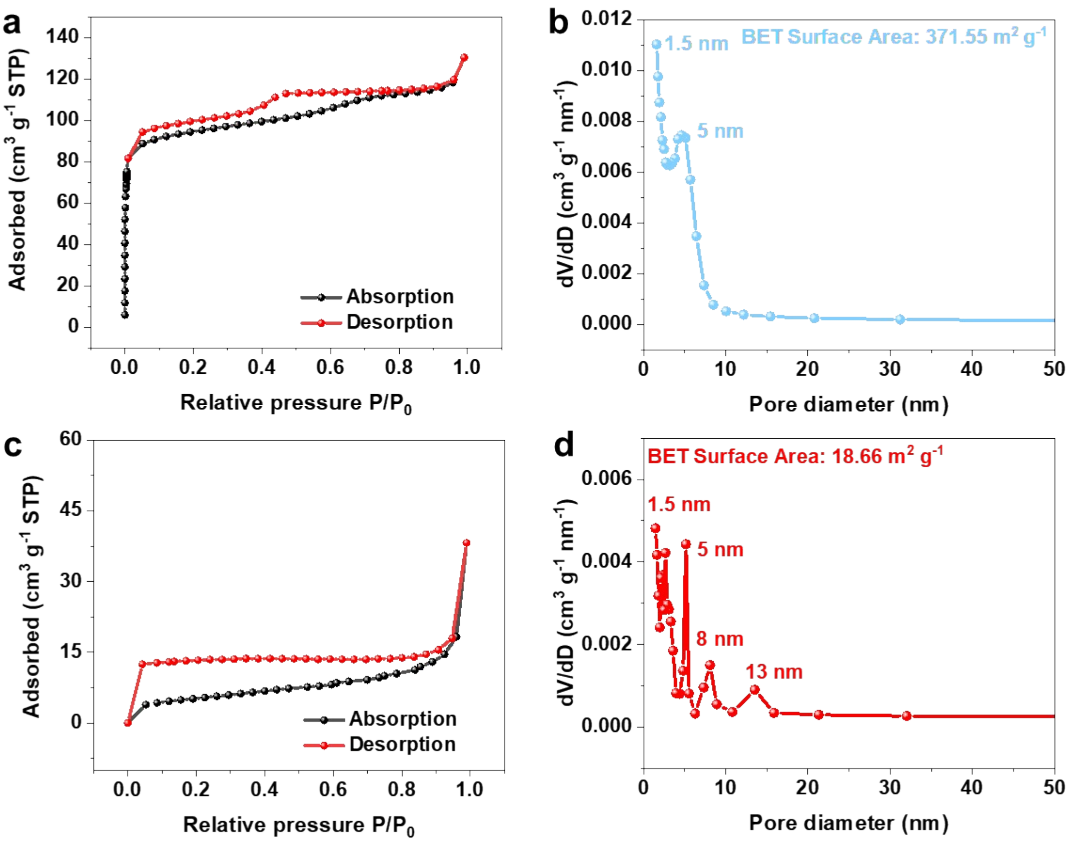

Figure S2. Nitrogen adsorption–desorption isotherms of (a) NMCSs and (c) $9MoO_2:2Co_2Mo_3O_8$. Pore size distribution of (b) NMCSs and (d) $9MoO_2:2Co_2Mo_3O_8$.

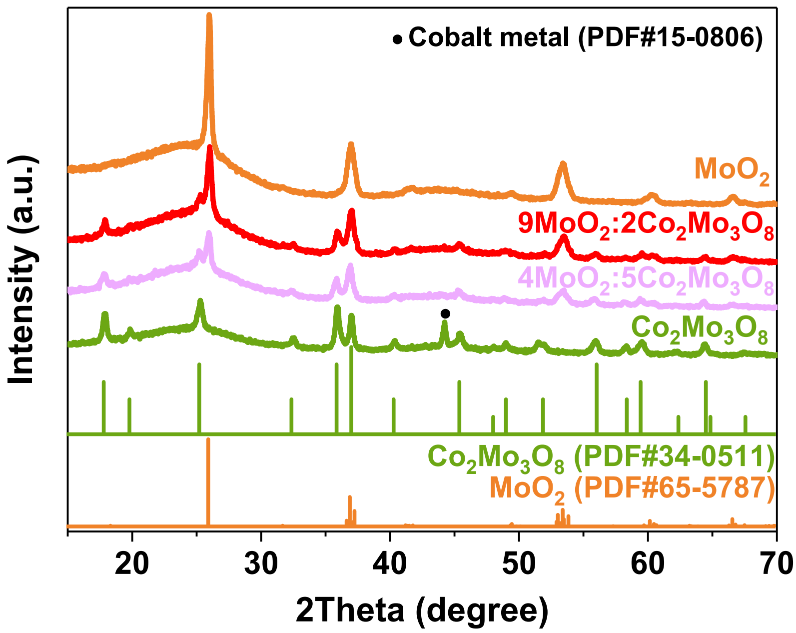

Figure S3. XRD patterns of various hosts.

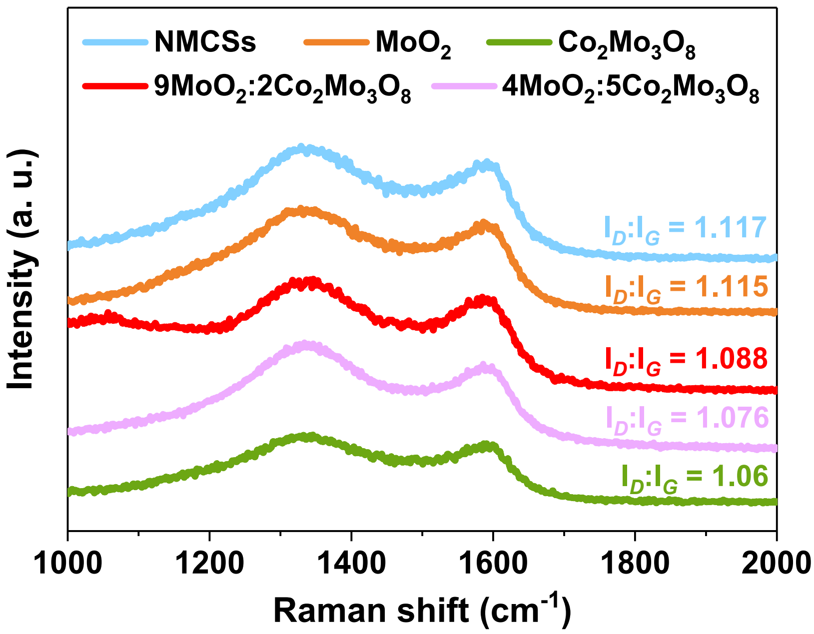

Figure S4. Raman spectra of the samples.

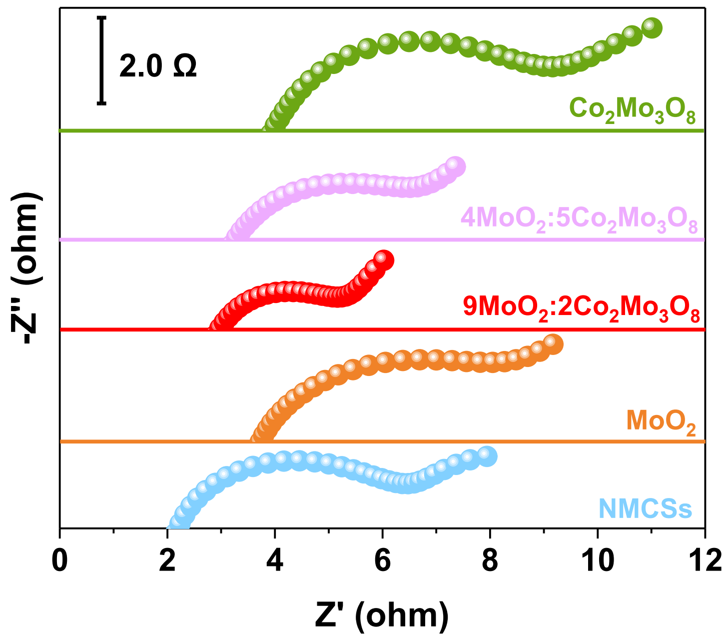

Figure S5. EIS spectra of symmetrical Li_2S_6–Li_2S_6 cells.

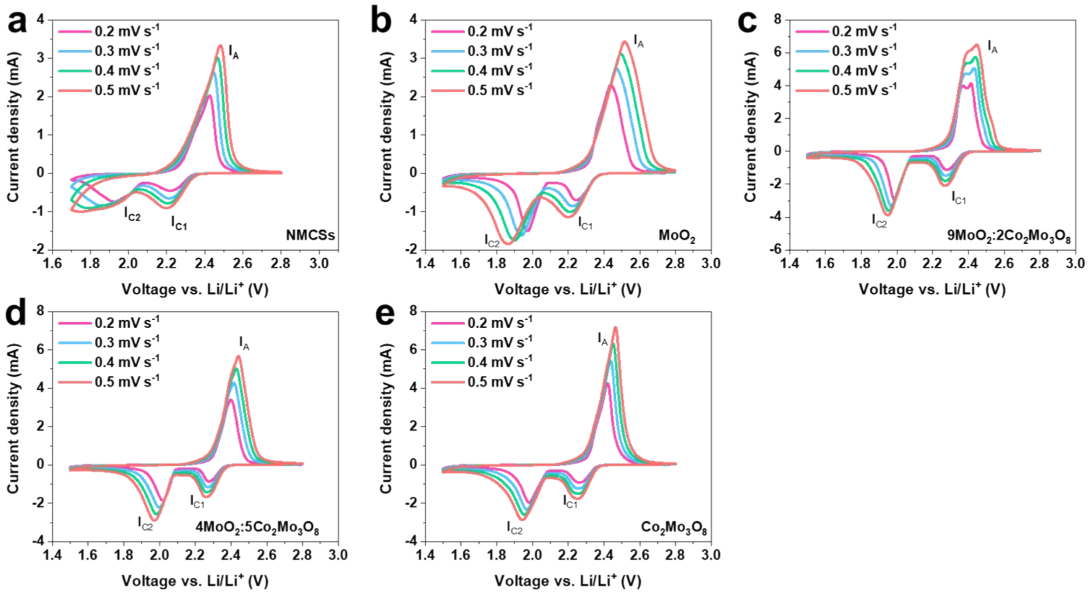

Figure S6. CV curves at various scanning speed: (a) NMCSs; (b) MoO_2; (c) $9MoO_2{:}2Co_2Mo_3O_8$; (d) $4MoO_2{:}5Co_2Mo_3O_8$ and (e) $Co_2Mo_3O_8$.

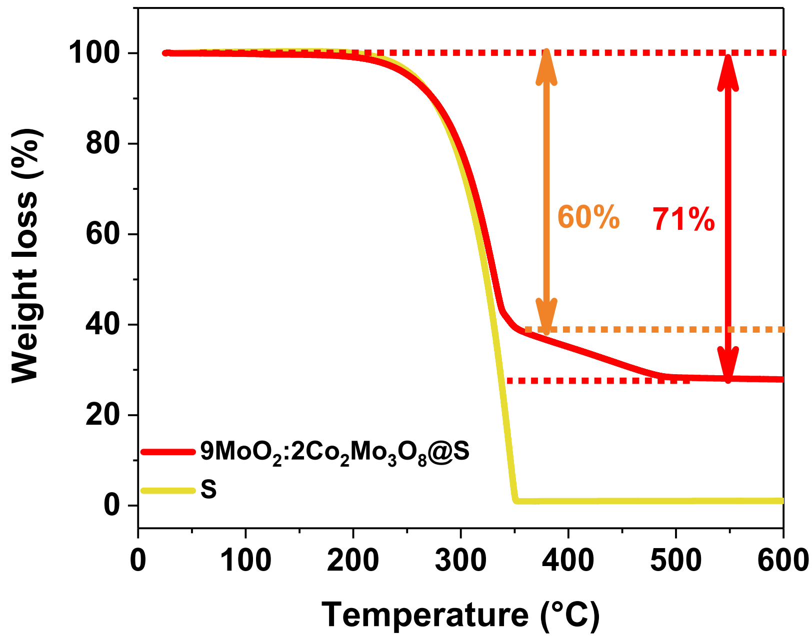

Figure S7. TGA curves of sulfur powder and $9MoO_2$:$2Co_2Mo_3O_8$@S.

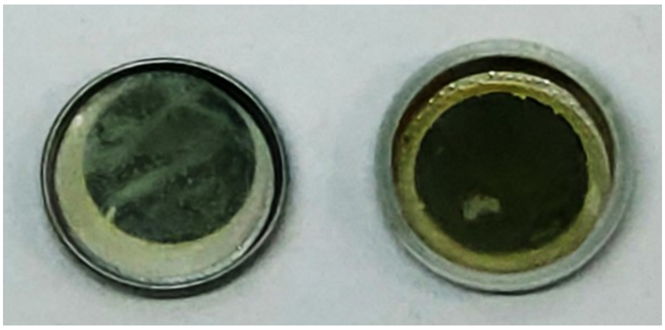

Figure S8. Digital images of separators after cycling: $9MoO_2$:$2Co_2Mo_3O_8$ (left) and NMCSs (right).

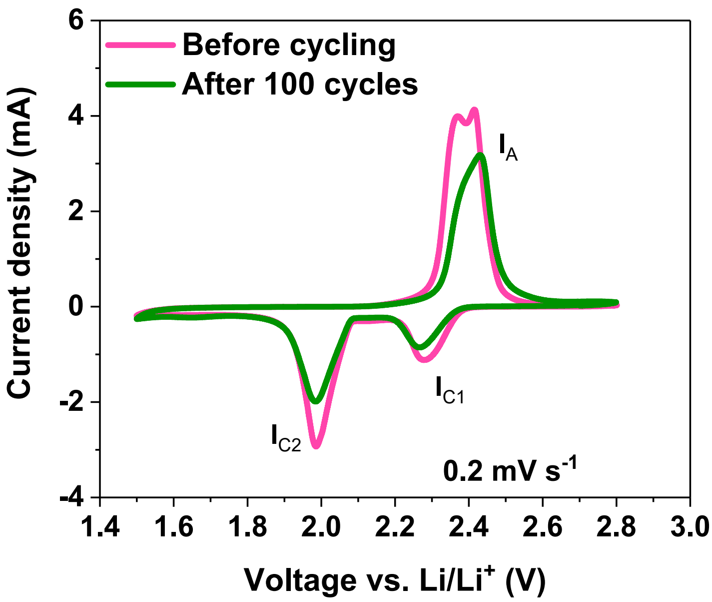

Figure S9. CV curves for $9MoO_2$:$2Co_2Mo_3O_8$ based cathode before and after cycling.

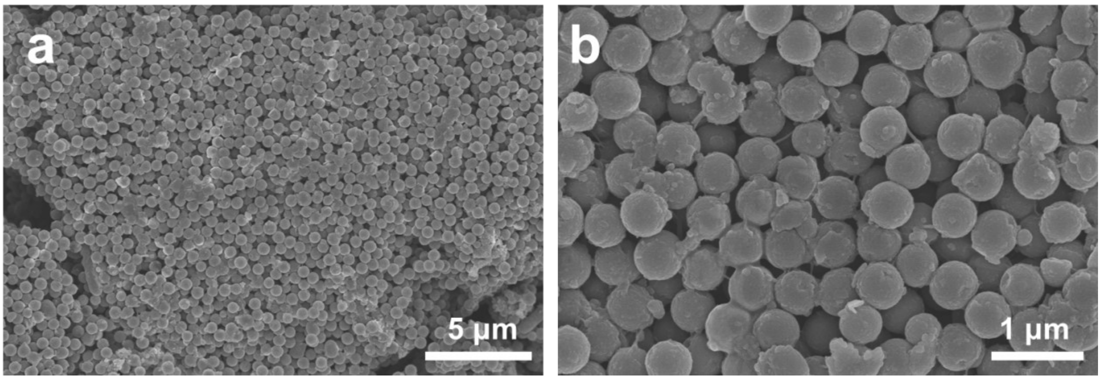

Figure S10. SEM images for $9MoO_2$:$2Co_2Mo_3O_8$ based cathode after cycling.

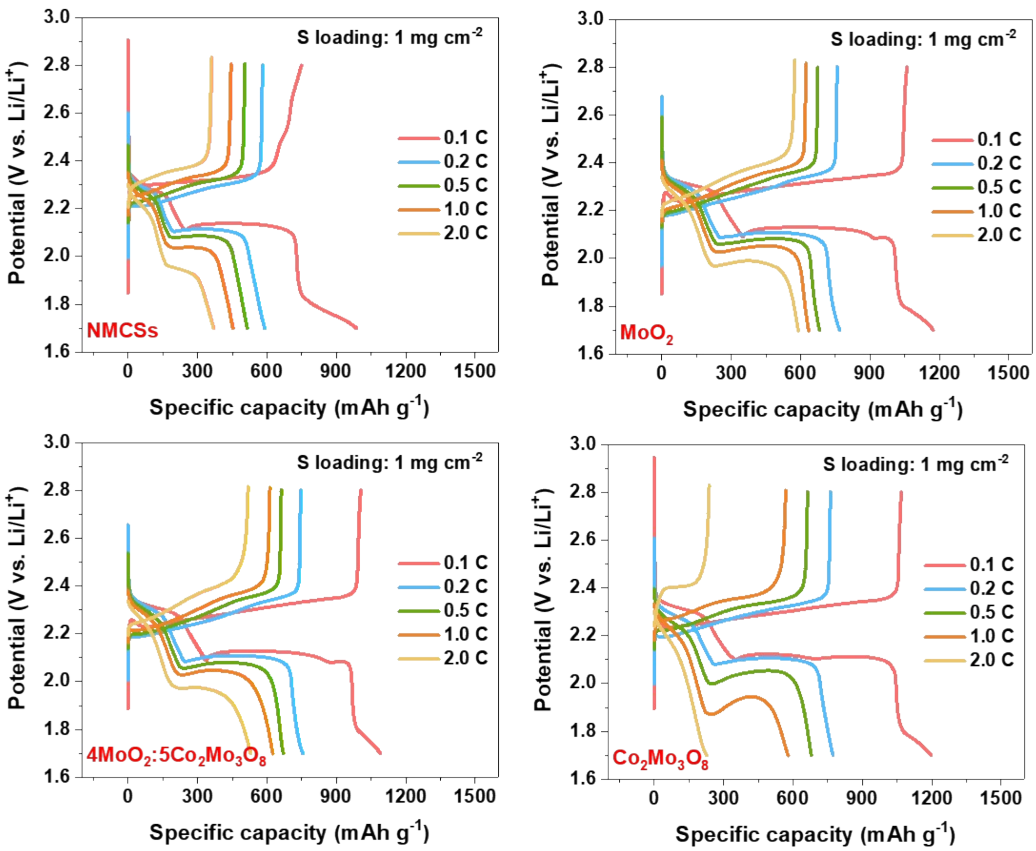

Figure S11. Galvanostatic discharge–charge curves at various current densities with S loading of 1.0 mg cm^{-2}: (a) NMCSs; (b) MoO_2; (c) $4MoO_2$:$5Co_2Mo_3O_8$ and (d) $Co_2Mo_3O_8$.

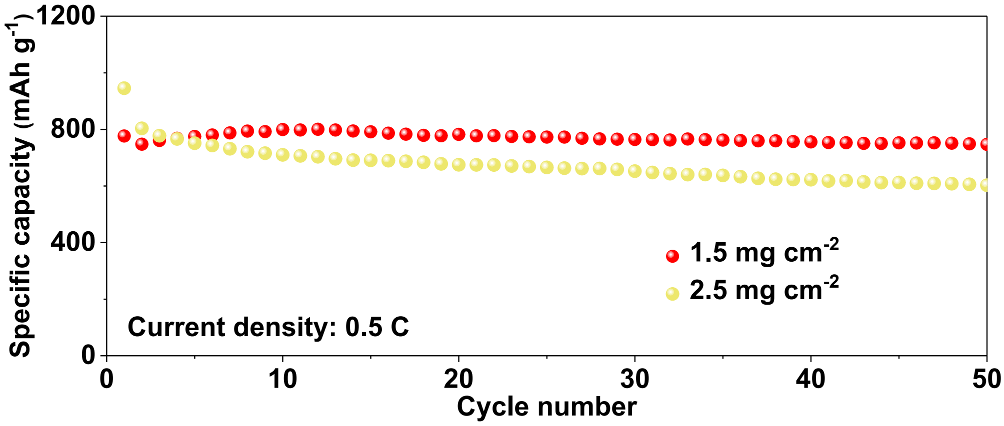

Figure S12. Cycling performance of the $9MoO_2{:}2Co_2Mo_3O_8$ based cathodes at 0.5 C with high sulfur loading.

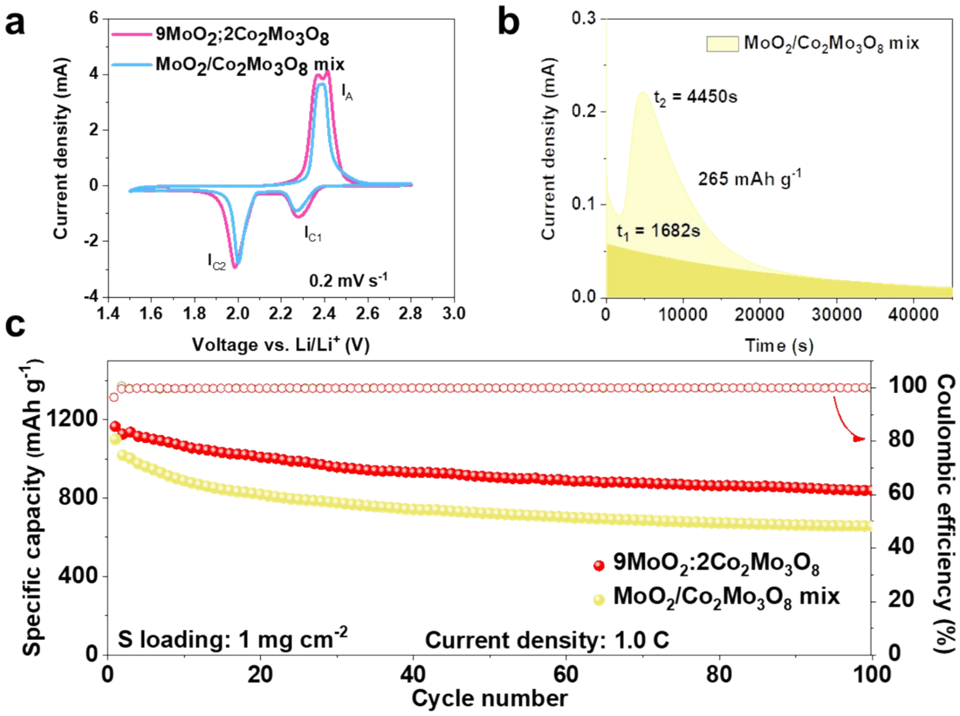

Figure S13. (a) CV curve of $9MoO_2$:$2Co_2Mo_3O_8$ and $MoO_2/Co_2Mo_3O_8$ mixture. (b) Potentiostatic discharge profiles of $MoO_2/Co_2Mo_3O_8$ mixture at 2.05 V. (c) Cyclic stability performance at 1 C.

Table S1. Lithium ion diffusion coefficient.

Samples	D_{Li^+} (× 10^{-8} cm^2 S^{-1})		
	I_{C1} peak	I_{C2} peak	I_A peak
NMCSs	0.29	0.089	2.48
MoO_2	0.29	0.18	1.89
$9MoO_2$:$2Co_2Mo_3O_8$	1.38	1.32	8.08
$4MoO_2$:$5Co_2Mo_3O_8$	0.97	1.6	7.63
$Co_2Mo_3O_8$	1.07	1.18	12.67

Table S2. Comparison of electrochemical performance between MoO_2–$Co_2Mo_3O_8$ and other molybdenum–based heterostructures reported by previous literatures.

Sample	S loading (mg cm^{-2})	Rate (C)	Discharge capacity (mAh g^{-1})	Decay rate per cycle	Reference
$9MoO_2$:$2Co_2Mo_3O_8$	1	1	509 (1000th)	0.056%	This work
$MoSe_2/MoO_2$	2.3	0.5	848 (500th)	0.046%	1
MoO_2/Mo_3N_2	1.2	0.5	760 (1000th)	0.024%	2
MoS_2–MoN	1.2	1	520 (1000th)	0.039%	3
MoO_2/Mo_2N	1	1	632 (300th)	0.028 %	4
MoO_3/MoO_2	0.616	0.5	828 (500th)	0.016%	5
MoP/MoS_2	1.5	1	650 (500th)	0.082%	6
MoN–VN	1.13	1	555 (500th)	0.055%	7
MoS_2/Ni_3S_2	1.2	1	739 (1000th)	0.029%	8
MoS_2/MoO_3	1.5	1	324 (600th)	0.009%	9
Co_9S_8@MoS_2	3	1	794 (400th)	0.091%	10
$FeMoO_4/FeS_2/Mo_2S_3$	2.3	1	781 (300th)	0.171%	11
MoO_2/MoS_2	4	1	640 (140th)	0.211%	12
Ni–MoS_2	1	1	422 (400th)	0.11%	13
NiO-$NiCo_2O_4$	/	0.5	717 (500th)	0.059%	14
Co_9S_8/CoO	2.5	1	470 (1000th)	0.049%	15
WO_3–WS_2	1	1	668 (500th)	0.04%	16
TiO_2–Ni_3S_2	3.9	0.5	600 (900th)	0.038%	17
Nb_2O_5/Nb_4N_5	/	1	913 (400th)	0.08%	18
Fe_9S_{10}/Fe_3O_4	1	1	585 (500th)	0.08%	19
V_2O_3–VN	1.2	1	618 (800th)	0.038%	20

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