

Revealing better organic sodium-ion battery performance in ionic liquid electrolyte

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All calculations presented in this paper are performed using the Gaussian 16 software at the B3LYP/6-311+G (d,p) level of theory.¹

Table S1 PY13TFSI (Zero-point Energy (E) = -2197.827940 hartrees)

Serial number	Symbol	X	Y	Z
1	S	1.820080	0.528473	0.742133
2	C	2.679291	1.501313	-0.633784
3	F	1.776230	2.255562	-1.294749
4	F	3.586286	2.317330	-0.089632
5	F	3.277689	0.700419	-1.504649
6	N	0.541959	-0.155129	0.015242
7	S	0.580704	-1.547559	-0.815473
8	O	1.810171	-1.847393	-1.530140
9	C	0.421137	-2.888891	0.510637
10	F	0.126962	-4.051758	-0.080800
11	F	-0.587330	-2.578715	1.351291
12	F	1.534624	-3.026478	1.215412
13	O	-0.710497	-1.612867	-1.507611
14	C	-1.900413	1.709791	-0.997452
15	C	-1.851949	1.971045	1.354458
16	C	-1.304775	3.283658	0.787754
17	C	-1.384526	3.129566	-0.755730
18	H	-1.085814	0.989537	-1.020615
19	H	-2.532058	1.591461	-1.874795
20	H	-2.462924	2.070163	2.250832
21	H	-1.041677	1.268681	1.532119
22	H	-1.881536	4.145070	1.127973
23	H	-0.278773	3.403846	1.128911
24	H	-2.052023	3.875573	-1.190965
25	H	-0.410435	3.248030	-1.224740
26	N	-2.708303	1.375588	0.247297
27	C	-2.870248	-0.116444	0.457503
28	H	-3.364272	-0.228675	1.426014
29	H	-1.859665	-0.507731	0.533892
30	C	-3.640307	-0.838353	-0.639006
31	H	-4.647519	-0.424581	-0.747152
32	H	-3.115781	-0.719750	-1.588512
33	C	-3.738722	-2.331752	-0.313432

34	H	-4.239739	-2.500649	0.644546
35	H	-4.308771	-2.850337	-1.086425
36	H	-2.746378	-2.779565	-0.272102
37	C	-4.035719	2.059845	0.212507
38	H	-4.591736	1.789402	1.108998
39	H	-3.884433	3.135924	0.185108
40	H	-4.582191	1.745498	-0.672404
41	O	2.829078	-0.380093	1.261576
42	O	1.267073	1.581184	1.598908

Table S2 EC (E = -342.430507 hartrees)

Serial number	Symbol	X	Y	Z
1	C	0.000000	0.000000	0.847836
2	C	-0.000785	-0.764621	-1.303485
3	C	0.000785	0.764621	-1.303485
4	H	0.769615	-1.206553	-1.932583
5	H	-0.977021	-1.183548	-1.558825
6	H	0.977021	1.183548	-1.558825
7	H	-0.769615	1.206553	-1.932583
8	O	-0.288865	1.077796	0.068506
9	O	0.288865	-1.077796	0.068506
10	O	0.000000	0.000000	2.035686

Table S3 DMC (E = -343.579344 hartrees)

Serial number	Symbol	X	Y	Z
1	C	-0.034039	0.621474	0.063845
2	O	-0.441546	1.812063	0.061459
3	O	1.231622	0.297788	-0.517730
4	O	-0.836623	-0.407783	0.648131
5	C	1.793309	-0.829266	0.159882
6	H	1.133518	-1.666488	0.066960
7	H	2.740342	-1.071465	-0.275282
8	H	1.926350	-0.593165	1.194994
9	C	-1.703840	-0.958510	-0.346622
10	H	-2.304375	-1.728652	0.090572
11	H	-2.337797	-0.188084	-0.733199
12	H	-1.118245	-1.370875	-1.141564

Table S4 C4Q (E= -1678.483360 hartrees)

Serial number	Symbol	X	Y	Z
1	C	2.668293	-0.000123	-0.913320
2	C	3.361694	-1.290120	-0.615296
3	C	4.616124	-1.270562	-0.126616
4	C	5.333556	-0.000185	0.132331
5	C	4.616203	1.270223	-0.126694
6	C	3.361765	1.289839	-0.615353
7	O	6.483167	-0.000203	0.564031
8	O	1.537174	-0.000102	-1.384363
9	H	5.164101	2.179304	0.104620
10	H	5.163938	-2.179668	0.104797
11	C	-2.668245	-0.000199	-0.913168
12	C	-3.361778	-1.290107	-0.615125
13	C	-4.616249	-1.270398	-0.126553
14	C	-5.333593	0.000062	0.132249
15	C	-4.616140	1.270390	-0.126894
16	C	-3.361661	1.289855	-0.615452
17	O	-6.483206	0.000169	0.563942
18	O	-1.537013	-0.000307	-1.383952
19	H	-5.163989	2.179538	0.104269
20	H	-5.164168	-2.179433	0.104888
21	C	-0.000105	-2.735220	-0.812206
22	C	1.284809	-2.548430	-0.067176
23	C	1.264482	-2.403574	1.270694
24	C	0.000007	-2.364242	2.035661
25	C	-1.264542	-2.403802	1.270847
26	C	-1.284972	-2.548595	-0.067032
27	O	0.000088	-2.271086	3.260663
28	O	-0.000154	-3.067347	-1.990027
29	H	-2.174292	-2.290422	1.854559
30	H	2.174266	-2.290070	1.854330
31	C	0.000097	2.734738	-0.812823
32	C	-1.284822	2.548453	-0.067664
33	C	-1.264498	2.404381	1.270294
34	C	-0.000016	2.365262	2.035249
35	C	1.264525	2.404361	1.270378
36	C	1.284957	2.548462	-0.067574
37	O	-0.000048	2.272691	3.260294
38	O	0.000124	3.066259	-1.990815
39	H	2.174273	2.291312	1.854159

40	H	-2.174296	2.291333	1.853998
41	C	-2.563924	2.538062	-0.879218
42	H	-2.290889	2.594720	-1.936933
43	H	-3.171205	3.417256	-0.642359
44	C	2.564144	2.538145	-0.879016
45	H	3.171440	3.417252	-0.641916
46	H	2.291207	2.594989	-1.936743
47	C	2.563905	-2.538346	-0.878765
48	H	3.171107	-3.417523	-0.641659
49	H	2.290832	-2.595257	-1.936453
50	C	-2.564138	-2.538471	-0.878483
51	H	-2.291212	-2.595563	-1.936204
52	H	-3.171458	-3.417515	-0.641192

Table S5 P5Q (E= -2098.144859 hartrees)

Serial number	Symbol	X	Y	Z
1	C	-2.699937	3.163740	1.213963
2	C	-3.626696	2.014544	1.239863
3	C	-4.099363	1.454871	-0.065780
4	C	-3.654448	1.989063	-1.213825
5	C	-2.720667	3.132575	-1.239724
6	C	-2.269719	3.709876	0.065941
7	H	-2.375845	3.534690	2.179757
8	H	-3.951219	1.595958	-2.179640
9	O	-3.999811	1.532252	2.298069
10	O	-2.326130	3.597514	-2.297928
11	C	2.460978	-3.586029	-0.065971
12	C	1.749956	-3.762226	1.239688
13	C	-0.344613	-4.335207	0.065767
14	C	0.359261	-4.132238	-1.239879
15	C	1.786751	-3.755645	-1.213996
16	H	2.257675	-3.611177	-2.179791
17	O	2.335509	-3.592055	2.297888
18	O	-0.233408	-4.275738	-2.298070
19	C	4.171778	1.232284	-0.065913
20	C	4.118727	0.501759	1.239802
21	C	4.044851	-0.972727	1.214016
22	C	4.017451	-1.667491	0.066030
23	C	4.042727	-0.935463	-1.239680
24	C	4.125563	0.538526	-1.213893
25	H	4.000913	-1.463273	2.179852

26	H	4.134142	1.030971	-2.179717
27	O	4.137007	1.111394	2.297933
28	O	3.996745	-1.543581	-2.297838
29	C	0.117116	4.347263	-0.065993
30	C	0.795737	4.071571	1.239706
31	C	2.175271	3.545818	1.213873
32	C	2.827504	3.305013	0.065875
33	C	2.138888	3.554703	-1.239829
34	C	0.762522	4.088710	-1.213994
35	H	2.628406	3.352775	2.179689
36	H	0.296734	4.248893	-2.179799
37	O	0.221756	4.277582	2.297879
38	O	2.702863	3.322639	-2.297991
39	C	-3.844441	-1.590345	1.214033
40	C	-3.037254	-2.826465	1.239689
41	C	-2.650417	-3.448305	-0.066077
42	C	-3.020884	-2.859805	-1.214002
43	C	-3.820633	-1.618857	-1.239658
44	C	-4.230696	-1.012087	0.066111
45	H	-4.097457	-1.167919	2.179923
46	H	-2.738376	-3.263115	-2.179886
47	O	-2.693842	-3.330553	2.297791
48	O	-4.140719	-1.099614	-2.297747
49	C	3.910431	-3.171292	0.000057
50	H	4.365421	-3.604913	0.890037
51	H	4.428564	-3.527138	-0.889898
52	C	4.224830	2.738963	-0.000038
53	H	4.777700	3.037923	0.889941
54	H	4.723306	3.121843	-0.890002
55	C	-1.299301	4.863641	-0.000040
56	H	-1.509311	5.456083	-0.889993
57	H	-1.412586	5.481860	0.889946
58	C	-5.028153	0.267344	0.000306
59	H	-5.656672	0.250712	-0.889525
60	H	-5.650939	0.350632	0.890423
61	C	-1.807807	-4.698467	-0.000257
62	H	-1.986021	-5.301087	-0.890311
63	H	-2.079461	-5.265408	0.889625
64	C	0.324759	-4.147433	1.213803
65	H	-0.155167	-4.258108	2.179632

Table S6 P5Q-10Na (E= -3722.028497 hartrees)

Serial number	Symbol	X	Y	Z
1	C	1.538683	-4.012490	1.090165
2	C	2.577706	-3.076403	1.294849
3	C	3.324196	-2.797886	0.117022
4	C	2.800165	-3.259494	-1.090542
5	C	1.482853	-3.729062	-1.295126
6	C	0.883438	-4.254087	-0.117364
7	H	1.157927	-4.567115	1.944682
8	H	3.469014	-3.187873	-1.945088
9	O	2.727163	-2.525402	2.513677
10	O	0.926730	-3.598660	-2.513759
11	C	-1.044659	4.217612	0.117358
12	C	-0.276967	4.003755	1.295019
13	C	1.785821	3.961187	-0.117380
14	C	0.992194	3.888856	-1.295006
15	C	-0.349548	4.283167	-1.090249
16	H	-0.932890	4.618284	-1.944741
17	O	-0.721698	3.645632	2.513699
18	O	1.365238	3.456634	-2.513730
19	C	-4.334078	0.309718	0.117635
20	C	-3.893332	0.973638	1.295328
21	C	-3.603096	2.341696	1.090727
22	C	-3.215540	2.922449	-0.116880
23	C	-3.392220	2.145455	-1.294613
24	C	-4.181826	0.991209	-1.089908
25	H	-3.621010	3.014150	1.945291
26	H	-4.680809	0.539958	-1.944380
27	O	-3.690057	0.439878	2.513929
28	O	-2.866020	2.366801	-2.513379
29	C	-1.633701	-4.026130	0.117183
30	C	-2.129076	-3.402197	1.295032
31	C	-3.340560	-2.703511	1.090556
32	C	-3.772979	-2.154897	-0.116892
33	C	-3.088602	-2.562765	-1.294779
34	C	-2.234751	-3.670399	-1.090288
35	H	-3.985658	-2.513183	1.945199
36	H	-1.959935	-4.284268	-1.944916
37	O	-1.558694	-3.374090	2.513700
38	O	-3.136560	-1.993678	-2.513475
39	C	4.291947	0.223481	1.090084

40	C	3.722567	1.500861	1.294706
41	C	3.688497	2.296894	0.116879
42	C	3.965729	1.655905	-1.090671
43	O	4.005222	0.257948	-1.295195
44	C	4.319280	-0.474375	-0.117418
45	H	4.701650	-0.310041	1.944638
46	H	4.104376	2.314103	-1.945290
47	O	3.244379	1.813147	2.513343
48	O	3.709241	-0.230678	-2.513743
49	C	-2.561096	4.292412	0.000306
50	H	-2.985171	4.795434	0.873746
51	H	-2.802483	4.904668	-0.872984
52	C	-4.873820	-1.109330	0.000609
53	H	-5.483024	-1.357260	0.874202
54	H	-5.530995	-1.149685	-0.872477
55	C	-0.451027	-4.978088	-0.000103
56	H	-0.615763	-5.615232	-0.873416
57	H	-0.403441	-5.634398	0.873255
58	C	4.595156	-1.967330	-0.000318
59	H	5.149985	-2.320835	-0.873790
60	H	5.234217	-2.125166	0.872873
61	C	3.291004	3.762203	-0.000433
62	H	3.798473	4.180687	-0.873993
63	H	3.638639	4.321245	0.872721
64	C	1.113800	4.150521	1.090244
65	H	1.747940	4.375333	1.944672
66	Li	-3.028333	0.105561	-3.041119
67	Li	-0.835777	2.911649	-3.040601
68	Li	2.511108	1.694309	-3.041008
69	Li	-1.036027	-2.846778	-3.041585
70	Li	2.387632	-1.864881	-3.041991
71	Li	-2.683768	-1.405592	3.041525
72	Li	-2.165831	2.118276	3.041862
73	Li	0.507370	-2.986386	3.040867
74	Li	1.345524	2.714627	3.041222
75	Li	2.997459	-0.440659	3.040328

Table S7 NaTFSI (E= -1989.860827 hartrees)

Serial number	Symbol	X	Y	Z
1	S	-1.908186	-0.596772	0.608476
2	C	-2.564744	-1.880344	-0.604814
3	F	-1.555114	-2.620546	-1.072816
4	F	-3.433929	-2.671925	0.019749
5	F	-3.166435	-1.267597	-1.618552
6	N	-0.819957	0.207422	-0.286353
7	S	-0.997264	1.697535	-0.926717
8	O	-2.356756	2.100510	-1.222451
9	C	-0.440100	2.734059	0.558431
10	F	-0.166945	3.979413	0.205174
11	F	0.715272	2.178607	1.067646
12	F	-1.339647	2.725635	1.533178
13	O	0.083603	1.866694	-1.883850
14	O	-3.057067	0.124755	1.116063
15	O	-1.056082	-1.371561	1.545326
16	Na	0.973991	-0.369642	1.029021

2. ^1H NMR of P5Q in CDCl_3 .

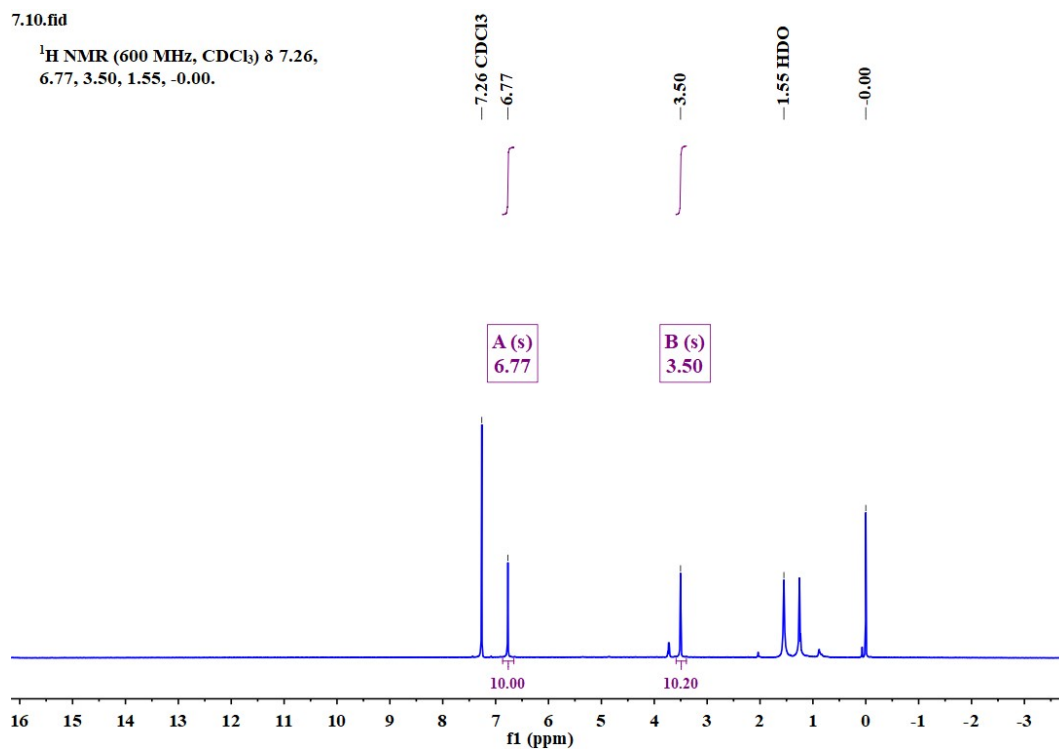


Fig. S1 ^1H NMR of P5Q in CDCl_3 , 3.50 (CH_2 -, 10H), 6.77 ($\text{CH}=\text{C}$ -, 10H).

3. ESI-MS positive ion mode spectrum of P5Q.

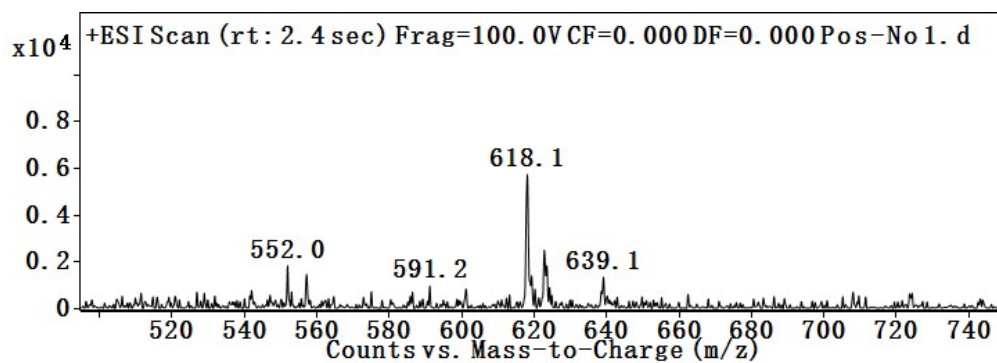


Fig. S2 ESI-MS positive ion mode spectrum of P5Q, ESI-MS (m/z): 618.1 ($\text{M} + \text{NH}_4^+$)

4. FTIR of P5Q.

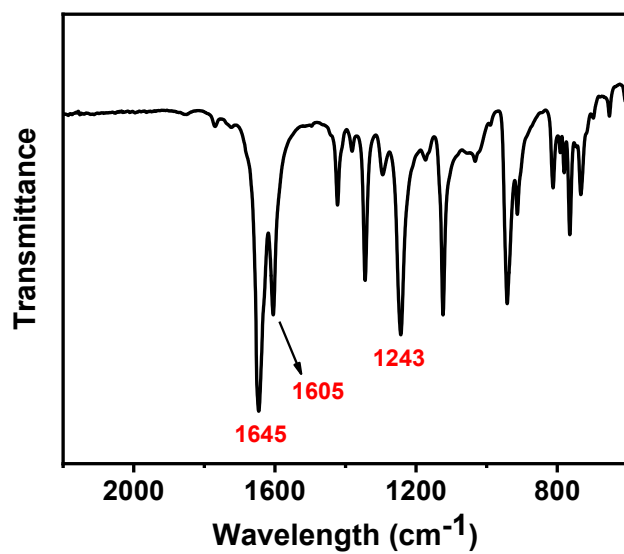


Fig. S3 FTIR of P5Q, 1645, 1605 (ph-C=O), 1243 (CH₂-)

5. The mechanism of P5Q's sodium storage

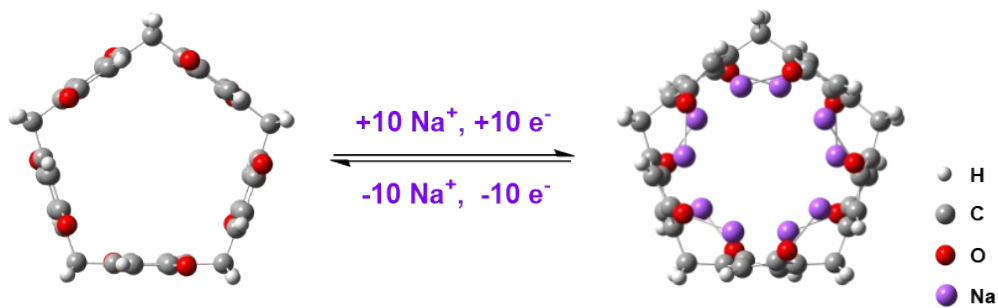


Fig. S4 The mechanism of P5Q's sodium storage

6. Visualized dissolution comparison of P5Q in different electrolytes.

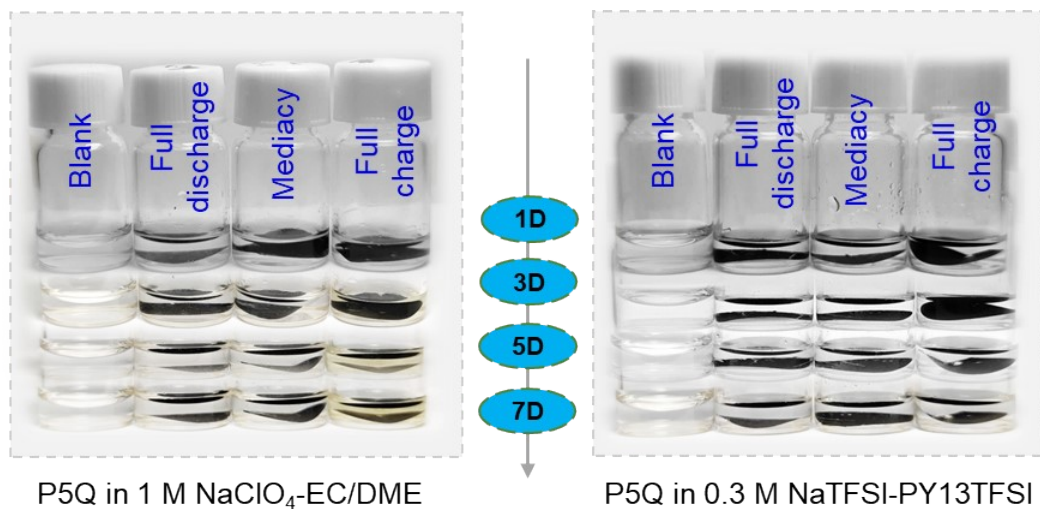


Fig. S5 Visualized dissolution comparison of P5Q in different electrolytes

7. Discharge-charge curves under different rate.

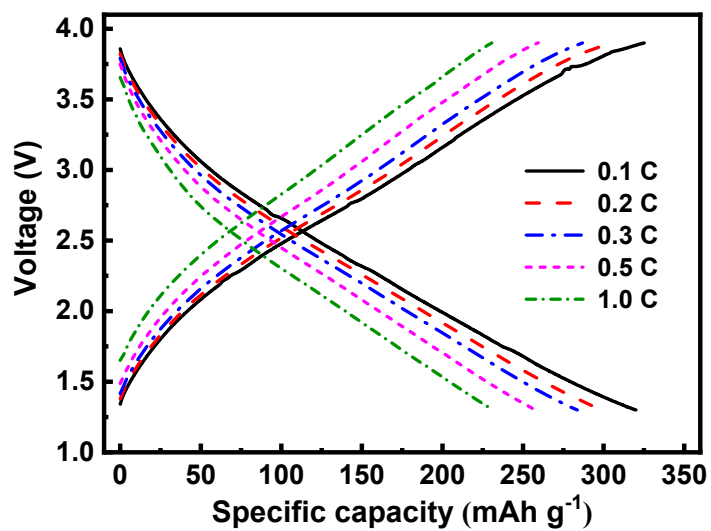
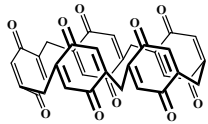
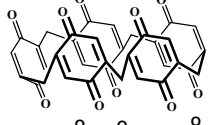
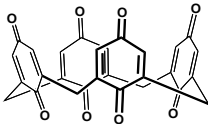
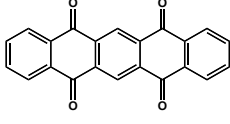
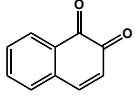
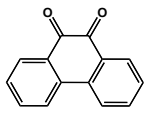
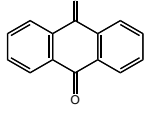
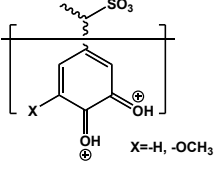


Fig. S6 Discharge-charge curves under different rate

8. Electrochemical cyclability comparison of organic cathodes of SIBs.

Table S8 Electrochemical cyclability comparison of organic cathodes of SIBs

Materials	Structure	Electrolytes	Voltage (V)	Capability/(mAh g ⁻¹), Cycle number, current density	Ref.
P5Q:KB:PVDF		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-3.8	258, 500, 0.2 C	This work
P5Q:CMK-3: SWCNTs:PVDF		1 M NaClO ₄ /EC+DMC/FEC	1.5-4.2	290, 300, 0.1 C	2
C4Q:KB:PTFE		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-3.7	~220, 300, 0.29 C	3
PT:KB:PTFE		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-3.4	245, 50, 0.09 C	3
NQ:KB:PTFE		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-3.7	~220, 10, 0.1 C	3
PQ:KB:PTFE		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-3.7	~260, 10, 0.1 C	3
AQ:KB:PTFE		0.3 M Na[TFSI]/[PY13][TFSI]	1.2-2.8	~220, 10, 0.1 C	3
Lignin:C ₆₅ :PDADMA -TFSI		20 mol% Na[TFSI]/[EMIm][FSI]	1.5-3.9	70, 100, 25 mA g ⁻¹	4

9. References

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