Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

Synthesis, Characterization and Electrochemical Lithium-ion Storage Property of Sulfonylcalix[4]quinone

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Contents

Experimental section

1. General methods

Melting points (mp) were performed using BUCHI M-565. Nuclear magnetic resonance (NMR) spectroscopy was conducted by Bruker 400 MHz (AV/400). Fourier transform infrared (FT-IR) spectrum was measured with Thermo Scientific Nicolet iS10. Electrospray ionization mass spectrometry (ESI-MS) was recorded with Agilent 1290II-6460. Elemental analysis (EA) was obtained on Perkin Elmer 2400.

2. Structural characterization

The thermogravimetric analysis (TG, NETZSCH, STA 449 F3) was employed to characterize the thermal stability of SC4Q. X-ray diffraction (XRD, Rigaku Mini-Flex 600) was performed to investigate its material crystallinity. Scanning electron microscopy (SEM, JEOL JSM7500F) and transmission electron microscopy (TEM, FEI Talos F200X G2, AEMC) were used to observe the structural morphology and element distribution of SC4Q.

3. Electrochemical characterization

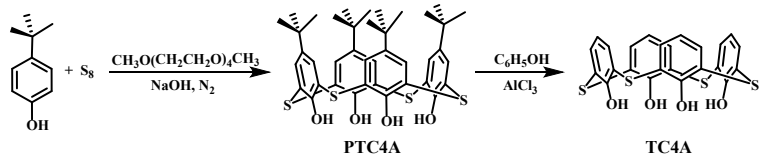
40 wt.% Sulfonylcalix[4]quinone (SC4Q), 40 wt.% ketjenblack (KB) and 20 wt.% poly(vinylidene fluoride) (PVDF) were ground evenly in 1-Methyl-2-pyrrolidinone (NMP) to prepare electrode slurry. Subsequently, it was coated on the collector aluminum foil, vacuum dried at 60 °C for 12 h, and cut into electrode sheets with a diameter of 12 mm. The mass loading of the active substance SC4Q on Al foil was around 0.6-1.0 mg cm^{-2}. The pure KB electrode (KB:PVDF=8:2) was prepared to deduct the capacity contribution of conductive carbon.

Within the vacuum glove box, CR2032 standard button batteries were fabricated with SC4Q as the cathode, metal lithium as the anode, and 0.3 M bis(trifluoromethane)sulfonimide lithium salt/N-methyl-N-propylpyrrolidinium bis(trifluoromethane)sulfonimide (LiTFSI/[PY13][TFSI]) as the electrolytes. The electrochemical measurements, including cyclic voltammetry (CV), rate capability, discharge-charge performance, galvanostatic intermittent titration technique (GITT), and electrochemical impedance spectroscopy (EIS) were conducted under 30 °C using the battery testing thermostat. The discharge-charge performance was performed on the Neware CT-4008T with a voltage range of 0.01–3.0 V. CV and EIS tests were performed through the CHI-660E electrochemical workstation with a scan rate of 0.2 mV s^{-1} and a frequency range of 10^{-2}-10^{5} Hz.

4. Density functional theory (DFT) calculation

The initial configuration and lithiation structure of SC4Q was constructed by GaussView·6.0 and optimized by Gaussian·16W.[1] The highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO), and the HOMO-LUMO energy gaps (*E*g) of SC4Q were calculated under the basis of the B3LYP/6-31G(d, p) group. Considering the dispersion and weak interaction of the organic system, DFT-D3(BJ) was used for molecular dispersion correction.[2] The molecular surface electrostatic potential (MESP) and dipole moment can be found in the output file.

5. Material synthesis



Scheme S1 One-step synthesis method of PTC4A and TC4A

Synthesis and characterization of p-tert-butylthiacalix[4]arene (PTC4A)

Under N_2 atmosphere, a mixture of 32.75 g (0.22 mol) *p*-tert-Butylphenol in 10 ml tetraethylene glycol dimethyl ether was stirred for 15 min and heated gradually to 110 °C for 1 h. Then, 13.75 g (0.054 mol) S8 and 4.43 g (0.12 mol) NaOH were gradually added to the mixture and kept at 230 °C for a further 4 h. The reaction was continuously monitored by TLC (hexane/chloroform, v:v=1:1). After that, the resulting dark brown mixture was cooled to 130 °C and diluted with 70 ml H_2SO_4 solution (15 ml conc. H_2SO_4 in 55 ml H_2O) and 17.5 ml toluene. After cooling down to room temperature, 140 ml diethyl ether was poured into the reaction mixture. The white product PTC4A was collected by filtration, washed with 1 M HCl, and further purified by recrystallization from chloroform and methanol. The yield obtained was 70%.

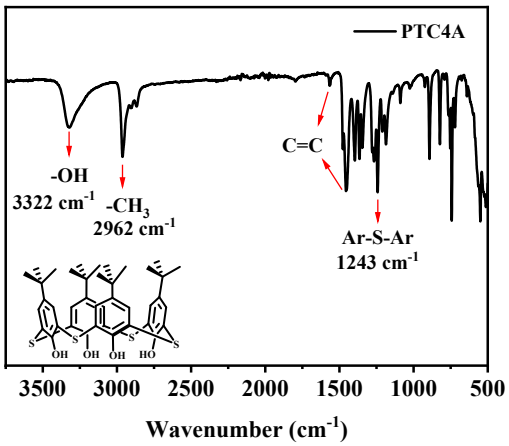


Figure S1 FT-IR spectrum of PTC4A

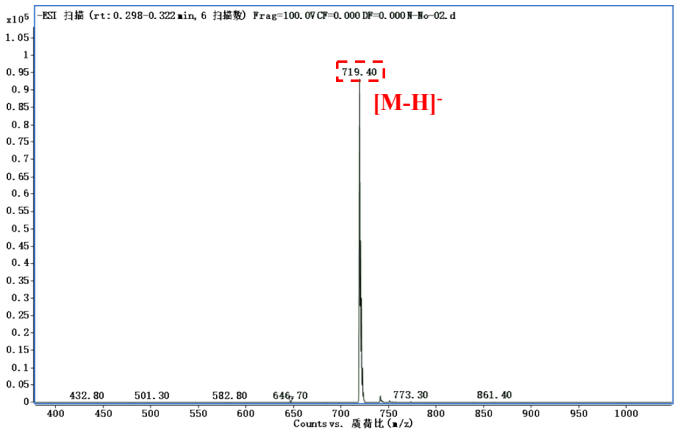


Figure S2 Mass Spectrometry (MS) image of PTC4A

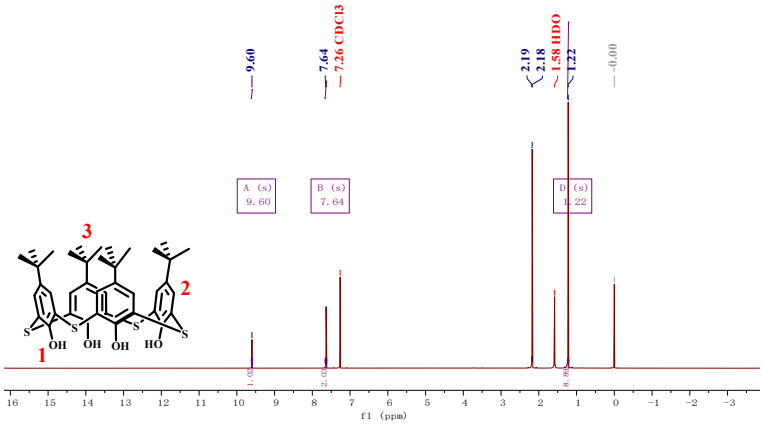


Figure S3 ^{1}H NMR (600 MHz, $CDCl_3$) of PTC4A: δ=9.6 (4H, s, -OH), 7.64 (8H, s, aromatic-H), 1.22 (36H, s, -$C(CH_3)_3$) ppm.

Synthesis and characterization of thiacalix[4]arene (TC4A)

A suspension of 5.0 g (6.94 mmol) PTCA, 3.15 g (3.67 mmol) phenol, and 9.73 g (73.0 mmol) $AlCl_3$ was stirred in 200 ml anhydrous toluene at 80 °C for 2 h. After cooling to room temperature, the reaction mixture was washed with water and HCl (v:v=1:10), then the solvent was evaporated in vacuo. The yellowish product was suspended in 100 ml MeOH and refluxed for 30 min. After cooling, the white precipitates were filtered to afford pure TCA with a yield of 73.5%.

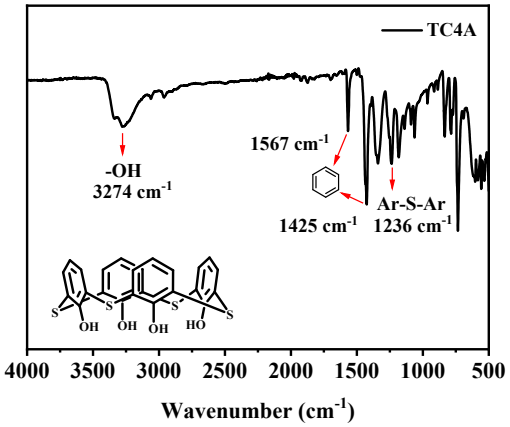


Figure S4 FT-IR spectrum of TC4A

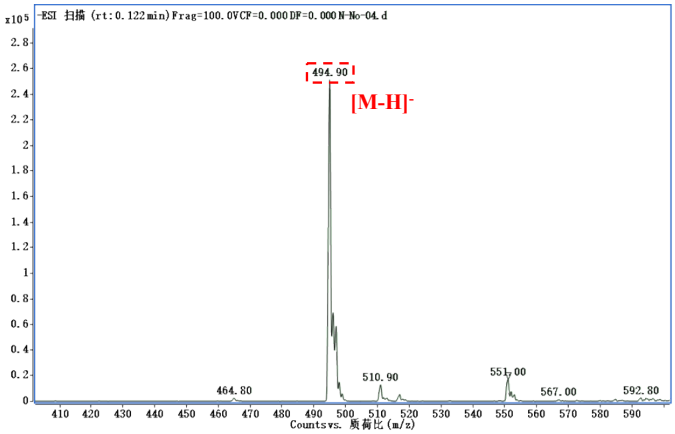


Figure S5 MS image of TC4A

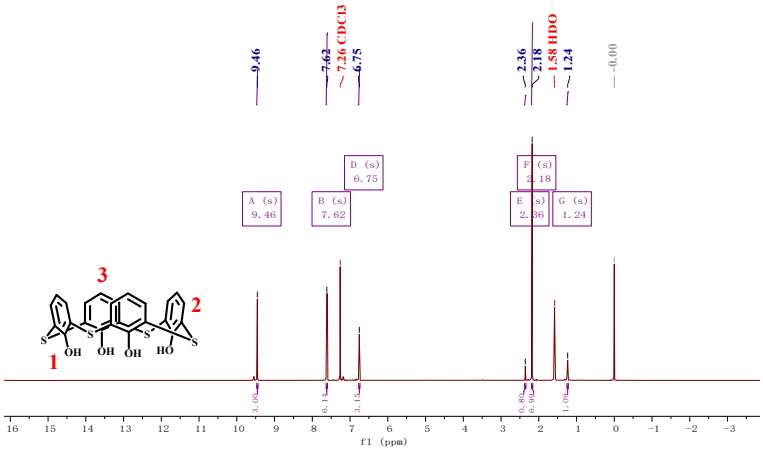


Figure S6 ^{1}H NMR (600 MHz, $CDCl_3$) of TC4A: δ=9.46 (4H, s, -OH), 7.62 (8H, s, aromatic-H), 6.75 (4H, s, aromatic-H) ppm.

Characterization of sulfonylcalix[4]arene (SC4A)

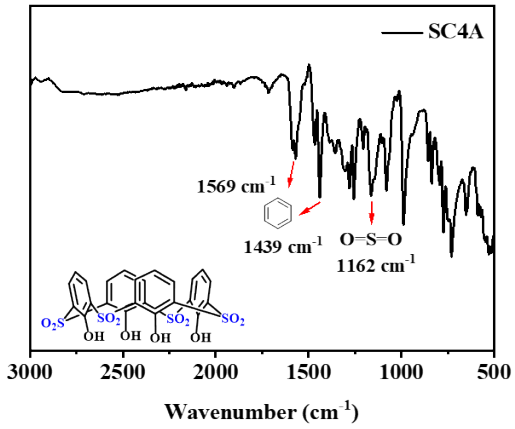


Figure S7 FT-IR spectrum of SC4A

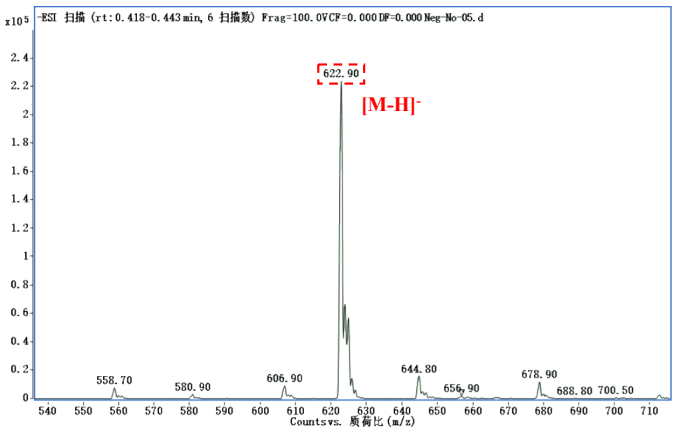


Figure S8 MS image of SC4A

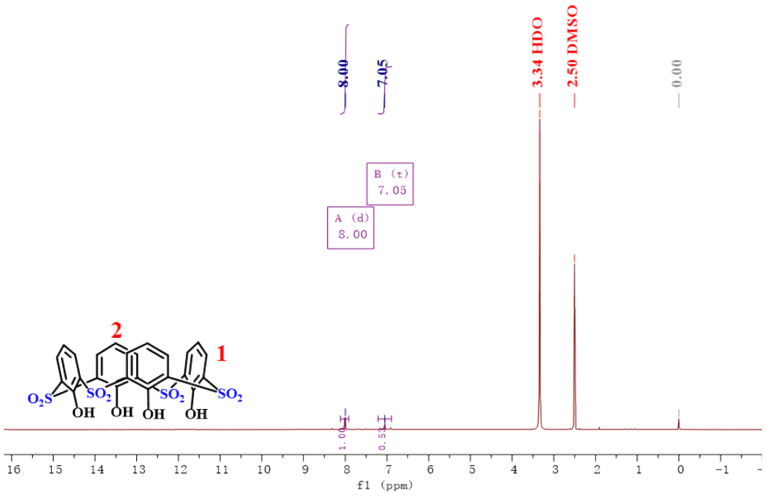


Figure S9 ^{1}H NMR (600 MHz, $(CD_3)_2SO$) of SC4A: δ=8.00 (d, 8H, aromatic-H), 7.05 (t, 4H, aromatic-H) ppm.

Characterization of 5,11,17,23-Tetrakis[(p-carboxyphenyl)azo]-25,26,27,28-tetrahydroxysulfonylcalix[4]arene (Azo-SC4A)

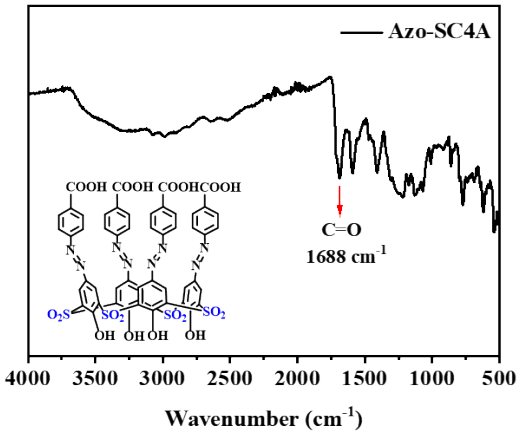


Figure S10 FT-IR spectrum of Azo-SC4A

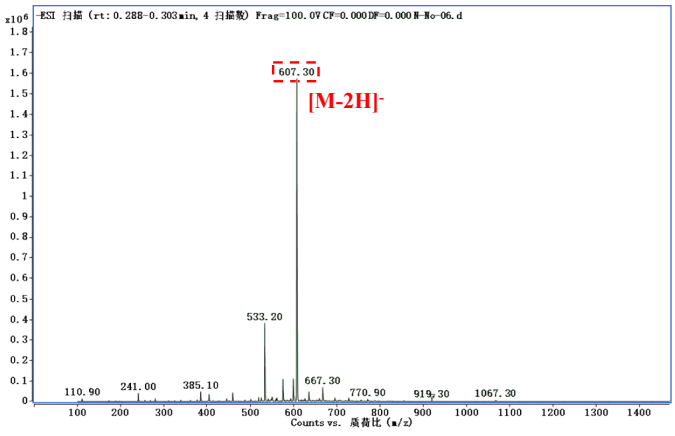


Figure S11 MS image of Azo-SC4A

Characterization of 5,11,17,23-Tetraaminosulfonylcalix[4]arene (ASC4A)

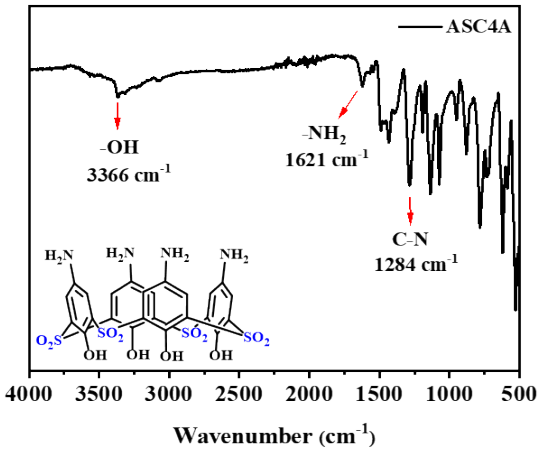


Figure S12 FT-IR spectrum of ASC4A.

Characterization of SC4Q

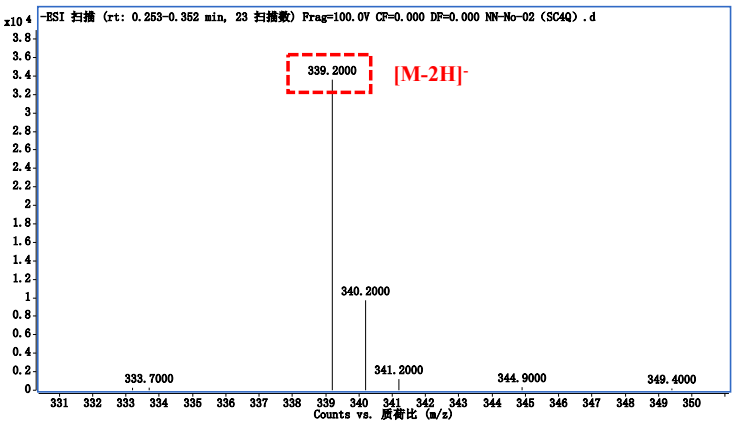


Figure S13 MS image of SC4Q.

Table S1. Element compositions of the theoretical calculation and elemental analysis (EA) results of SC4Q.

	C	O	S	H
Theoretical (wt. %)	42.35	37.65	18.82	1.18
EA	41.83	38.51	17.72	1.94

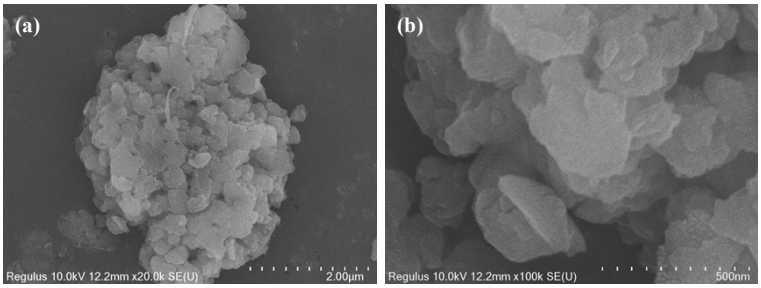


Figure S14 SEM images of pristine SC4Q particle.

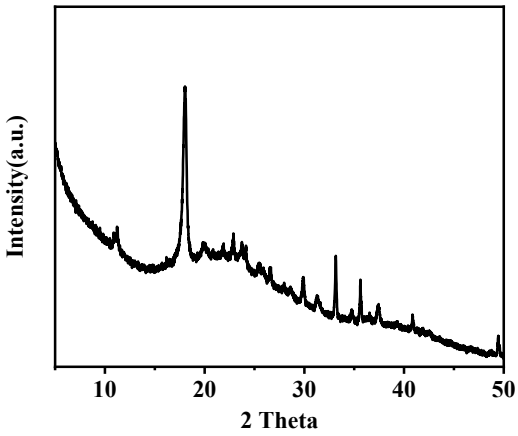


Figure S15 XRD patterns of pristine SC4Q.

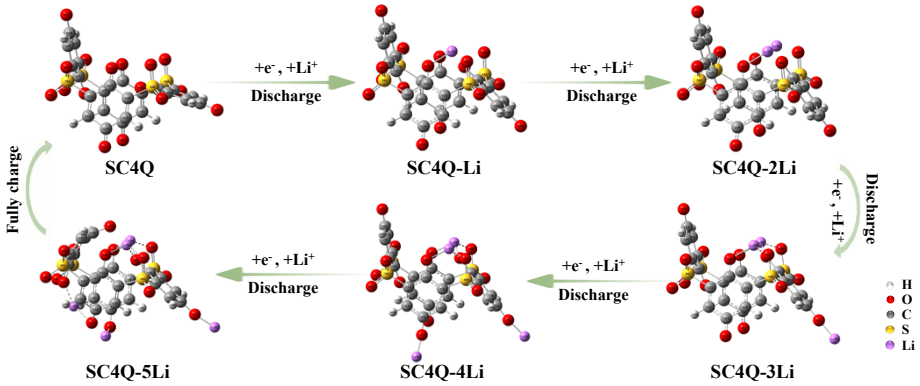


Figure S16 Proposed redox mechanism and structural evolution of SC4Q cathodes in organic LIBs based on DFT calculations.

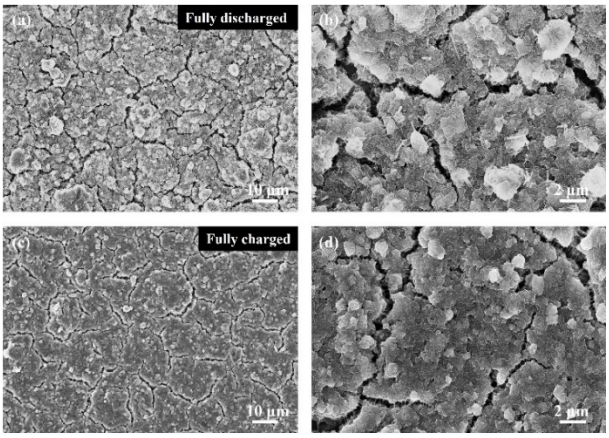


Figure S17 SEM images of SC4Q-based electrodes under (a, b) fully discharged and (c, d) fully charged states.

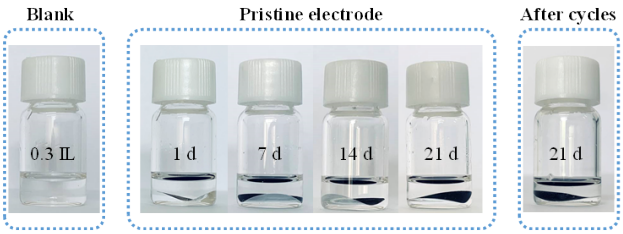


Figure S18 Dissolution test of SC4Q electrodes under pristine and reduction states.

Reaction kinetics of the SC4Q electrodes

To elucidate the reaction kinetics of the SC4Q electrodes, the Li^+ diffusion coefficient D_{Li^+} can be verified by the galvanostatic intermittent titration technique (GITT) measurement. The D_{Li^+} calculated by the GITT method was based on the following equation:

$$D^{GITT} = \frac{4}{\pi\tau}\left(\frac{m_B V_m}{M_B S}\right)^2\left(\frac{\Delta E_S}{\Delta E_t}\right)^2$$

where τ is the pulse time, M_B is the mole mass, V_m is the molar volume, S is the electrode-electrolyte interface area, ΔE_S is the voltage difference between the steady state and the initial state of every step, and ΔE_t is the change of total voltage during a pulse step excluding the IR drop. The V_m (532.93 $cm^3\ mol^{-1}$) of per SC4Q molecule was calculated by measuring the mass and the total volume of a pressed SC4Q pellet.

The weight, thickness and diameter were 78.5 mg, 0.486 mm, and 12.699 mm, respectively. The V_m of SC4Q molecule is about 532.93 $cm^3\ mol^{-1}$.

Figure S19 The SC4Q pellet obtained by powder pressing method under 11 MPa.

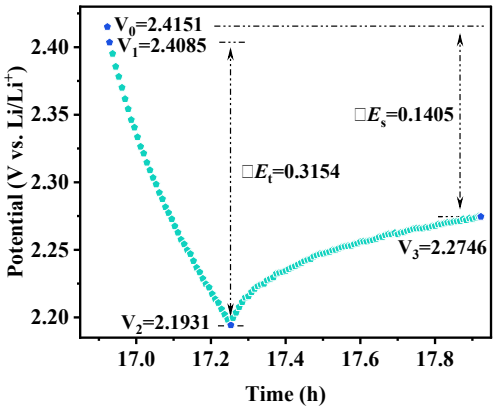


Figure S20 The partially enlarged image of a complete cycle in the GITT test.

The ionic conductivities of the SC4Q cathode can be calculated with the following equation:

$$\sigma = \frac{L}{R_{ct}S}$$

where σ refers to the ionic conductivity, L refers to the thickness of active material, R_{ct} corresponds to the charge transfer impedance (425 Ω for SC4Q), and S corresponds to the area of active material (S=1.13 cm^2). Thus, the ionic conductivities of SC4Q are calculated to be 1.041×10^{-3} S m^{-1}, respectively.

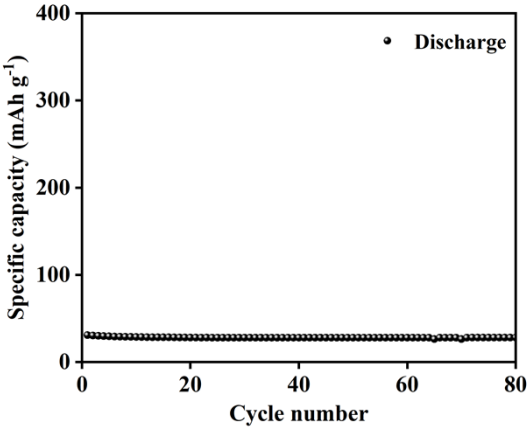


Figure S21 Cycle performance of pure KetjenBlack-based LIBs at the current density of 1 C.

Table S2. The atomic coordinates of optimized SC4Q.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	0.4502	4.8292	-0.2801	27	O	8.7596	0.0003	-6.7937
2	C	2.4515	5.3620	1.6274	28	O	3.9900	0.0001	2.0473
3	C	1.9903	6.0105	4.0206	29	H	7.6790	-4.1566	-4.3230
4	C	-0.6457	6.3953	4.8819	30	H	7.6786	4.1571	-4.3231
5	C	-2.6721	6.2065	2.9355	31	C	-4.8842	-0.0001	-0.9370
6	C	-2.1728	5.4536	0.5752	32	C	-6.3793	-2.3740	-1.0832
7	O	-1.1577	6.8678	7.0674	33	C	-8.8998	-2.3994	-0.9070
8	O	0.9637	3.9374	-2.3165	34	C	-10.3530	-0.0003	-0.7275
9	H	-4.5634	6.7118	3.5390	35	C	-8.9000	2.3989	-0.9070
10	H	3.4958	6.2675	5.3863	36	C	-6.3795	2.3736	-1.0832
11	C	0.4507	-4.8294	-0.2802	37	O	-12.6297	-0.0004	-0.4639
12	C	2.4520	-5.3619	1.6274	38	O	-2.6241	0.0000	-0.5470
13	C	1.9907	-6.0103	4.0206	39	H	-9.9655	4.1492	-0.8855
14	C	-0.6452	-6.3953	4.8819	40	H	-9.9651	-4.1499	-0.8855
15	C	-2.6717	-6.2066	2.9355	41	S	5.7088	-5.3099	0.5745
16	C	-2.1724	-5.4538	0.5751	42	O	7.2815	-5.1871	2.8377
17	O	-1.1572	-6.8680	7.0673	43	O	6.0052	-7.3447	-1.2638
18	O	0.9641	-3.9379	-2.3168	44	S	5.7083	5.3104	0.5744
19	H	-4.5629	-6.7118	3.5390	45	S	-4.8126	5.3938	-1.6293
20	H	3.4963	-6.2671	5.3864	46	S	-4.8122	-5.3940	-1.6293
21	C	5.3012	0.0002	0.1612	47	O	7.2811	5.1877	2.8375
22	C	6.1013	2.3648	-1.1086	48	O	6.0044	7.3451	-1.2640
23	C	7.2029	2.4029	-3.3779	49	O	-6.5979	7.2982	-0.7213
24	C	7.8004	0.0003	-4.7118	50	O	-3.8863	5.4063	-4.2114
25	C	7.2032	-2.4024	-3.3779	51	O	-6.5973	-7.2986	-0.7213
26	C	6.1016	-2.3644	-1.1085	52	O	-3.8859	-5.4065	-4.2114

Table S3. The atomic coordinates of optimized SC4Q-Li.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	0.2384	2.6140	-0.1901	28	O	1.9299	0.0473	1.1606
2	C	1.2638	2.9175	0.8495	29	H	4.2572	-2.2864	-1.8791
3	C	0.9788	3.3522	2.0834	30	H	4.2765	2.1102	-2.0553
4	C	-0.4261	3.6267	2.4637	31	C	-2.5718	0.0525	-0.9883
5	C	-1.4564	3.4670	1.4022	32	C	-3.2672	-1.1978	-0.6930
6	C	-1.1606	2.9857	0.1830	33	C	-4.4833	-1.2475	-0.0845
7	O	-0.7308	4.0073	3.5822	34	C	-5.1793	-0.0187	0.3076
8	O	0.5550	2.0737	-1.2344	35	C	-4.4991	1.2489	-0.0064
9	H	-2.4667	3.7652	1.6630	36	C	-3.2824	1.2679	-0.6033
10	H	1.7525	3.5158	2.8269	37	O	-6.2800	-0.0416	0.8673
11	C	0.2028	-2.5546	-0.1242	38	O	-1.4478	0.0964	-1.5329
12	C	1.1563	-2.8903	0.9350	39	H	-5.0069	2.1716	0.2536
13	C	0.7911	-3.3797	2.1379	40	H	-4.9779	-2.1930	0.1091
14	C	-0.6207	-3.6936	2.4231	41	S	2.9207	-2.8134	0.5681
15	C	-1.5715	-3.4918	1.3213	42	O	3.6290	-2.7130	1.8471
16	C	-1.1895	-2.9437	0.1356	43	O	3.2061	-3.9007	-0.3750
17	O	-0.9830	-4.1287	3.5170	44	S	3.0045	2.8229	0.3840
18	O	0.5939	-1.9703	-1.1542	45	S	-2.5546	2.8807	-0.9949
19	H	-2.5943	-3.8085	1.4941	46	S	-2.4762	-2.7503	-1.1177
20	H	1.5232	-3.5702	2.9160	47	O	3.7767	2.7830	1.6295
21	C	2.7329	0.0044	0.2407	48	O	3.2415	3.8583	-0.6258
22	C	3.2410	1.2303	-0.4263	49	O	-3.5275	3.8692	-0.5111
23	C	3.9575	1.1998	-1.5578	50	O	-2.0636	2.9056	-2.3674
24	C	4.3340	-0.0974	-2.1788	51	O	-3.4552	-3.8154	-0.9082
25	C	3.9481	-1.3367	-1.4541	52	O	-1.8314	-2.6002	-2.4473
26	C	3.2188	-1.2755	-0.3320	53	Li	-0.4983	-1.1994	-2.4798
27	O	4.9236	-0.1440	-3.2459					

Table S4. The atomic coordinates of optimized SC4Q-2Li.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	0.1947	2.6102	-0.1251	28	O	1.8920	0.0020	1.2135
2	C	1.1645	2.9049	0.9274	29	H	4.2599	-2.1878	-1.9027
3	C	0.8213	3.3692	2.1476	30	H	4.2540	2.2099	-1.8942
4	C	-0.5847	3.6821	2.4659	31	C	-2.5255	-0.0031	-1.1819
5	C	-1.5542	3.5175	1.3703	32	C	-3.1679	-1.2152	-0.7162
6	C	-1.1847	3.0101	0.1645	33	C	-4.2864	-1.2298	0.0785
7	O	-0.9254	4.0888	3.5752	34	C	-4.9292	-0.0052	0.5319
8	O	0.5586	2.0462	-1.1831	35	C	-4.2913	1.2206	0.0750
9	H	-2.5732	3.8338	1.5627	36	C	-3.1727	1.2078	-0.7197
10	H	1.5681	3.5373	2.9164	37	O	-5.9424	-0.0062	1.2473
11	C	0.2033	-2.6100	-0.1276	38	O	-1.4785	-0.0023	-1.9487
12	C	1.1766	-2.9040	0.9217	39	H	-4.7449	2.1591	0.3705
13	C	0.8383	-3.3754	2.1406	40	H	-4.7361	-2.1692	0.3770
14	C	-0.5655	-3.6959	2.4608	41	S	2.9302	-2.8170	0.5216
15	C	-1.5387	-3.5283	1.3688	42	O	3.6662	-2.7582	1.7875
16	C	-1.1740	-3.0155	0.1640	43	O	3.2006	-3.8692	-0.4653
17	O	-0.9015	-4.1108	3.5685	44	S	2.9193	2.8266	0.5308
18	O	0.5626	-2.0391	-1.1840	45	S	-2.4970	2.8355	-1.0659
19	H	-2.5563	-3.8483	1.5628	46	S	-2.4899	-2.8415	-1.0630
20	H	1.5872	-3.5435	2.9074	47	O	3.6530	2.7676	1.7980
21	C	2.6972	0.0048	0.2944	48	O	3.1872	3.8825	-0.4529
22	C	3.1997	1.2595	-0.3196	49	O	-3.5152	3.8351	-0.7518
23	C	3.9344	1.2773	-1.4403	50	O	-1.8899	2.8458	-2.4264
24	C	4.3058	0.0115	-2.1229	51	O	-3.5057	-3.8428	-0.7464
25	C	3.9375	-1.2579	-1.4453	52	O	-1.8856	-2.8506	-2.4246
26	C	3.2028	-1.2465	-0.3245	53	Li	-0.5752	-1.5396	-2.5709
27	O	4.8729	0.0144	-3.2045	54	Li	-0.5778	1.5377	-2.5707

Table S5. The atomic coordinates of optimized SC4Q-3Li.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	0.2886	2.6185	-0.1392	29	H	4.3453	-2.2027	-1.8610
2	C	1.2399	2.9040	0.9294	30	H	4.3449	2.1954	-1.8659
3	C	0.8848	3.3444	2.1583	31	C	-2.4638	0.0057	-1.2468
4	C	-0.5223	3.6270	2.4693	32	C	-3.1262	-1.1821	-0.8184
5	C	-1.4821	3.4463	1.3698	33	C	-4.3180	-1.1912	-0.0908
6	C	-1.1052	2.9649	0.1573	34	C	-4.9648	0.0011	0.2828
7	O	-0.8858	4.0132	3.5838	35	C	-4.3205	1.1958	-0.0866
8	O	0.6804	2.1032	-1.2125	36	C	-3.1285	1.1909	-0.8145
9	H	-2.5116	3.7230	1.5674	37	O	-6.0919	-0.0001	0.9546
10	H	1.6262	3.5030	2.9339	38	O	-1.3426	0.0078	-1.9432
11	C	0.2894	-2.6148	-0.1418	39	H	-4.7656	2.1428	0.1939
12	C	1.2365	-2.9070	0.9278	40	H	-4.7613	-2.1402	0.1860
13	C	0.8775	-3.3529	2.1540	41	S	2.9945	-2.8240	0.5564
14	C	-0.5303	-3.6339	2.4603	42	O	3.7129	-2.7510	1.8332
15	C	-1.4858	-3.4488	1.3585	43	O	3.2959	-3.8824	-0.4158
16	C	-1.1048	-2.9617	0.1490	44	S	2.9969	2.8206	0.5522
17	O	-0.8976	-4.0274	3.5717	45	S	-2.4249	2.8063	-1.0838
18	O	0.6852	-2.0937	-1.2118	46	S	-2.4209	-2.7962	-1.0943
19	H	-2.5160	-3.7261	1.5514	47	O	3.7186	2.7494	1.8272
20	H	1.6168	-3.5162	2.9306	48	O	3.2943	3.8783	-0.4219
21	C	2.7707	-0.0017	0.3178	49	O	-3.4279	3.8199	-0.7475
22	C	3.2766	1.2519	-0.2980	50	O	-1.7934	2.8685	-2.4336
23	C	4.0211	1.2644	-1.4118	51	O	-3.4258	-3.8110	-0.7666
24	C	4.4020	-0.0040	-2.0838	52	O	-1.7868	-2.8503	-2.4432
25	C	4.0217	-1.2707	-1.4088	53	Li	-0.4906	-1.5123	-2.5584
26	C	3.2765	-1.2563	-0.2954	54	Li	-0.4996	1.5304	-2.5631
27	O	4.9914	-0.0049	-3.1542	55	Li	-7.4929	-0.0776	1.8000
28	O	1.9654	-0.0003	1.2364					

Table S6. The atomic coordinates of optimized SC4Q-4Li.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	-0.2154	-2.6650	-0.0224	29	H	-4.4233	1.9454	-1.9905
2	C	-1.1644	-2.8825	1.0722	30	H	-4.3184	-2.4422	-1.7554
3	C	-0.7940	-3.1938	2.3307	31	C	2.4634	-0.0955	-1.2820
4	C	0.6275	-3.3942	2.6616	32	C	3.0756	1.1386	-0.9111
5	C	1.5845	-3.2965	1.5423	33	C	4.2854	1.2189	-0.2298
6	C	1.1962	-2.9459	0.2938	34	C	5.0027	0.0677	0.1597
7	O	1.0031	-3.6562	3.8036	35	C	4.3978	-1.1650	-0.1210
8	O	-0.6237	-2.2660	-1.1294	36	C	3.1839	-1.2347	-0.8160
9	H	2.6206	-3.5263	1.7647	37	O	6.1633	0.1532	0.7776
10	H	-1.5275	-3.3055	3.1218	38	O	1.3396	-0.1754	-1.9617
11	C	-0.3990	2.5251	-0.3444	39	H	4.8854	-2.0811	0.1900
12	C	-1.3183	2.8975	0.6902	40	H	4.6930	2.1964	0.0003
13	C	-0.9589	3.4684	1.8917	41	S	-3.0604	2.7445	0.3594
14	C	0.3965	3.7791	2.1619	42	O	-3.7751	2.7046	1.6463
15	C	1.3341	3.5074	1.1402	43	O	-3.4591	3.7270	-0.6601
16	C	0.9610	2.9077	-0.0589	44	S	-2.9230	-2.8868	0.6786
17	O	0.7585	4.3172	3.3015	45	S	2.5069	-2.8648	-0.9704
18	O	-0.8138	1.9074	-1.3899	46	S	2.2862	2.7139	-1.2527
19	H	2.3666	3.7983	1.2953	47	O	-3.6498	-2.7813	1.9488
20	H	-1.7195	3.6803	2.6352	48	O	-3.1618	-4.0174	-0.2284
21	C	-2.7713	-0.0843	0.2854	49	O	3.5160	-3.8486	-0.5668
22	C	-3.2478	-1.3831	-0.2613	50	O	1.8549	-3.0396	-2.3005
23	C	-4.0071	-1.4808	-1.3602	51	O	3.2785	3.7651	-0.9884
24	C	-4.4340	-0.2581	-2.0914	52	O	1.6969	2.6494	-2.6239
25	C	-4.0738	1.0462	-1.4942	53	Li	0.3981	1.3118	-2.6237
26	C	-3.3021	1.1196	-0.3994	54	Li	0.5443	-1.7299	-2.5308
27	O	-5.0548	-0.3407	-3.1426	55	Li	7.6862	0.2539	1.3574
28	O	-1.9864	-0.0340	1.2208	56	Li	0.9856	4.9398	4.8031

Table S7. The atomic coordinates of optimized SC4Q-5Li.

Center Number	Atom	Coordinates (Angstroms)			Center Number	Atom	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	C	0.2285	-2.7540	-0.3895	30	H	-2.0508	-2.4703	-2.5329
2	C	-0.7792	-2.9390	0.6451	31	C	2.4263	0.4982	-0.8720
3	C	-0.5095	-2.7337	1.9740	32	C	2.8250	1.7355	-0.3014
4	C	0.7898	-2.2986	2.4078	33	C	4.0314	1.9561	0.3623
5	C	1.8351	-2.2519	1.4194	34	C	4.9757	0.9220	0.5142
6	C	1.5640	-2.4503	0.0940	35	C	4.5997	-0.3393	0.0117
7	O	0.9904	-1.8878	3.6099	36	C	3.3834	-0.5262	-0.6441
8	O	-0.0559	-2.7717	-1.6139	37	O	6.1334	1.1173	1.1097
9	H	2.8289	-1.9722	1.7534	38	O	1.2696	0.3174	-1.4846
10	H	-1.2967	-2.8741	2.7113	39	H	5.2631	-1.1878	0.1401
11	C	-1.0684	2.6603	-0.1843	40	H	4.2438	2.9439	0.7564
12	C	-2.1906	2.5117	0.7184	41	S	-3.8363	2.2766	0.0234
13	C	-2.0198	2.0654	2.0108	42	O	-4.7660	2.0572	1.1357
14	C	-0.7455	1.6454	2.4707	43	O	-4.1356	3.2545	-1.0226
15	C	0.4007	2.0359	1.7042	44	S	-2.4965	-3.2296	0.1512
16	C	0.2432	2.5579	0.4462	45	S	2.9368	-2.1812	-1.0767
17	O	-0.6708	0.8140	3.4954	46	S	1.7178	3.0968	-0.4726
18	O	-1.2062	2.7338	-1.4343	47	O	-3.2850	-3.3010	1.3876
19	H	1.3950	1.8539	2.1031	48	O	-2.5589	-4.3002	-0.8447
20	H	-2.8993	1.8833	2.6199	49	O	4.0166	-3.1061	-0.7163
21	C	-3.1308	-0.4609	0.0557	50	O	2.4255	-2.1854	-2.4704
22	C	-2.7774	-1.6604	-0.6988	51	O	2.2505	4.2742	0.2230
23	C	-2.3523	-1.5849	-1.9927	52	O	1.3723	3.2128	-1.9131
24	C	-2.0695	-0.2654	-2.5441	53	Li	0.1936	1.6718	-2.4072
25	C	-2.8909	0.8145	-2.0425	54	Li	0.6958	-1.1795	-2.5978
26	C	-3.3888	0.7179	-0.7665	55	Li	7.6636	1.3856	1.6179
27	O	-1.0508	-0.0713	-3.2781	56	Li	-2.0469	-0.3722	2.7432
28	O	-3.1499	-0.4403	1.3142	57	Li	0.6336	-0.2379	4.1994
29	H	-2.9664	1.7418	-2.5933					

References

1 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, Williams, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman and D. J. Fox, Gaussian 16 Revision A.03, *Gaussian, Inc.,* Wallingford, CT, USA, 2016.

2 L. Goerigk, A. Hansen, C. Bauer, S. Ehrlich, A. Najibi and S. Grimme, A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions, *Phys. Chem. Chem. Phys.*, 2017, **19**, 32184-32215.