

Supporting Information

Multifunctional Separator Based on Scandium Oxide Nanocrystals Decorated Carbon Nanotubes for High Performance Lithium-Sulfur Batteries

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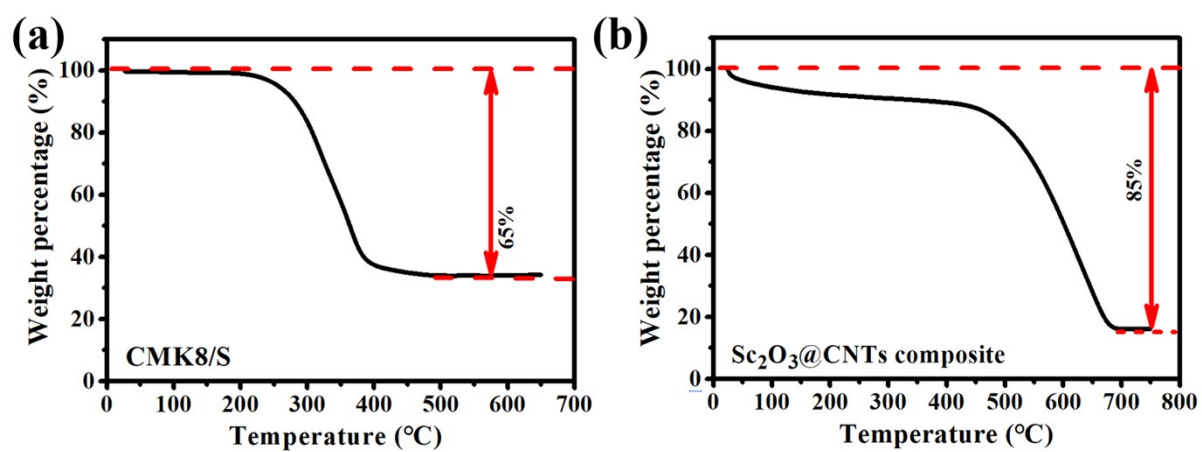


Fig. S1. TGA plots for (a) CMK8/S and (b) Sc₂O₃@CNTs composites.

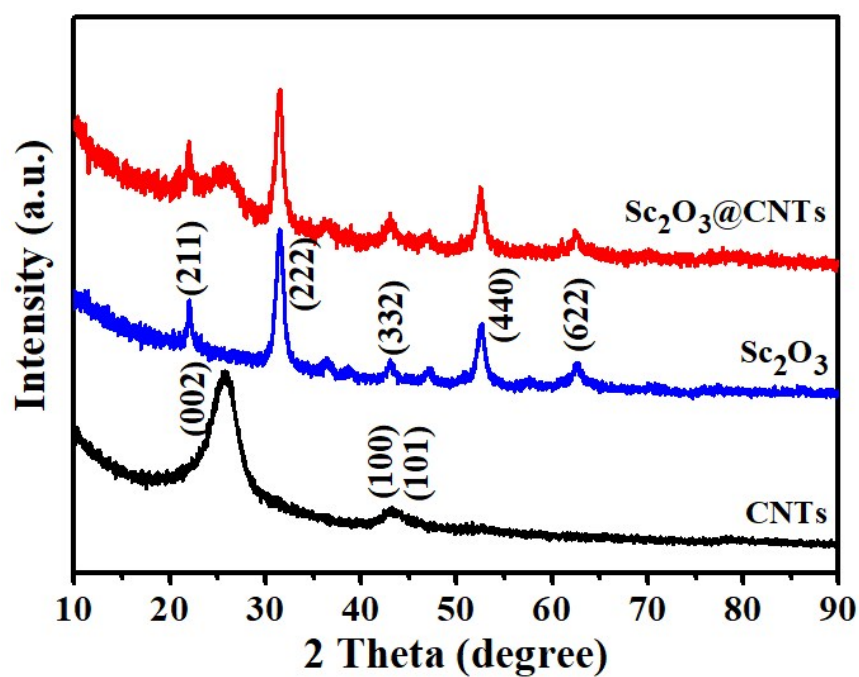


Fig. S2. XRD patterns of CNTs, Sc_2O_3 , and $\text{Sc}_2\text{O}_3@\text{CNTs}$ composite.

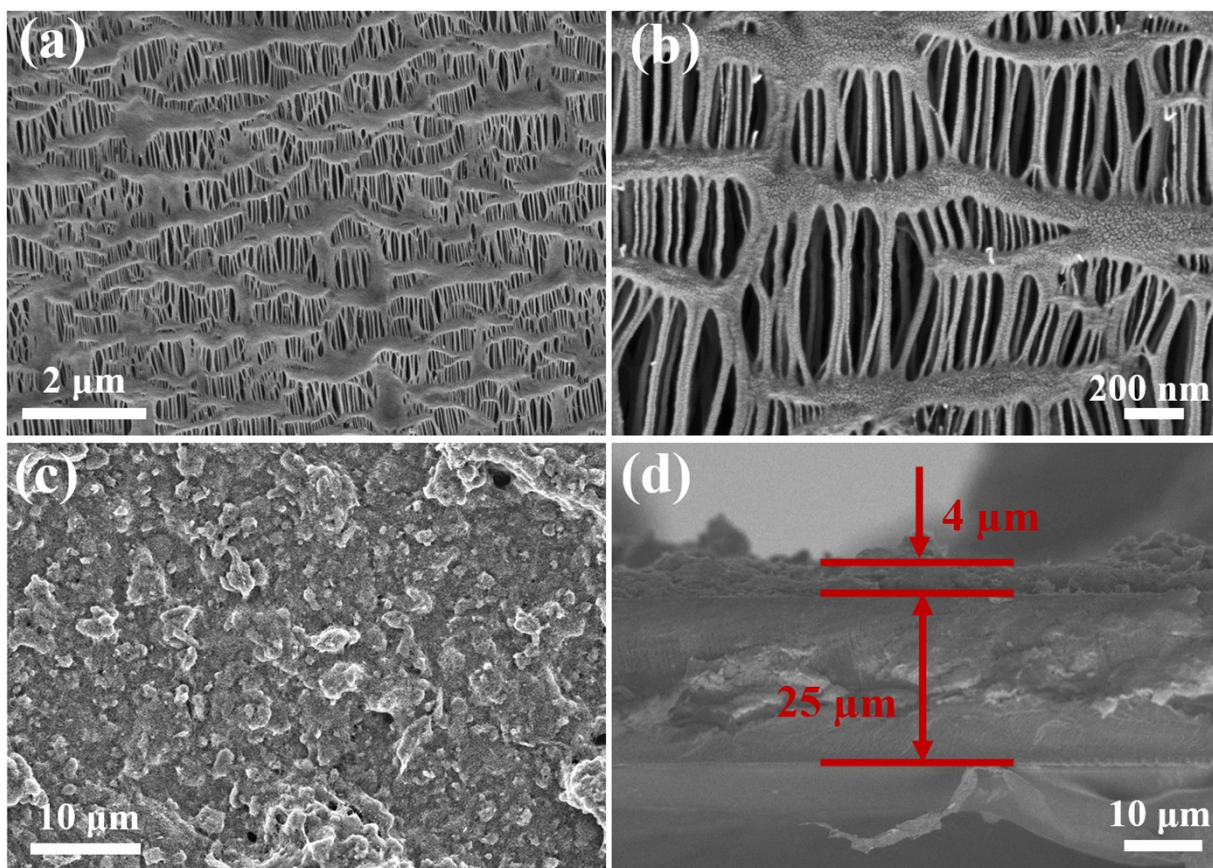


Fig. S3. Top-surface SEM images of commercial PP separator (a, b), and top surface (c) and cross-sectional (d) SEM images of $\text{Sc}_2\text{O}_3@\text{CNTs}$ -coated separator.

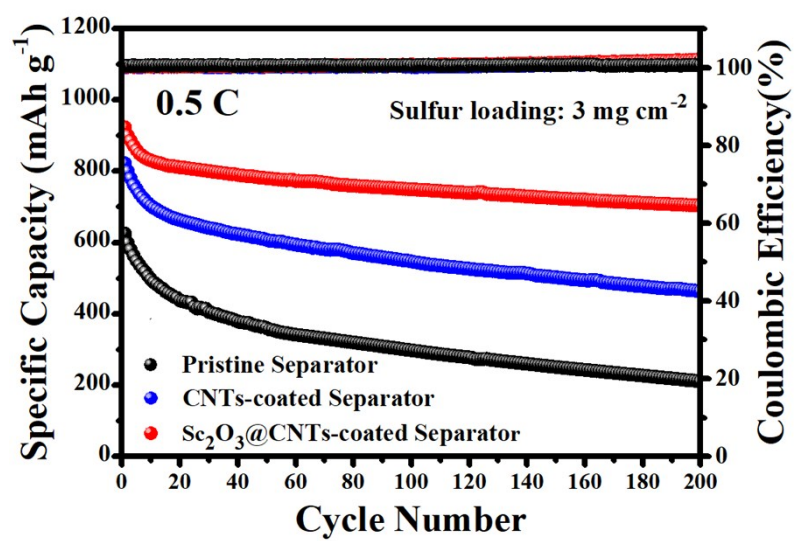


Fig. S4 Cycle performance of Li-S cells with pristine/CNTs-coated/Sc₂O₃@CNTs-coated separators at a sulfur loading of 3 mg/cm².

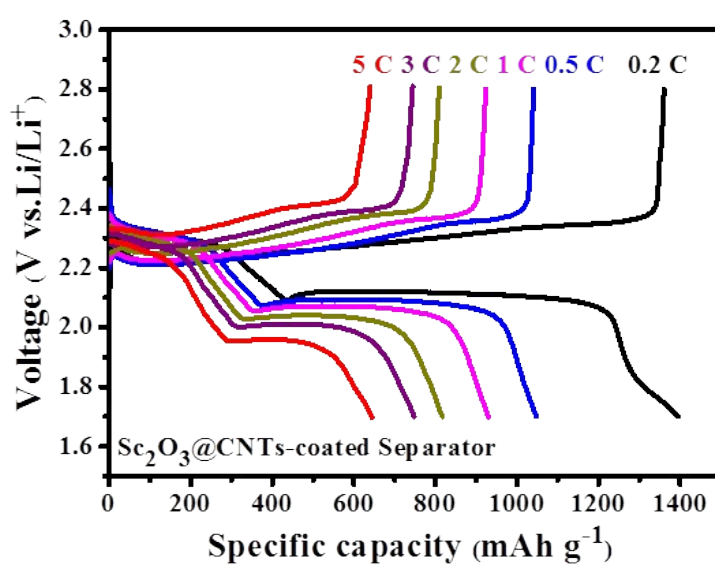


Fig. S5. Charge-discharge voltage profiles of Li-S cell using Sc₂O₃@CNTs-coated separator at different current rates.

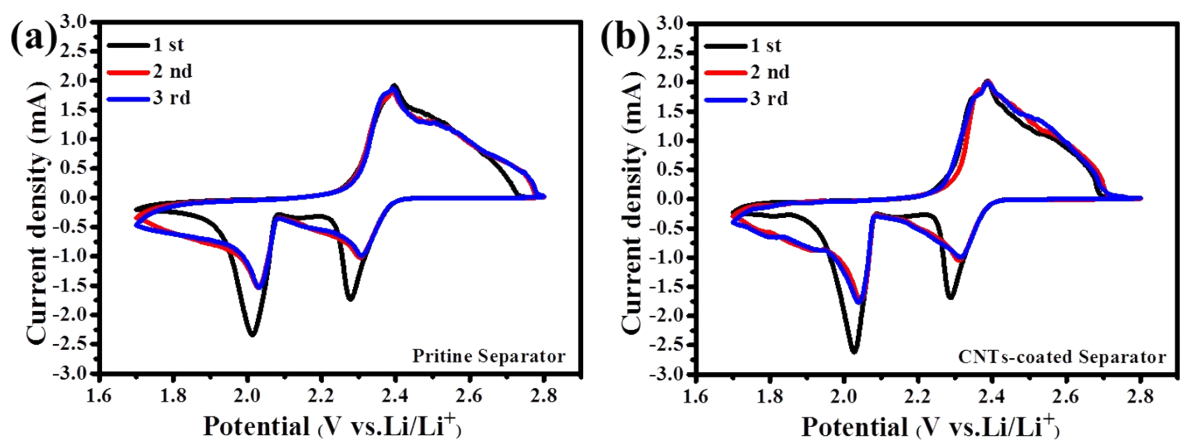


Fig. S6. CV profiles of Li-S cells with pristine and CNTs-coated separators. Measured between 1.7 and 2.8 V at a scan rate of 0.1 mV s^{-1} for the first three cycles.

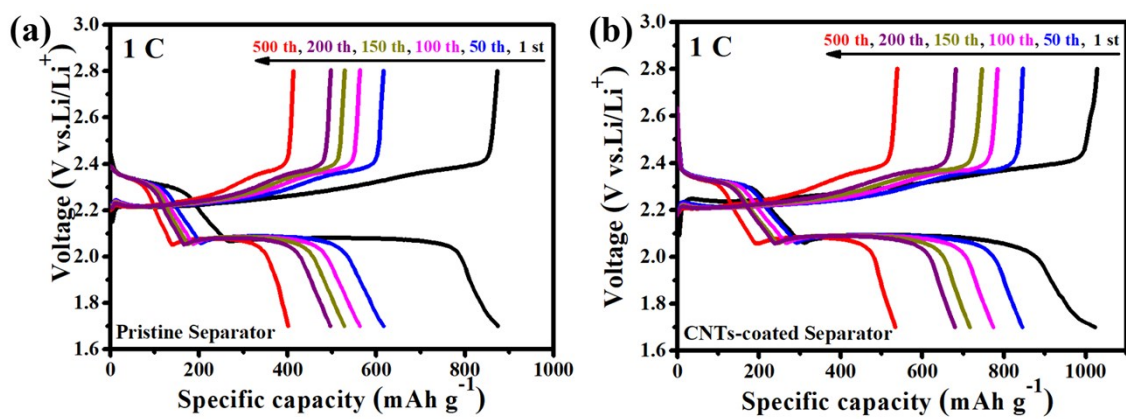


Fig. S7 Charge-discharge voltage profiles of Li-S cells using pristine and CNTs-coated separators at 1C for different cycles.

Table S1 The fitted data of Li-S cells using identical cathodes but different separators

Fitted data	Li-S cell using Sc ₂ O ₃ @CNTs-coated separator			Li-S cell using CNTs-coated separator			Li-S cell using Pristine separator		
	R _e (Ω)	R _{ct} (Ω)	R _f (Ω)	R _e (Ω)	R _{ct} (Ω)	R _f (Ω)	R _e (Ω)	R _{ct} (Ω)	R _f (Ω)
Before cycling	1.85	13.88	/	1.62	17.82	/	1.76	25.12	/
After 50 cycles	3.08	11.68	19.65	3.23	13.84	22.20	4.38	21.11	26.48

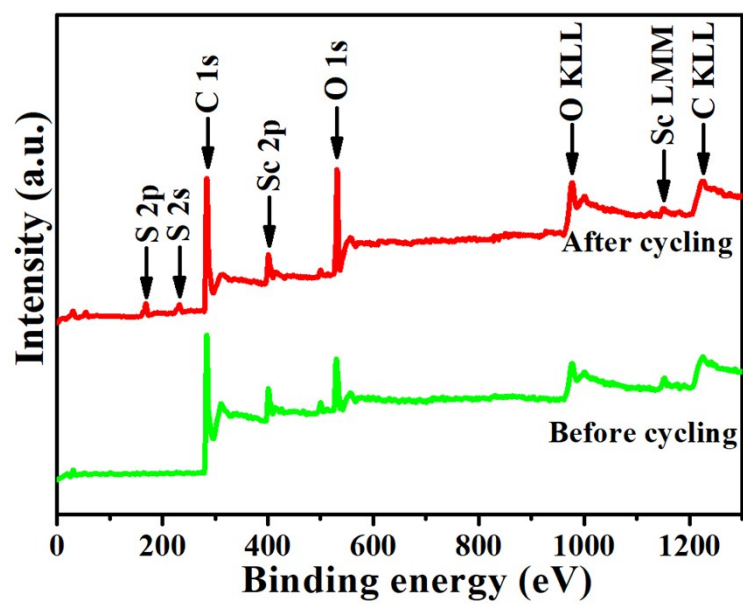


Fig. S8 Full XPS spectrum of $\text{Sc}_2\text{O}_3@\text{CNTs}$ -coated separator before and after cycling.

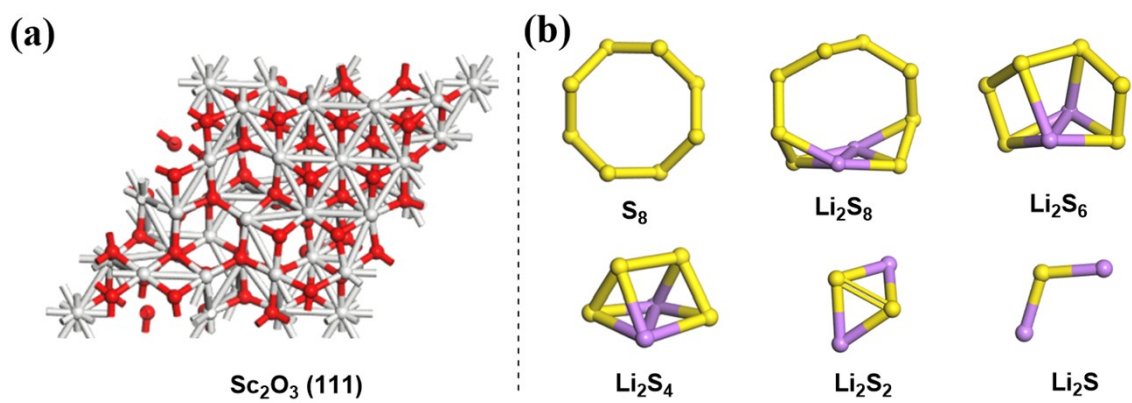


Fig. S9 (a) The optimized $\text{Sc}_2\text{O}_3(111)$ surface model and (b) the optimized structures of S_8 and polysulfide species.

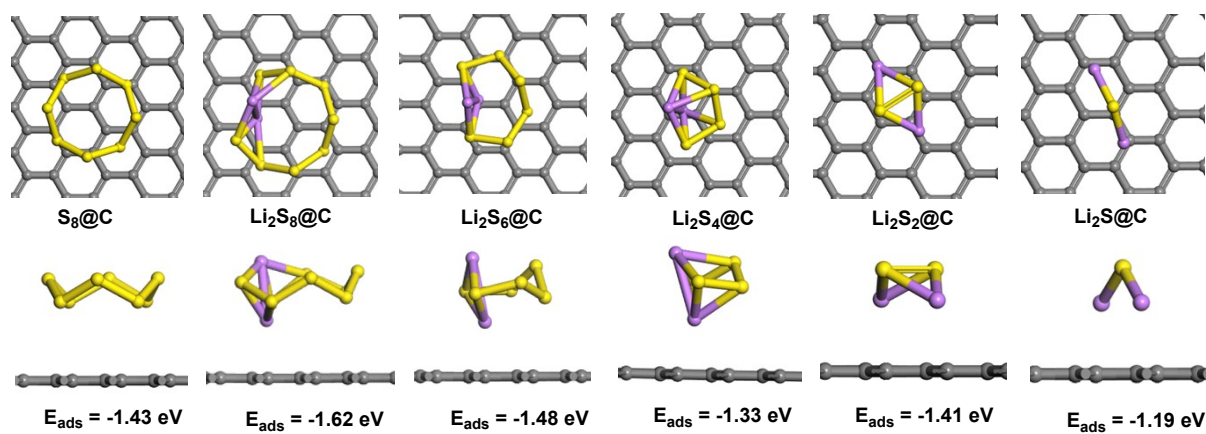


Fig. S10 Binding geometric configurations and adsorption energies of S_8 and polysulfide species with graphene surface.

Table S2 Electronic Energies of related compounds

	Electronic Energy (Hartree)
S ₈	-3185.747731
Li ₂ S ₈	-3200.959077
Li ₂ S ₆	-2404.520454
Li ₂ S ₄	-1608.066235
Li ₂ S ₂	-811.5944191
Li ₂ S	-413.3474638
Sc ₂ O ₃ (111)	-4209.243063
Graphene (refers to C)	-1219.966595
S ₈ @Sc ₂ O ₃	-7395.217711
Li ₂ S ₈ @Sc ₂ O ₃	-7410.399629
Li ₂ S ₆ @Sc ₂ O ₃	-6613.856565
Li ₂ S ₄ @Sc ₂ O ₃	-5817.402273
Li ₂ S ₂ @Sc ₂ O ₃	-5020.93556
Li ₂ S@Sc ₂ O ₃	-4622.667909
S ₈ @C	-4405.766727
Li ₂ S ₈ @C	-4420.985094
Li ₂ S ₆ @C	-3624.541524
Li ₂ S ₄ @C	-2828.081792
Li ₂ S ₂ @C	-2031.61269
Li ₂ S@C	-1633.357987

Table S3 Cartesian Coordinates of related compounds**S₈**

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	5.056469	3.463830	13.061103
2	S	5.934586	2.517052	9.930627
3	S	6.658167	3.195555	11.758889
4	S	5.770149	4.135509	8.631433
5	S	4.511816	5.472268	13.061103
6	S	3.633699	6.419046	9.930627
7	S	2.910118	5.740544	11.758889
8	S	3.798136	4.800590	8.631433

Li₂S₈

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	4.053565	5.692344	12.482087
2	S	5.448478	4.106555	12.494457
3	S	4.729330	2.474685	11.411665
4	S	4.853181	7.375244	11.540382
5	S	5.576021	2.389911	9.496103
6	S	4.123749	7.574200	9.587539
7	S	4.299488	3.128296	8.022188
8	S	5.479856	6.903697	8.151800
9	Li	6.208576	4.594446	8.410428
10	Li	3.556629	5.417495	8.378384

Li₂S₆

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	3.995729	5.664730	12.580343
2	S	5.436404	3.987693	12.656598
3	S	4.582386	2.459906	11.567938
4	S	4.967884	7.206634	11.618039
5	S	4.820690	2.925118	9.552862
6	S	4.984431	6.750833	9.587484
7	Li	6.346369	4.768809	10.104627
8	Li	3.409760	4.900271	9.929599

Li₂S₄

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	4.775983	5.778676	12.272838
2	S	4.904359	3.658042	12.250876
3	S	3.950744	3.075341	10.474040
4	S	5.692604	6.395714	10.487742
5	Li	6.138688	4.014595	10.051935
6	Li	3.496740	5.466108	10.087990

Li₂S₂

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	3.847644	5.571856	12.388333
2	S	5.023034	3.739536	12.541049
3	Li	6.151261	5.770450	12.646746
4	Li	4.077019	4.257900	10.486744

Li₂S

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	S	4.273244	5.609337	11.625341
2	Li	6.407432	5.883458	12.102454
3	Li	3.553320	3.572933	11.188537

Sc₂O₃(111)

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.517533	6.848176	4.082499
2	O	-5.245831	11.040550	1.053596
3	O	1.755960	0.756142	3.580297
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.220460	4.044631	3.705787
7	O	10.574362	3.998960	3.789105
8	O	3.575638	7.858353	-0.478818
9	O	0.233139	9.880429	4.082499
10	O	-0.015881	1.926997	1.053596
11	O	12.312382	1.142635	3.580297
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.530076	9.777056	3.705787
15	O	5.094818	7.158186	3.789105
16	O	-1.670752	11.157712	-0.478818
17	O	-1.750672	7.251985	4.082499
18	O	5.261712	11.013043	1.053596
19	O	6.699458	10.091518	3.580297
20	O	6.690016	2.037027	0.601349

21	O	10.656790	2.296397	1.011111
22	O	-3.309617	10.158903	3.705787
23	O	5.098620	0.833149	3.789105
24	O	-1.904886	4.964525	-0.478818
25	O	-1.426278	9.174139	2.018673
26	O	5.069898	3.308429	2.675138
27	O	0.090834	11.856022	2.195916
28	O	10.032173	0.136379	2.500127
29	O	-0.309299	6.168032	2.018673
30	O	8.445068	2.736446	2.675138
31	O	-3.390434	6.140948	2.195916
32	O	-5.134194	8.619927	2.500127
33	O	1.735577	8.638418	2.018673
34	O	7.252835	5.945420	2.675138
35	O	3.299600	5.983619	2.195916
36	O	2.024621	3.233989	2.500127
37	Sc	0.000000	7.993530	3.248593
38	Sc	3.434587	1.818108	3.073293
39	Sc	6.779834	8.106801	3.073293
40	Sc	10.553379	2.065385	3.073293
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.116586	8.236238	2.813388
48	Sc	6.597927	1.799364	2.783342
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.348101	5.173133	2.813388

52	Sc	8.987941	4.814290	2.783342
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.768485	10.571219	2.813388
56	Sc	5.181932	5.376641	2.783342
57	Sc	0.233487	2.136403	3.157824
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.167270	7.778387	3.394737
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.955677	11.124299	3.157824
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.397315	10.844037	3.394737
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.189164	10.719887	3.157824
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.769954	5.358166	3.394737
68	Sc	5.141416	9.216226	0.067316

Graphene

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.000077	0.001464	-1.970671
2	C	1.229921	0.708674	-1.970671
3	C	-1.229923	2.131886	-1.970671
4	C	-0.000079	2.839096	-1.970671
5	C	-2.459923	4.262309	-1.970671
6	C	-1.230079	4.969519	-1.970671
7	C	-3.689923	6.392731	-1.970671
8	C	-2.460079	7.099941	-1.970671
9	C	2.460077	0.001464	-1.970671

10	C	3.689921	0.708674	-1.970671
11	C	1.230077	2.131886	-1.970671
12	C	2.459921	2.839096	-1.970671
13	C	0.000077	4.262309	-1.970671
14	C	1.229921	4.969519	-1.970671
15	C	-1.229923	6.392731	-1.970671
16	C	-0.000079	7.099941	-1.970671
17	C	4.920077	0.001464	-1.970671
18	C	6.149921	0.708674	-1.970671
19	C	3.690077	2.131886	-1.970671
20	C	4.919921	2.839096	-1.970671
21	C	2.460077	4.262309	-1.970671
22	C	3.689921	4.969519	-1.970671
23	C	1.230077	6.392731	-1.970671
24	C	2.459921	7.099941	-1.970671
25	C	7.380077	0.001464	-1.970671
26	C	8.609921	0.708674	-1.970671
27	C	6.150077	2.131886	-1.970671
28	C	7.379921	2.839096	-1.970671
29	C	4.920077	4.262309	-1.970671
30	C	6.149921	4.969519	-1.970671
31	C	3.690077	6.392731	-1.970671
32	C	4.919921	7.099941	-1.970671

S₈@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.386285	6.831738	4.005529
2	O	-5.245831	11.040550	1.053596
3	O	1.821482	0.712554	3.485200

4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.410055	4.038882	3.234074
7	O	10.502273	4.009696	3.768398
8	O	3.575638	7.858353	-0.478818
9	O	0.230340	9.916584	4.076683
10	O	-0.015881	1.926997	1.053596
11	O	12.309132	1.120088	3.548278
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.523019	9.832234	3.764925
15	O	5.101096	7.275840	3.710562
16	O	-1.670752	11.157712	-0.478818
17	O	-1.768413	7.360602	4.013431
18	O	5.261712	11.013043	1.053596
19	O	6.709827	10.101339	3.528261
20	O	6.690016	2.037027	0.601349
21	O	10.656790	2.296397	1.011111
22	O	-3.310602	10.132502	3.730803
23	O	5.131067	0.756745	3.629313
24	O	-1.904886	4.964525	-0.478818
25	O	-1.474866	9.203148	1.966107
26	O	5.174749	3.256161	2.560261
27	O	0.163710	11.817561	2.136334
28	O	10.032767	0.149643	2.479592
29	O	-0.230972	6.285220	1.929044
30	O	8.454737	2.754597	2.623385
31	O	-3.418852	6.172341	2.184944
32	O	-5.123934	8.618491	2.456260
33	O	1.671118	8.805191	1.980050
34	O	7.233985	5.959307	2.650818

35	O	3.202983	5.987001	2.136562
36	O	2.019168	3.251943	2.466708
37	Sc	0.004046	8.011594	3.197337
38	Sc	3.458632	1.944590	3.282069
39	Sc	6.799752	8.101703	3.071077
40	Sc	10.590696	2.075349	3.085861
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.124996	8.266733	2.855913
48	Sc	6.605954	1.783897	2.779427
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.330305	5.165782	2.901811
52	Sc	8.957804	4.835269	2.793232
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.784859	10.586211	2.948265
56	Sc	5.047138	5.369193	2.937477
57	Sc	0.276891	2.151668	3.395903
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.168101	7.810145	3.889704
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.968411	11.128897	3.194458
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.406665	10.823986	3.385454
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.175489	10.748474	3.182298

66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.818645	5.376121	3.531049
68	Sc	5.141416	9.216226	0.067316
69	S	2.856929	7.874410	6.502060
70	S	3.841912	2.859378	5.588969
71	S	4.276422	4.873122	5.231984
72	S	0.863956	2.789173	5.857034
73	S	0.819946	8.129116	6.725959
74	S	-1.536740	5.178972	6.202792
75	S	-0.235412	6.569217	7.514143
76	S	-1.063235	3.202810	6.566791

Li₂S₈@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.438391	6.823835	4.108924
2	O	-5.245831	11.040550	1.053596
3	O	1.792058	0.739954	3.489849
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.441341	3.999472	3.043186
7	O	10.475540	3.976393	3.817909
8	O	3.575638	7.858353	-0.478818
9	O	0.222805	9.896585	4.083773
10	O	-0.015881	1.926997	1.053596
11	O	12.295719	1.104624	3.539490
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.482529	9.806684	3.766352
15	O	5.068490	7.307543	3.556259

16	O	-1.670752	11.157712	-0.478818
17	O	-1.764317	7.324171	4.050711
18	O	5.261712	11.013043	1.053596
19	O	6.700482	10.101660	3.536203
20	O	6.690016	2.037027	0.601349
21	O	10.656790	2.296397	1.011111
22	O	-3.313221	10.156577	3.712944
23	O	5.098619	0.842789	3.781437
24	O	-1.904886	4.964525	-0.478818
25	O	-1.447380	9.206453	2.003180
26	O	5.099915	3.257251	2.594274
27	O	0.087026	11.850340	2.185548
28	O	10.017364	0.139764	2.489138
29	O	-0.223232	6.337021	1.939935
30	O	8.442236	2.732933	2.637074
31	O	-3.418236	6.140248	2.217670
32	O	-5.117823	8.626267	2.471489
33	O	1.750554	8.678237	2.031399
34	O	7.219257	5.941553	2.672270
35	O	3.224368	6.008559	2.168066
36	O	2.032874	3.251513	2.504828
37	Sc	-0.038281	8.007714	3.209838
38	Sc	3.435696	1.854415	3.085114
39	Sc	6.813601	8.113136	3.056471
40	Sc	10.556071	2.063986	3.079362
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027

47	Sc	-3.112906	8.241887	2.825436
48	Sc	6.599750	1.793894	2.790654
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.312260	5.177576	2.741318
52	Sc	8.960704	4.827311	2.793422
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.758557	10.584307	2.870440
56	Sc	5.102387	5.371364	2.924148
57	Sc	0.207688	2.117860	3.189455
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.122692	7.804653	3.457910
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.940797	11.108174	3.183073
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.412820	10.855370	3.421975
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.180790	10.730882	3.171147
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.830455	5.307874	3.585237
68	Sc	5.141416	9.216226	0.067316
69	S	1.250237	1.763628	8.722968
70	S	1.822530	5.924538	8.208475
71	S	3.837052	6.453279	8.113617
72	S	0.032799	1.545006	7.076965
73	S	4.358232	6.685511	6.147500
74	S	0.400254	3.136730	5.782827
75	S	4.420384	4.708001	5.279691
76	S	-0.838528	4.868734	6.010801
77	Li	1.140243	6.363346	5.928644

78	Li	2.305145	3.642811	7.565066
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Li₂S₆@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.395227	6.774712	4.048318
2	O	-5.245831	11.040550	1.053596
3	O	1.761259	0.749292	3.578247
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.231499	4.054683	3.679400
7	O	10.567371	4.006980	3.802707
8	O	3.575638	7.858353	-0.478818
9	O	0.255293	9.847068	4.118535
10	O	-0.015881	1.926997	1.053596
11	O	12.308606	1.170125	3.575321
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.564553	9.805949	3.560621
15	O	5.112170	7.151470	3.772266
16	O	-1.670752	11.157712	-0.478818
17	O	-1.745335	7.287659	4.025371
18	O	5.261712	11.013043	1.053596
19	O	6.699506	10.107623	3.566399
20	O	6.690016	2.037027	0.601349
21	O	10.656790	2.296397	1.011111
22	O	-3.307562	10.175358	3.690395
23	O	5.107083	0.840240	3.807949
24	O	-1.904886	4.964525	-0.478818
25	O	-1.418947	9.197025	2.019628

26	O	5.075682	3.302346	2.668200
27	O	0.071087	11.835580	2.207333
28	O	10.027444	0.161984	2.485491
29	O	-0.319014	6.149775	2.010960
30	O	8.428527	2.741587	2.658989
31	O	-3.396258	6.130437	2.195511
32	O	-5.149318	8.625813	2.494202
33	O	1.741651	8.593074	2.040866
34	O	7.252087	5.932909	2.666436
35	O	3.291504	5.999882	2.221684
36	O	2.037360	3.220199	2.491493
37	Sc	-0.026184	7.976038	3.128472
38	Sc	3.439681	1.817518	3.076264
39	Sc	6.786514	8.103973	3.081850
40	Sc	10.539858	2.074097	3.079326
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.126044	8.241798	2.792066
48	Sc	6.593715	1.798950	2.782785
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.355416	5.157731	2.766827
52	Sc	8.984124	4.811929	2.784676
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.777217	10.569492	2.754497
56	Sc	5.169445	5.385109	2.780135

57	Sc	0.237928	2.140962	3.162175
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.170293	7.788483	3.578284
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.973747	11.153362	3.146430
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.401334	10.852281	3.418444
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.189804	10.728193	3.153607
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.784497	5.360017	3.394848
68	Sc	5.141416	9.216226	0.067316
69	S	0.633756	6.279924	9.402888
70	S	2.686228	6.720918	9.123734
71	S	3.220673	6.568167	7.085477
72	S	-0.516136	7.908423	8.875503
73	S	3.127886	8.503511	6.190231
74	S	-0.922173	7.731287	6.818281
75	Li	0.689110	9.427097	5.863184
76	Li	1.089815	6.634642	5.857566

Li₂S₄@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.425220	6.794774	4.079135
2	O	-5.245831	11.040550	1.053596
3	O	1.754125	0.758834	3.581037
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.215822	4.048363	3.689238

7	O	10.570727	3.999004	3.796846
8	O	3.575638	7.858353	-0.478818
9	O	0.232199	9.879425	4.119817
10	O	-0.015881	1.926997	1.053596
11	O	12.312868	1.152695	3.575920
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.549068	9.796220	3.624858
15	O	5.140278	7.139988	3.764073
16	O	-1.670752	11.157712	-0.478818
17	O	-1.749627	7.254669	4.049022
18	O	5.261712	11.013043	1.053596
19	O	6.706958	10.097563	3.562732
20	O	6.690016	2.037027	0.601349
21	O	10.656790	2.296397	1.011111
22	O	-3.308521	10.165813	3.706458
23	O	5.100021	0.830904	3.802089
24	O	-1.904886	4.964525	-0.478818
25	O	-1.423669	9.189649	2.018905
26	O	5.072824	3.297571	2.672310
27	O	0.078971	11.848898	2.197318
28	O	10.026787	0.150596	2.494291
29	O	-0.327673	6.172765	2.000008
30	O	8.441574	2.738106	2.673180
31	O	-3.393866	6.136168	2.193513
32	O	-5.129762	8.623504	2.499971
33	O	1.713406	8.631729	2.035063
34	O	7.260201	5.943394	2.659900
35	O	3.300661	5.990582	2.224041
36	O	2.028803	3.227572	2.497169
37	Sc	-0.012018	7.979537	3.156592

38	Sc	3.436932	1.815046	3.072123
39	Sc	6.793706	8.108348	3.071536
40	Sc	10.552462	2.068475	3.075078
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.119940	8.235054	2.808774
48	Sc	6.595859	1.796556	2.781589
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.357739	5.169020	2.754283
52	Sc	8.987316	4.814564	2.783910
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.781585	10.568879	2.765604
56	Sc	5.172219	5.377481	2.772129
57	Sc	0.233384	2.142798	3.156368
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.210131	7.791984	3.613783
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.970157	11.134140	3.147687
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.413830	10.849498	3.385596
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.187883	10.726736	3.155917
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.771568	5.357263	3.387517
68	Sc	5.141416	9.216226	0.067316

69	S	1.196457	8.495281	8.533749
70	S	2.653683	9.304308	7.263719
71	S	3.626829	7.714140	6.298450
72	S	-0.283936	7.771325	7.225312
73	Li	0.528447	9.632698	5.923139
74	Li	1.400912	6.571808	5.921210

Li₂S₂@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.386255	6.769523	4.059560
2	O	-5.245831	11.040550	1.053596
3	O	1.756422	0.758003	3.585769
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111
6	O	-0.228754	4.042660	3.676807
7	O	10.567187	3.999442	3.800901
8	O	3.575638	7.858353	-0.478818
9	O	0.257461	9.884492	4.121993
10	O	-0.015881	1.926997	1.053596
11	O	12.308995	1.144517	3.579825
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.508765	9.813578	3.664713
15	O	5.151369	7.155388	3.760984
16	O	-1.670752	11.157712	-0.478818
17	O	-1.751147	7.260039	4.066747
18	O	5.261712	11.013043	1.053596
19	O	6.702205	10.100701	3.561596
20	O	6.690016	2.037027	0.601349

21	O	10.656790	2.296397	1.011111
22	O	-3.305500	10.169673	3.711867
23	O	5.102802	0.832715	3.810650
24	O	-1.904886	4.964525	-0.478818
25	O	-1.422670	9.196504	2.023304
26	O	5.071929	3.298304	2.672025
27	O	0.070380	11.847741	2.196364
28	O	10.027345	0.150619	2.486497
29	O	-0.350894	6.175972	1.991241
30	O	8.441304	2.734848	2.673784
31	O	-3.394630	6.139253	2.196234
32	O	-5.124984	8.627304	2.500703
33	O	1.704612	8.624601	2.024364
34	O	7.262973	5.943835	2.657454
35	O	3.298250	5.977719	2.228632
36	O	2.023487	3.222021	2.498294
37	Sc	-0.006607	7.974627	3.162592
38	Sc	3.435423	1.815577	3.072650
39	Sc	6.798005	8.110318	3.069164
40	Sc	10.552017	2.067736	3.072344
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.116295	8.239669	2.809570
48	Sc	6.593495	1.796202	2.781271
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.346480	5.167849	2.725678

52	Sc	8.987738	4.813392	2.783370
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.778965	10.562499	2.727292
56	Sc	5.164954	5.381033	2.776171
57	Sc	0.230412	2.139438	3.152916
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.210944	7.783286	3.674369
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.955396	11.129873	3.153284
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.402056	10.850345	3.404673
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.187974	10.728995	3.157061
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.775556	5.361203	3.386225
68	Sc	5.141416	9.216226	0.067316
69	S	1.821901	8.246649	7.342205
70	S	3.564544	7.617916	6.246440
71	Li	1.031757	9.801076	5.803147
72	Li	1.489535	6.431532	5.876540

Li₂S@Sc₂O₃

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	O	1.645104	6.776643	4.260876
2	O	-5.245831	11.040550	1.053596
3	O	1.746874	0.768321	3.591946
4	O	8.736075	4.775211	0.601349
5	O	6.528067	8.080853	1.011111

6	O	-0.182906	4.047220	3.817825
7	O	10.589404	3.971106	3.769334
8	O	3.575638	7.858353	-0.478818
9	O	0.208561	10.037468	4.272643
10	O	-0.015881	1.926997	1.053596
11	O	12.302081	1.131136	3.582489
12	O	5.341708	5.178057	0.601349
13	O	3.582943	1.613046	1.011111
14	O	3.506802	9.798601	3.783980
15	O	5.107940	7.184896	3.772803
16	O	-1.670752	11.157712	-0.478818
17	O	-1.815927	7.186489	4.198341
18	O	5.261712	11.013043	1.053596
19	O	6.708958	10.087402	3.583489
20	O	6.690016	2.037027	0.601349
21	O	10.656790	2.296397	1.011111
22	O	-3.324091	10.140214	3.804364
23	O	5.070756	0.843052	3.784818
24	O	-1.904886	4.964525	-0.478818
25	O	-1.557815	9.307803	1.989030
26	O	5.065265	3.317592	2.684590
27	O	0.080532	11.847062	2.195847
28	O	10.022575	0.102503	2.492399
29	O	-0.351005	5.968395	1.983554
30	O	8.438909	2.729929	2.683360
31	O	-3.374688	6.148841	2.195101
32	O	-5.098621	8.631719	2.493795
33	O	1.882409	8.671373	1.996128
34	O	7.261467	5.943908	2.683430
35	O	3.286764	5.990718	2.195588
36	O	1.997731	3.250136	2.493240

37	Sc	-0.008390	7.997641	4.508305
38	Sc	3.424218	1.834099	3.066423
39	Sc	6.809028	8.101097	3.064953
40	Sc	10.536413	2.046374	3.065707
41	Sc	0.000000	0.000000	0.103863
42	Sc	-3.515113	6.090352	0.168551
43	Sc	7.031956	-0.000999	0.168551
44	Sc	3.405757	5.900942	0.168551
45	Sc	-0.196980	5.929368	0.031186
46	Sc	10.433529	0.131040	0.436027
47	Sc	-3.070131	8.235500	2.843166
48	Sc	6.588264	1.798922	2.770227
49	Sc	1.886106	8.855021	0.031186
50	Sc	8.514951	8.970181	0.436027
51	Sc	1.334353	5.192741	2.816175
52	Sc	9.002413	4.811907	2.774629
53	Sc	-1.689126	9.196200	0.031186
54	Sc	1.819319	2.889073	0.436027
55	Sc	1.742887	10.545488	2.794608
56	Sc	5.182041	5.388287	2.770053
57	Sc	0.229613	2.144849	3.171229
58	Sc	7.168248	6.133917	0.573465
59	Sc	3.188885	7.816800	3.344145
60	Sc	-3.629594	11.834779	0.067316
61	Sc	4.949048	11.116173	3.164012
62	Sc	4.948948	3.140927	0.573465
63	Sc	-1.453379	10.859427	3.355446
64	Sc	-1.511822	2.929585	0.067316
65	Sc	-5.183619	10.720454	3.169384
66	Sc	8.650604	2.715452	0.573465
67	Sc	-1.747633	5.325991	3.374675

68	Sc	5.141416	9.216226	0.067316
69	S	0.303843	8.101776	6.905756
70	Li	0.593262	10.295398	6.107246
71	Li	1.808243	6.485201	6.121647

S₈@C

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.116760	-0.045798	-1.674915
2	C	1.344134	0.662603	-1.671488
3	C	-1.112996	2.084951	-1.675911
4	C	0.114334	2.792960	-1.665403
5	C	-2.343250	4.215019	-1.682314
6	C	-1.115549	4.922904	-1.680010
7	C	-3.573311	6.345302	-1.680481
8	C	-2.346020	7.053567	-1.683991
9	C	2.576752	-0.045938	-1.677009
10	C	3.803909	0.662377	-1.672598
11	C	1.347173	2.084776	-1.661281
12	C	2.573920	2.792626	-1.657122
13	C	0.117372	4.214764	-1.668138
14	C	1.344638	4.922615	-1.664138
15	C	-1.113066	6.345267	-1.683015
16	C	0.114494	7.053400	-1.677923
17	C	5.036908	-0.045948	-1.677459
18	C	6.264101	0.662270	-1.678407
19	C	3.806213	2.084472	-1.660435
20	C	5.033842	2.792732	-1.666653
21	C	2.576778	4.214641	-1.659843
22	C	3.803582	4.922702	-1.661004

23	C	1.347316	6.344942	-1.669366
24	C	2.574107	7.053341	-1.669168
25	C	7.496752	-0.045917	-1.677047
26	C	8.723996	0.662437	-1.677285
27	C	6.266586	2.084772	-1.677231
28	C	7.493973	2.792925	-1.680287
29	C	5.036350	4.214861	-1.668073
30	C	6.263883	4.923049	-1.678610
31	C	3.806656	6.345065	-1.664683
32	C	5.033808	7.053419	-1.673240
33	S	0.410471	5.646024	-5.115524
34	S	3.781208	6.004836	-5.145395
35	S	2.011381	6.513163	-6.122305
36	S	4.662046	4.391729	-6.112850
37	S	-0.130565	3.882157	-6.082734
38	S	2.522504	1.749520	-6.084025
39	S	0.755392	2.273756	-5.108875
40	S	4.131294	2.638169	-5.113696

Li₂S₈@C

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.016102	0.069034	-1.826618
2	C	1.245381	0.774767	-1.819843
3	C	-1.214995	2.200190	-1.806418
4	C	0.013017	2.909006	-1.799958
5	C	-2.443638	4.331073	-1.814765
6	C	-1.215372	5.039211	-1.812463
7	C	-3.673457	6.460959	-1.830300
8	C	-2.444432	7.168192	-1.828092

9	C	2.477271	0.069290	-1.821369
10	C	3.706601	0.777150	-1.810084
11	C	1.245190	2.199862	-1.806852
12	C	2.477531	2.908693	-1.800566
13	C	0.015843	4.332643	-1.800305
14	C	1.245367	5.040304	-1.804046
15	C	-1.213257	6.461797	-1.819603
16	C	0.015806	7.169346	-1.817432
17	C	4.937631	0.070127	-1.817117
18	C	6.165969	0.778096	-1.816363
19	C	3.709726	2.199624	-1.797519
20	C	4.937114	2.908364	-1.799250
21	C	2.477975	4.333665	-1.803698
22	C	3.707646	5.039532	-1.811168
23	C	1.247047	6.462909	-1.814788
24	C	2.475890	7.169016	-1.822017
25	C	7.396820	0.070252	-1.823445
26	C	8.625362	0.777406	-1.819579
27	C	6.166803	2.200727	-1.806347
28	C	7.394914	2.908098	-1.808069
29	C	4.937320	4.331174	-1.807742
30	C	6.165328	5.038171	-1.820621
31	C	3.707020	6.461495	-1.822083
32	C	4.935597	7.168274	-1.830117
33	S	1.623807	6.908871	-6.574554
34	S	-0.050735	6.389724	-5.418368
35	S	-1.128258	4.818011	-6.290435
36	S	3.414096	6.387896	-5.637335
37	S	-0.823564	3.052767	-5.223164
38	S	4.209109	4.619984	-6.433332
39	S	0.517169	1.717531	-6.093973

40	S	4.014644	3.009985	-5.125396
41	Li	1.699699	2.840046	-4.399193
42	Li	2.611952	2.602535	-7.005470

Li₂S₆@C

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.001231	0.058957	-1.957237
2	C	1.233133	0.771369	-1.943675
3	C	-1.228485	2.189702	-1.955407
4	C	0.002044	2.902833	-1.942333
5	C	-2.457667	4.319910	-1.960488
6	C	-1.226066	5.032813	-1.959303
7	C	-3.687993	6.450378	-1.960986
8	C	-2.455868	7.163073	-1.960588
9	C	2.462116	0.058383	-1.948183
10	C	3.694867	0.769964	-1.944154
11	C	1.228435	2.187854	-1.933742
12	C	2.463537	2.902093	-1.928906
13	C	0.001216	4.319703	-1.945927
14	C	1.232245	5.034263	-1.941225
15	C	-1.227777	6.450089	-1.961792
16	C	0.003839	7.163384	-1.959528
17	C	4.922736	0.058636	-1.956717
18	C	6.154286	0.772487	-1.960501
19	C	3.695021	2.187942	-1.934347
20	C	4.926940	2.903260	-1.940983
21	C	2.461880	4.323330	-1.933824
22	C	3.695425	5.034820	-1.939997
23	C	1.231719	6.450957	-1.953321

24	C	2.463955	7.163900	-1.958251
25	C	7.381931	0.059536	-1.964215
26	C	8.613756	0.772586	-1.960701
27	C	6.153353	2.189499	-1.955162
28	C	7.384399	2.902711	-1.959014
29	C	4.923320	4.320446	-1.943377
30	C	6.154965	5.033389	-1.957305
31	C	3.692199	6.451482	-1.954084
32	C	4.924184	7.163702	-1.959858
33	S	3.709659	5.153255	-6.807535
34	S	2.061465	5.549464	-5.431459
35	S	0.420379	4.485170	-6.084690
36	S	5.092943	4.047343	-5.743098
37	S	0.690990	2.478233	-5.590712
38	S	4.492846	2.049584	-5.698529
39	Li	2.705249	2.903456	-4.353079
40	Li	2.551170	2.344359	-7.151094

Li₂S₄@C

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.057744	-0.041723	-1.966059
2	C	1.169590	0.669513	-1.959700
3	C	-1.287566	2.089057	-1.962628
4	C	-0.061562	2.800694	-1.950963
5	C	-2.516846	4.219585	-1.961269
6	C	-1.290001	4.931425	-1.962251
7	C	-3.746909	6.349983	-1.963646
8	C	-2.519561	7.061621	-1.969349
9	C	2.403065	-0.041665	-1.964308

10	C	3.631126	0.668695	-1.960015
11	C	1.169242	2.086911	-1.948122
12	C	2.399902	2.799339	-1.937097
13	C	-0.058226	4.219724	-1.950959
14	C	1.167165	4.933374	-1.945363
15	C	-1.286937	6.349836	-1.967787
16	C	-0.059899	7.061654	-1.966511
17	C	4.863631	-0.041910	-1.966454
18	C	6.090570	0.670479	-1.966814
19	C	3.636420	2.087250	-1.944836
20	C	4.863009	2.801465	-1.942758
21	C	2.402883	4.222438	-1.935452
22	C	3.633677	4.933742	-1.938863
23	C	1.172367	6.350721	-1.957432
24	C	2.400369	7.061753	-1.961037
25	C	7.322960	-0.041649	-1.968984
26	C	8.550133	0.670298	-1.967725
27	C	6.094220	2.088966	-1.959331
28	C	7.320602	2.801365	-1.962670
29	C	4.865484	4.220547	-1.938870
30	C	6.091337	4.931804	-1.954239
31	C	3.633528	6.351403	-1.954456
32	C	4.860692	7.061944	-1.963436
33	S	3.739930	5.062892	-6.635228
34	S	1.899119	5.398885	-5.652567
35	S	0.833884	3.594080	-5.824031
36	S	4.613062	3.432930	-5.639169
37	Li	2.614038	3.460446	-4.264496
38	Li	2.784268	2.628616	-6.992281

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	-0.068951	0.047066	-1.917469
2	C	1.160307	0.757159	-1.912834
3	C	-1.298509	2.176980	-1.927170
4	C	-0.069775	2.886801	-1.918946
5	C	-2.529236	4.308822	-1.921242
6	C	-1.300463	5.018934	-1.928658
7	C	-3.759120	6.439051	-1.912433
8	C	-2.529918	7.149081	-1.919953
9	C	2.390083	0.046545	-1.914969
10	C	3.619129	0.756111	-1.911870
11	C	1.160135	2.175855	-1.906407
12	C	2.388602	2.884916	-1.905158
13	C	-0.071873	4.306182	-1.930114
14	C	1.159269	5.018839	-1.930551
15	C	-1.299861	6.438578	-1.926994
16	C	-0.070605	7.149396	-1.929391
17	C	4.849922	0.046474	-1.923003
18	C	6.080557	0.755215	-1.931904
19	C	3.618251	2.174639	-1.909907
20	C	4.848942	2.889175	-1.919619
21	C	2.392563	4.306572	-1.911412
22	C	3.622290	5.021500	-1.903140
23	C	1.160980	6.441407	-1.929985
24	C	2.391629	7.150096	-1.917548
25	C	7.311829	0.047081	-1.926812
26	C	8.541067	0.757502	-1.924377
27	C	6.082295	2.176679	-1.934905
28	C	7.312695	2.889362	-1.931282

29	C	4.852322	4.311484	-1.906705
30	C	6.081130	5.020333	-1.908360
31	C	3.622021	6.440108	-1.903852
32	C	4.851015	7.149524	-1.910763
33	S	2.936005	2.806764	-5.487308
34	S	4.079815	4.600383	-5.485261
35	Li	5.055578	2.723056	-4.448375
36	Li	1.980090	4.672473	-4.410892

Li₂S@C

Final Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	0.004716	-0.004220	-1.909524
2	C	1.234231	0.705750	-1.903117
3	C	-1.225389	2.125091	-1.918076
4	C	0.003917	2.834968	-1.911785
5	C	-2.455878	4.257555	-1.924681
6	C	-1.228193	4.968997	-1.928676
7	C	-3.685622	6.388493	-1.915712
8	C	-2.456179	7.098374	-1.918791
9	C	2.463894	-0.004425	-1.909275
10	C	3.693189	0.704804	-1.908833
11	C	1.234631	2.124850	-1.894182
12	C	2.462675	2.836022	-1.887056
13	C	0.002422	4.256013	-1.920722
14	C	1.235327	4.969204	-1.907143
15	C	-1.226528	6.388363	-1.924635
16	C	0.003842	7.099269	-1.917122
17	C	4.924378	-0.003974	-1.914898
18	C	6.155237	0.705116	-1.915832

19	C	3.691901	2.124013	-1.902246
20	C	4.924216	2.836911	-1.915291
21	C	2.466451	4.256613	-1.890458
22	C	3.694275	4.970500	-1.892661
23	C	1.235221	6.391393	-1.908991
24	C	2.465036	7.099207	-1.904029
25	C	7.385464	-0.003878	-1.911922
26	C	8.614721	0.706211	-1.913086
27	C	6.157421	2.124848	-1.920339
28	C	7.385944	2.837209	-1.922218
29	C	4.924493	4.260464	-1.909596
30	C	6.155069	4.969878	-1.917794
31	C	3.694872	6.388184	-1.898409
32	C	4.924248	7.098323	-1.908463
33	S	2.978611	3.772472	-5.620784
34	Li	4.685647	3.027085	-4.388518
35	Li	1.212116	4.417842	-4.409354

Table S4 Summary of the electrochemical performances of Li-S cells improved by $\text{Sc}_2\text{O}_3@\text{CNTs}$ -coated separator, and other types of functional separators reported in literature over the past three years

Functional separator	Sulfur content (%)	Areal sulfur loading (mg cm^{-2})	Rate (C)	Initial capacity (mAh g^{-1})	Cycled capacity (mAh g^{-1})	Cycle number (n)	Capacity retention (%)	Capacity decay per cycle (%)	Rate capacity (mAh g^{-1})	Refs
MWCNT/NCQD ^a	48.8	2.0	0.5	1330	650 507	500 1000	48.8 38.1	0.05	0.2~3 C 3C: 666	[17]
$\text{MoO}_3@\text{CNT}$	60	1.0	0.3	1218	755	200	62	0.19	0.3~3 C 3C: 655	[19]
MoS_2/CNT	50	1.4	0.5	1237	859	500	69.5	0.061	0.2~10 C 10 C: 784	[25]
MoP_2/CNT	50	1.2	1.0	619	543	500	87	0.025	0.1~5 C 5C: 360	[56]
CoP/KB^b	70	1.5	1.0	928	550	500	59.2	0.078	0.1~5 C 5C: 725	[57]
CNT/CH^c	78	1.2	0.5	890	534	200	60	0.2	0.1~1 C 1C: 843	[58]
$\text{SnS}_2@\text{CNT}/\text{S}-\text{SnS}_2@\text{CNT}$	78	1.4	0.5	1000	963	200	96.3	0.019	0.1~2 C 2C: 783	[59]
SSNS/CNT^d	65	1	1.0	790	403	1000	51	0.049	0.2~2 C 2C: 530	[60]
$\text{CNT}@\text{TiO}_2$	66.4	1.7	0.1	1351	803	200	59	0.2	0.2~2 C 2C: 740	[61]

PCCNT@NPS ^e	78.8	1.1-1.2	1	1067	657	500	61.5	0.077	0.1~2 C 2C: 655	[62]
Sc₂O₃@CNTs	65	1.5	1	1037	788	500	75.7	0.048	0.2~5 C 2C: 813 5C: 647.5	our work

Note: a. multiwall carbon nanotube/N-doped carbon quantum dot b. KB: Ketjen black c. carbon nanotubes/chitosan modified separator d. Sb₂S₃

Nanosheet/carbon nanotube e. P-doped carbon coated CNT skeleton coupled with nickel phosphide (Ni₂P) nanospheres.

