Supplementary Information

Lithium Passivated MoO_3 Nanobelts Decorated Polypropylene Separator for Fast-Charging Long-Life Li-S Battery

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P.S. ¶ Share equal authorship. * Share equal corresponding authorship

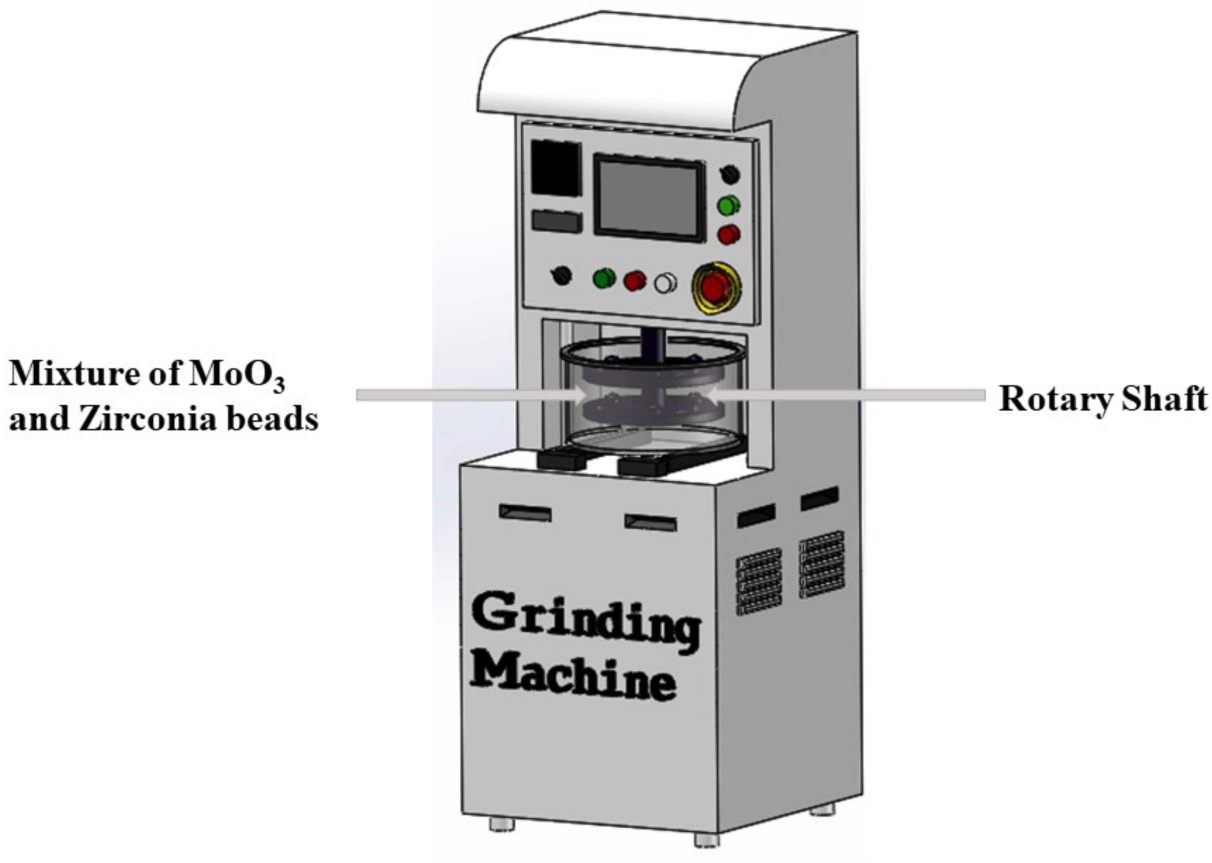

Fig. S1 Homemade grinder machine used to prepare the MNBs.

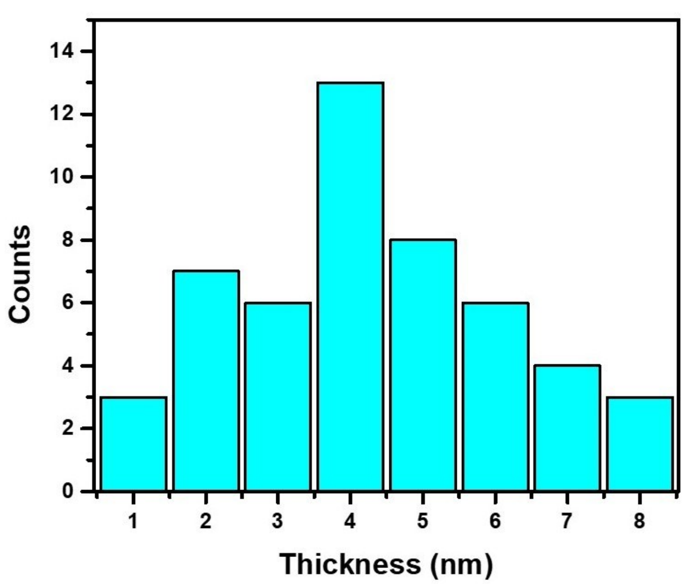

Fig. S2 Height histogram of 50 different MNBs.

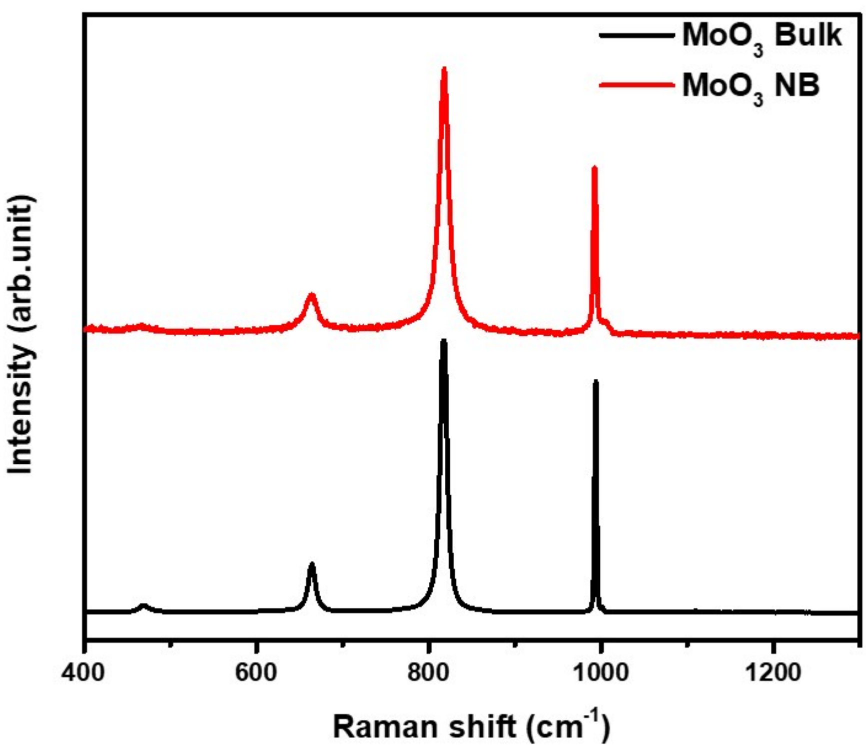

Fig. S3 Raman spectra of commercial bulk MoO_3 particles and as-prepared MNBs.

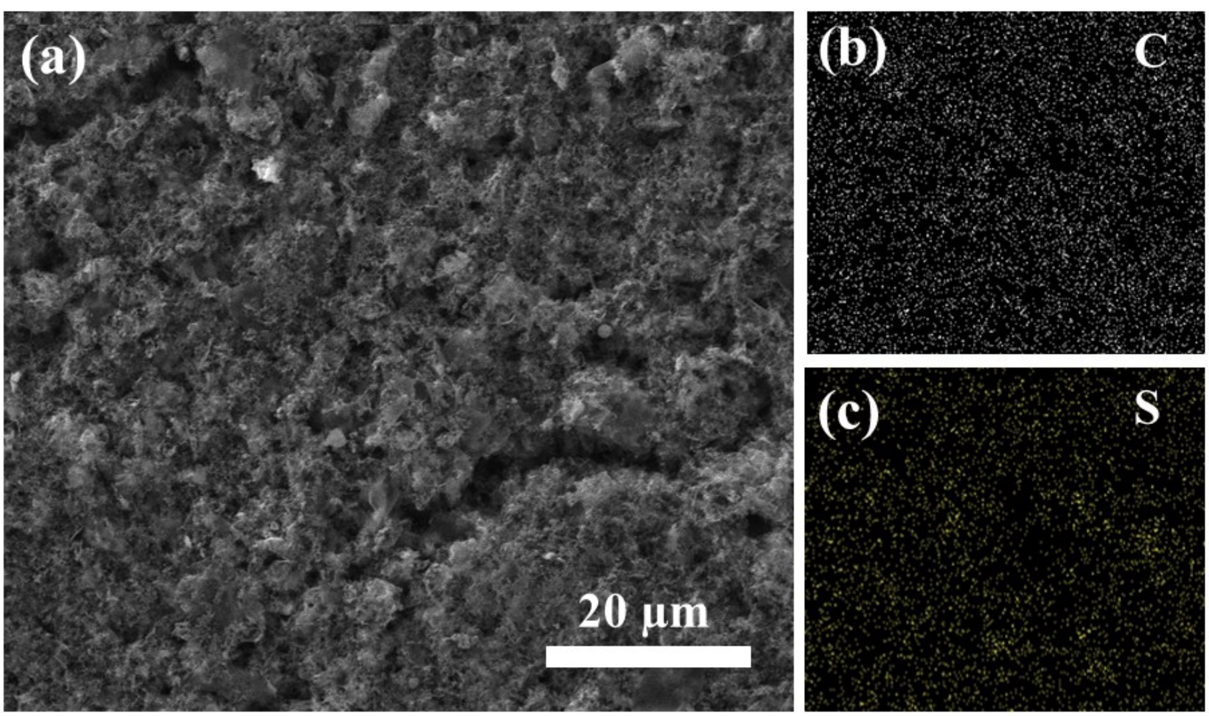

Fig. S4 (a) FE SEM image of S-EG cathode and (b-c) corresponding EDS mapping of Carbon and Sulfur.

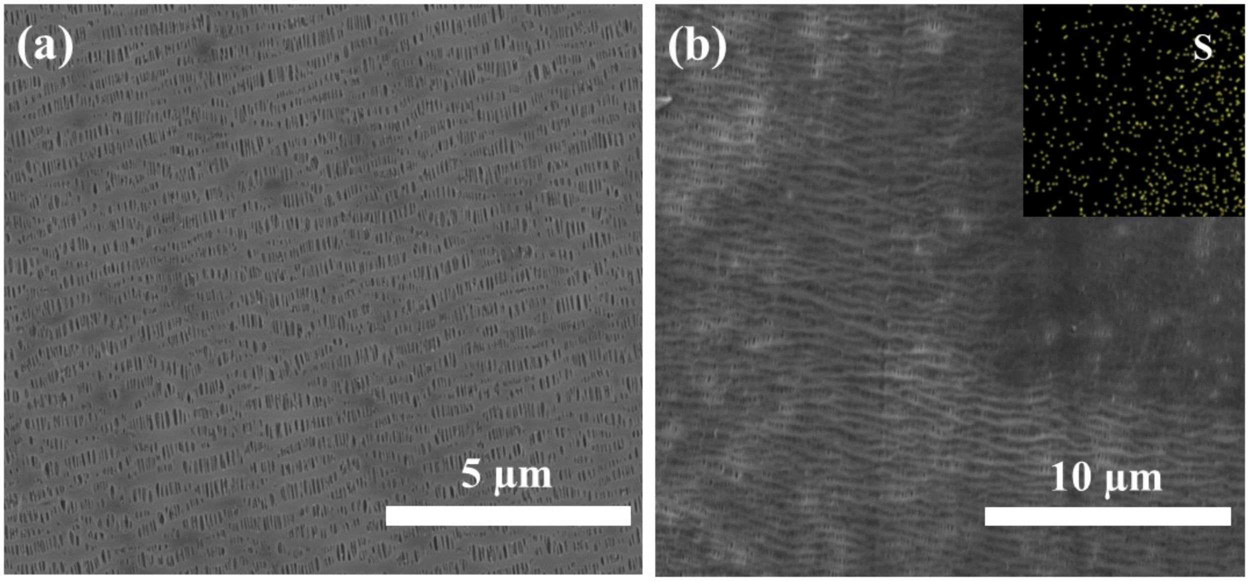

Fig. S5 FESEM images of pristine separator (a) before cycle, (b) after cycle; inset: EDS mapping of S on top of pristine separator after 500 charge-discharge cycle at 5C rate.

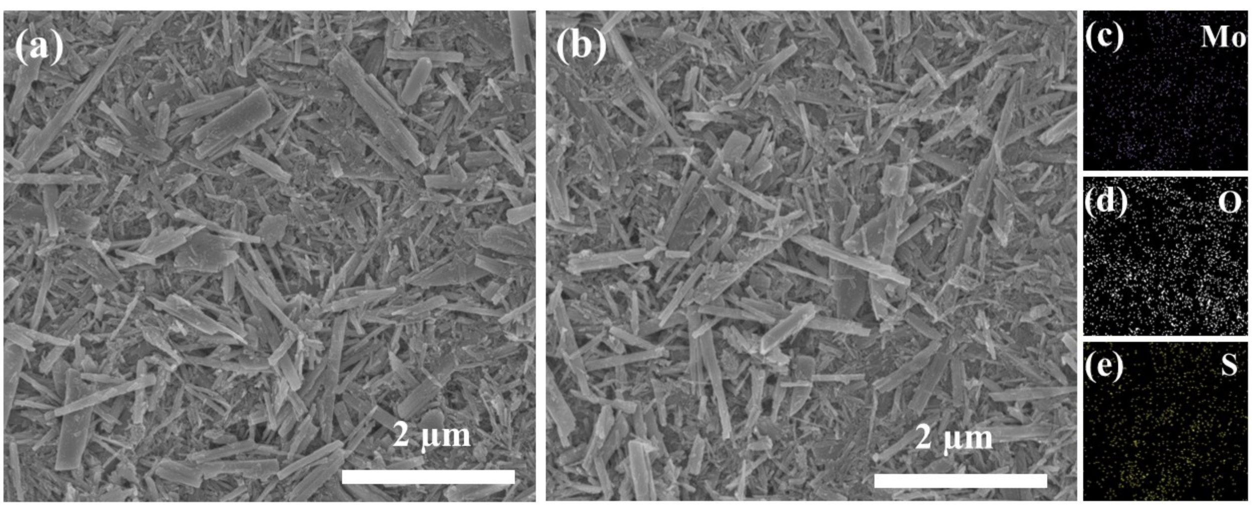

Fig. S6 FESEM (top view) image of MNBs coated onto a PP separator using a spray gun (a) before cycle (b) after cycle (c-e) corresponding EDS mapping of Mo, O, and S.

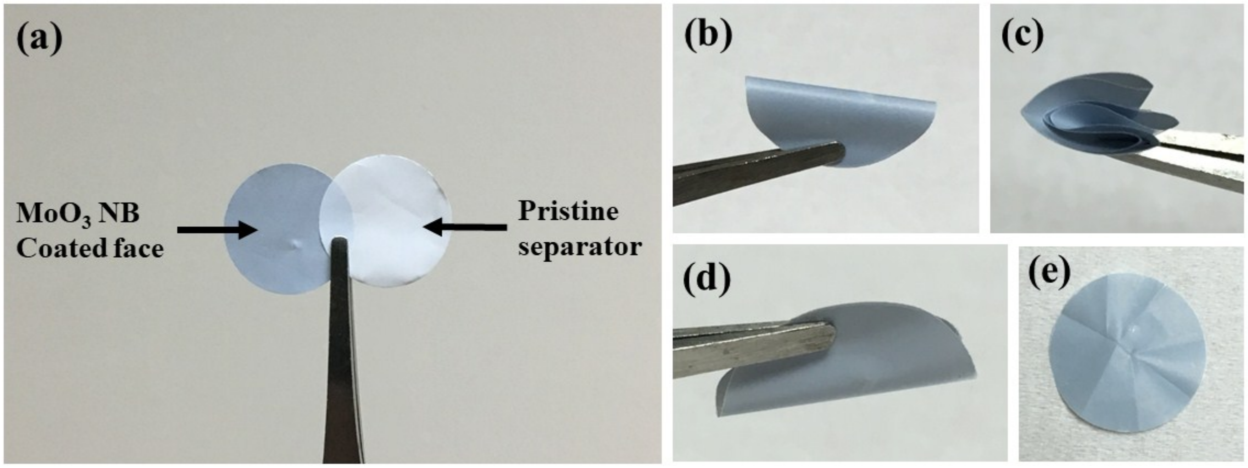

Fig. S7 Photograph of a pristine PP separator and an MNBs-coated PP separator and bending test.

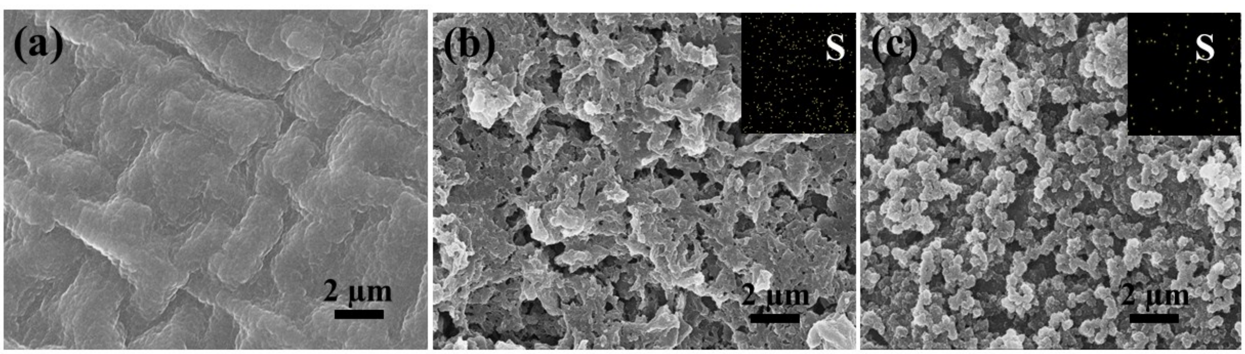

Fig. S8 FE-SEM images of Li foil (a) before cycle, (b-c) after cycle, incorporated pristine separator and MNBs separator respectively; inset: corresponding EDS mapping of S. Li-S battery was dissembled after 500 charge-discharge at 5C rate.

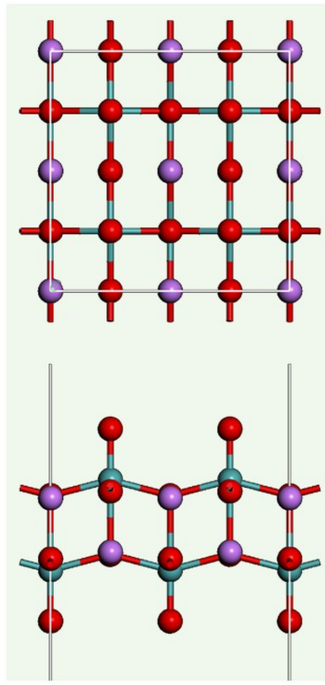

Fig. S9 Top and side views of the electronic structure of the Li-passivated MoO_3 (pink: Li; cyan: Mo; red: O).

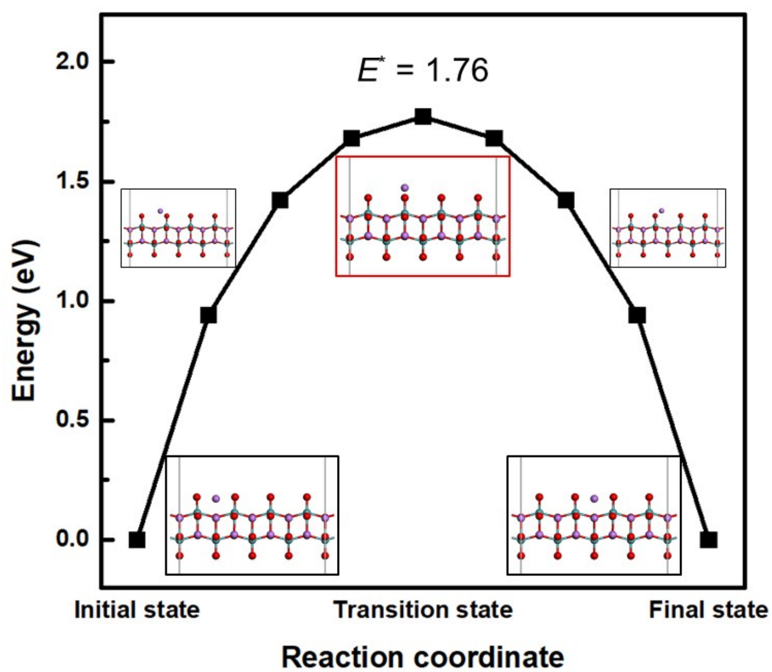

Fig. S10 Reaction coordinate and transition state structure for the surface diffusion of Li on the Li-passivated MoO_3.

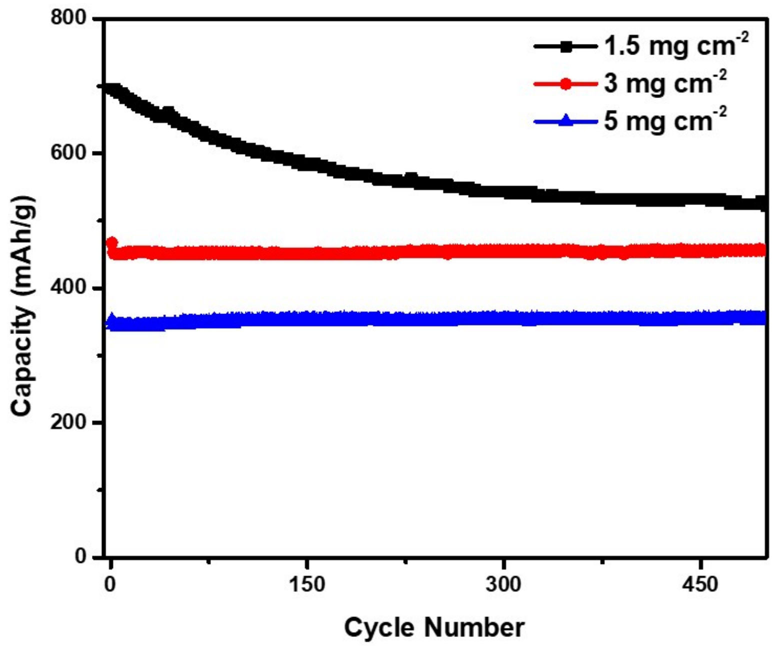

Fig. S11 Cycling performance of LSB using different amount of S loading in cathode, using MNBs-coated separator.

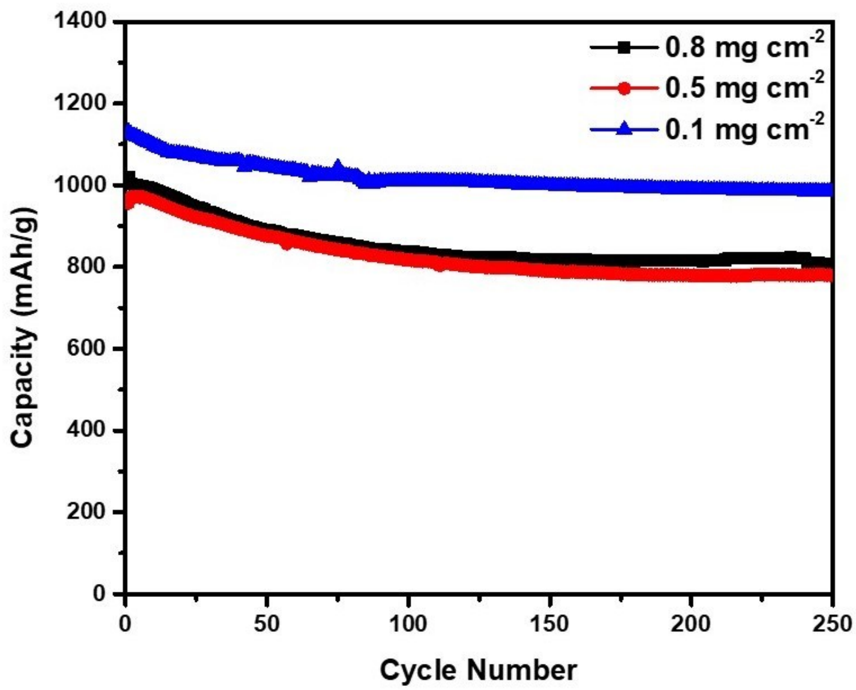

Fig. S12 Cycling performance of LSB incorporating different MNBs-loaded separators, measured at a rate of 1C.

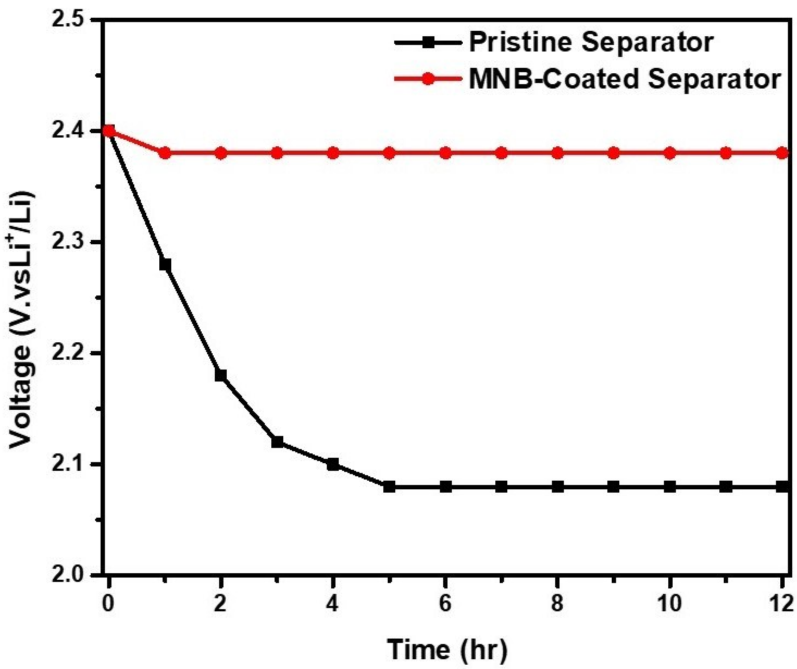

Fig. S13 Self-discharge phenomenon of an LSB, characterized through its open-circuit voltage.

Table S1 Population analyses of atoms near the bond sites in (a) Li_2S_8/MoO_3 with charge 0, (b) Li_2S_8/MoO_3 with charge +2, (c) Li_2S_4/MoO_3 with charge 0, and (d) Li_2S_4/ MoO_3 with charge +2.

(a) Li_2S_8, Charge = 0

	Before adsorption	As adsorption
S	-0.11	0.031
Li	+0.44	+0.66
O	-0.94	-1.23
Mo	+2.74	+2.75

(b) Li_2S_8, Charge = +2

	Before adsorption	As adsorption

S	-0.10	-0.021
Li	+0.56	+0.79
O	-0.86	-1.13
Mo	+2.77	+2.78

(c) Li_2S_4, Charge = 0

	Before adsorption	As adsorption
S	-0.20	-0.028
Li	+0.40	+0.53
O	-0.94	-1.14
Mo	+2.74	+2.75

(d) Li_2S_4, Charge = +2

	Before adsorption	As adsorption
S	-0.18	-0.016
Li	+0.51	+0.65
O	-0.86	-1.03
Mo	+2.75	+2.76

Table S2: Comparison of Electrochemical performance of this work with previous work on modification of separator in order to achieve stable Li-S battery.

Modified Separator	*Sulfur Loading (mg cm^{-2})*	*Sulfur Content (wt %)*	*Current rate (1C = 1675 mAhg^{-1})*	*Number of cycles*	*Degradation rate per cycle (%)*	*Reference*
Carbon Black	1.1-1.3	-	0.5 C	200	0.19	1
Single-Wall Carbon Nanotube	1.5	75	0.2 C	300	0.18	2
MWCNT	2	65	1 C	300	0.14	3
PVDF CB	1.5	65	0.2 C	500	0.09	4
Nafion	0.53	50	0.5 C	500	0.08	5
GO/Nafion	4	60	0.5 C	200	0.18	6
Mesoporous carbon	1.5	50	1 C	500	0.071	7
Microporous/ PEG	2	65	0.2 C	500	0.109	8
PVDF KOH activated CB	7	70	0.5 C	500	0.084	9
PEDOT:PSS	1	64	0.25 C	1000	0.0364	10
Silica Nanoparticles	1.2	48	0.2 C	200	0.175	11
N-Rich Porous Carbon	1.4	70	0.2 C	200	0.254	12
Black Phosphorous	1.5-2	80	0.2 C	100	0.14	13
$BaTiO_3$	3	60	0.1 C	50	0.34	14
MoS_2	-	65	0.5 C	600	0.083	15
COF-CNT		75	0.2 C	300	0.13	16
rGO/CeO_2	2	80	0.1 C	100	0.22	17

Carbon Flakes	1	60	0.5 C	500	0.071	18
MOF/Nafion	-	70.5	0.1 C	200	0.1225	19
C-WS_2	1.5-4.2	70	1 C	1000	0.045	20
MoO_3 NBs	1.5	64	1 C	1000	0.026	This Work
MoO_3 NBs	1.5	64	2 C	1000	0.028	This Work
MoO_3 NBs	1.5	64	3 C	1000	0.033	This Work
MoO_3 NBs	1.5	64	4 C	1000	0.038	This Work
MoO_3 NBs	1.5	64	5 C	5000	0.014	This Work

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