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Dual-role Magnesium Aluminate Ceramic Film as an Advanced Separator and Polysulfide Trapper in Li-S battery: Experimental and DFT investigations

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Table S1. Porosity calculation for Celgard®, MAO, and MAO/MWCNT separator

Separator	Mass of dry separator (mg)	Mass of DME/DOL absorbed separator (mg)	Mass of DME/DOL absorbed (mg)	Porosity (%) estimated using eq. 1
Celgard®	4.2	7.1	2.9	38.5
MAO	46.3	66.8	20.5	62.6
MAO/MWCNT	48.8	76.4	27.5	68.1

When the thickness of the MAO separator is less than 100 microns, the mechanical strength of the separator is poor and tend to break (brittle). Therefore, we have limited the thickness of the separator to be 100 μm and it is highly flexible. Further studies are required to fabricate a thin MAO separator for realistic future application in battery, and we will work towards it in future.

Table S2. Electrical parameters of Li|Celgard®|Li symmetric cell over time (derived from Nyquist plot Fig. 2d).

R_{el} - electrolyte resistance,

R_{pass} - passivation layer resistance

R_i - interfacial charge transfer resistance

Y_{pass}, Y_i - admittance

n_{pass}, n_i - CPE index

Time (h)	χ^2	R_{el}(Ω)/ % Error	R_{pass}(Ω)/ % Error	Y_{pass} (mho×S^n)/ % Error	n_{pass}/ % Error	R_i (Ω)/ % Error	Y_i (mho×S^n)/ % Error	n_i/ % Error
0	7.5×10^{-5}	3.4/0.8	17.3/15.6	1.9×10^{-1}/ 12.2	0.67/ 11.4	140.3/0.2	4.9×10^{-6}/ 1.4	0.82/ 0.1
24	1.0×10^{-3}	4.1/1.3	31.9/16.6	7.8×10^{-2}/ 44	0.59/ 49	281.1/0.9	3.7×10^{-6}/ 4.1	0.83/ 0.4
48	4.2×10^{-3}	4.4/2.4	33.1/11.1	5.5×10^{-2}/ 18.7	0.56/ 10.1	319.5/3	2.9×10^{-6}/ 15.3	0.88/ 2.1
72	1.3×10^{-3}	3.3/9.3	81.2/33.2	1.7×10^{-2}/ 47.2	0.33/ 20.7	342.2/3.5	5.9×10^{-6}/ 13.3	0.77/ 2.4
144	6.2×10^{-3}	3.9/3.3	55.1/17	2.1×10^{-4}/ 11.7	0.15/ 19.1	360.6/17.2	2.6×10^{-6}/ 29.1	0.85/ 3.7
216	3.1×10^{-3}	3.7/3	56.4/8.1	7.9×10^{-4}/ 12.1	0.64/ 10.2	470/2.8	1.7×10^{-6}/ 7.2	0.84/ 0.8
408	7.5×10^{-3}	2.7/7.6	52.2/13.1	9.5×10^{-4}/ 18.3	0.61/ 16.3	469.2/4.7	2.0×10^{-1}/ 16.1	0.83/ 2.0

Table S3. Electrical parameters of Li|MAO/MWCNT|Li symmetric cell over time (derived from Nyquist plot Fig. 2e)

Time (h)	**χ^2**	**R_{el}(Ω)/ % Error**	**R_{pass}(Ω)/ % Error**	**Y_{pass}(mho×S^n)/ % Error**	**n_{pass}/ % Error**	**R_i(Ω)/ % Error**	**Y_i(mho×S^n) / % Error**	**n_i/ % Error**
0	4.3×10^{-4}	8.5/1.3	39.6/15.7	3.2×10^{-2}/ 14.8	0.53/ 15.8	121.2/6.5	6.9×10^{-5}/ 13.2	0.59/ 1.9
24	5.7×10^{-4}	10.2/1.8	53.4/70	3.9×10^{-2}/ 42	0.36/ 56.1	136.5/12.6	1.3×10^{-4}/ 21.2	0.53/ 4.2
48	9.8×10^{-4}	4.9/2.1	19.5/14	2.6×10^{-3}/ 12.1	0.32/ 56.5	111.4/14.0	9.6×10^{-6}/ 21	0.78/ 2.29
72	2.9×10^{-3}	3.8/6.0	16.1/9.4	4.5×10^{-2}/ 49.7	0.39/ 46.3	90.8/21.72	2.5×10^{-4}/ 34.5	0.5/ 6.5
144	1.8×10^{-3}	4.1/8.9	8.3/56.1	6.3×10^{-3}/ 3.6	0.46/ 1.1	82.4/5.6	9.2×10^{-6}/ 8.5	0.81/ 5.3
216	1.0×10^{-3}	4.4/2.1	10.5/10.9	1.2×10^{-5}/ 17.9	0.78/ 2.1	89.2/9.8	2.6×10^{-7}/ 53.1	0.11/ 5.7
408	9.8×10^{-4}	4.1/2.5	16.2/15.4	1.2×10^{-5}/27.7	0.76/ 3.2	68.4/7.6	6.3×10^{-7}/ 51.2	0.94/ 4

Table S4. CV results of S electrode at various scan rate using MAO/MWCNT separator and Li-ion diffusivity values

Scan rate/ (mV s^{-1})	**Vo(I'))/ V**	**Io(I')/ mA**	**Vo(II') / V**	**Io(II')/ mA**	**Vr(I)/ V**	**Ir(I)/ mA**	**Vr(II)/ V**	**Ir(II)/ mA**	**Voltage difference V(I-I')**	**Voltage difference V(II-II')**
0.01	2.4	0.28	2.35	0.59	2.35	0.23	2.05	0.62	0.05	0.29
0.02	2.41	0.39	2.33	0.83	2.34	0.33	2.04	0.82	0.07	0.28
0.04	2.42	0.59	2.35	1.1	2.33	0.48	2.01	1.04	0.09	0.33
0.08	2.43	1.02	2.37	1.63	2.32	0.75	2.0	1.42	0.12	0.37
0.1	2.44	1.23	2.38	1.85	2.31	0.83	1.99	1.59	0.13	0.38
0.2	2.49	1.94	2.43	2.64	2.28	1.21	1.96	2.1	0.21	0.47
Diffusion coefficient/ cm^2 s^{-1}	**3.7×10^{-7}**		**2.04×10^{-8}**		**1.3×10^{-7}**		**1.1×10^{-8}**			

Table S5. CV results of S electrode at various scan rates using Celgard® separator and Li-ion diffusivity values

Scan rate/ mV s^{-1}	**Vo(I')/ V**	**Io(I')/ mA**	**Vo(II')/ V**	**Io(II')/ mA**	**Vr(I)/ V**	**Ir(I)/ mA**	**Vr(II)/ V**	**Ir(II)/ mA**	**Voltage difference V(I-I')**	**Voltage difference V(II-II')**
0.01	2.39	0.27	2.29	0.44	2.32	0.15	2.06	0.64	0.07	0.23
0.02	2.42	0.41	2.34	0.63	2.31	0.32	2.03	0.72	0.11	0.31
0.04	2.47	0.74	2.39	0.90	2.28	0.46	1.98	0.82	0.19	0.42
0.08	2.53	1.19	2.47	1.24	2.25	0.66	1.92	1.06	0.28	0.55
0.1	2.56	1.32	2.51	1.33	2.23	0.70	1.89	1.11	0.33	0.62
Diffusion coefficient/ cm^2 s^{-1}	**4×10^{-7}**		**9.9×10^{-9}**		**9.8×10^{-8}**		**2.9×10^{-9}**			

*Vo,Vr – oxidation and reduction potential

Io, Ir – Peak current for oxidation and reduction process

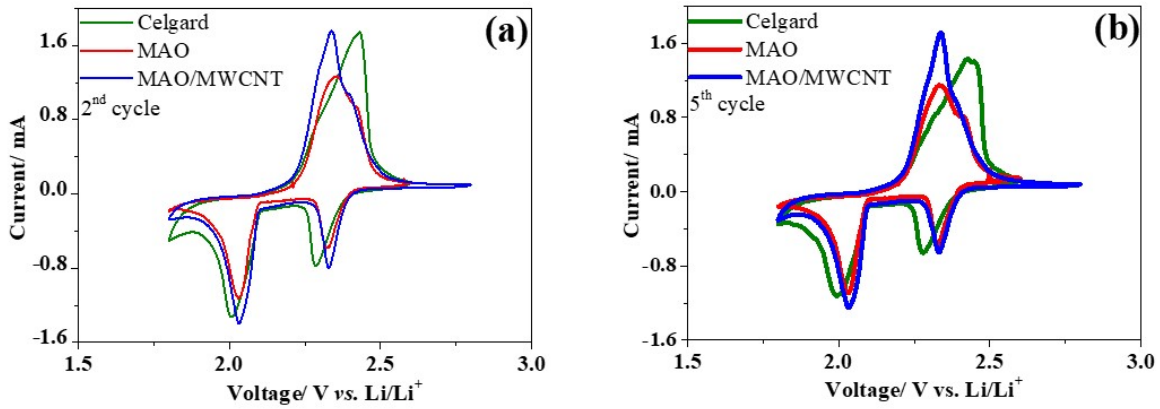

Fig. S1: CV of Li-S cell using Celgard®, MAO and MAO/MWCNT separator at 0.05 mV s^{-1} scan rate for 2nd cycle and 5th cycle

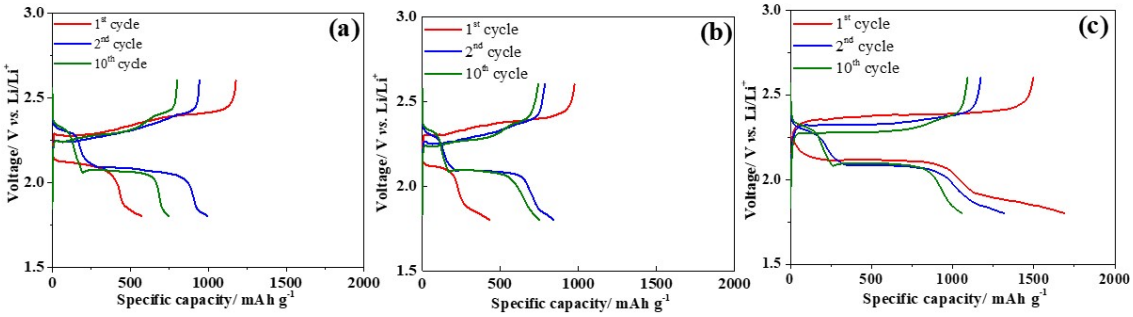

Fig. S2: Galvanostatic charge-discharge profile of Li-S cell for 1st, 2nd, and 10th cycle at 0.2 C rate while using (a) Celgard®, (b) MAO, and (c) MAO/MWCNT separators

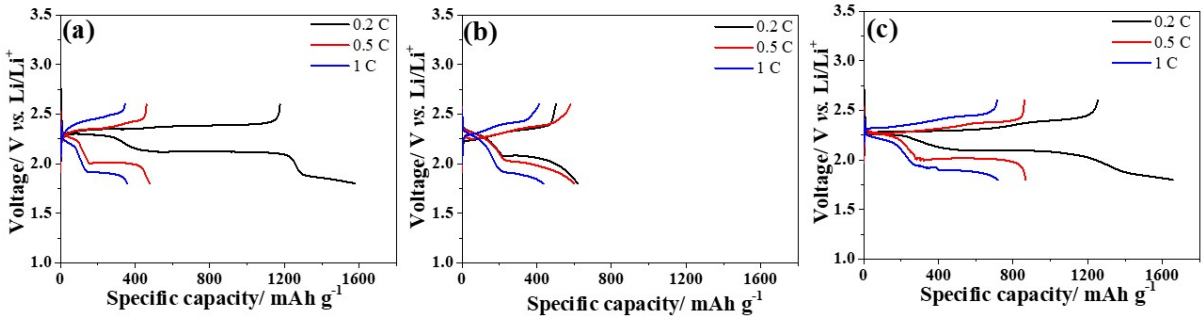

Fig. S3: Galvanostatic charge-discharge profile of Li-S cell at 0.2 C, 0.5 C, 1 C rate while using (a) Celgard®, (b) MAO, and (c) MAO/MWCNT separators