Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Sodium Phthalate as an Anode Material for Sodium Ions Batteries: Effect of the Bridging Carbonyl Group

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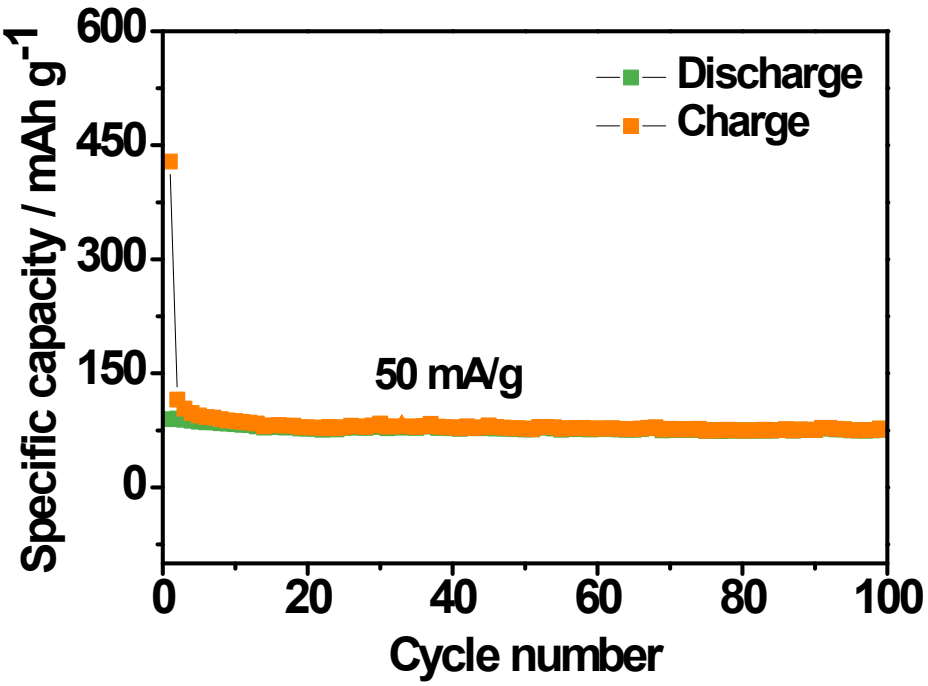


Figure S1. Cycling performance of sodium phthalate at a current density of 50 mA g^{-1}

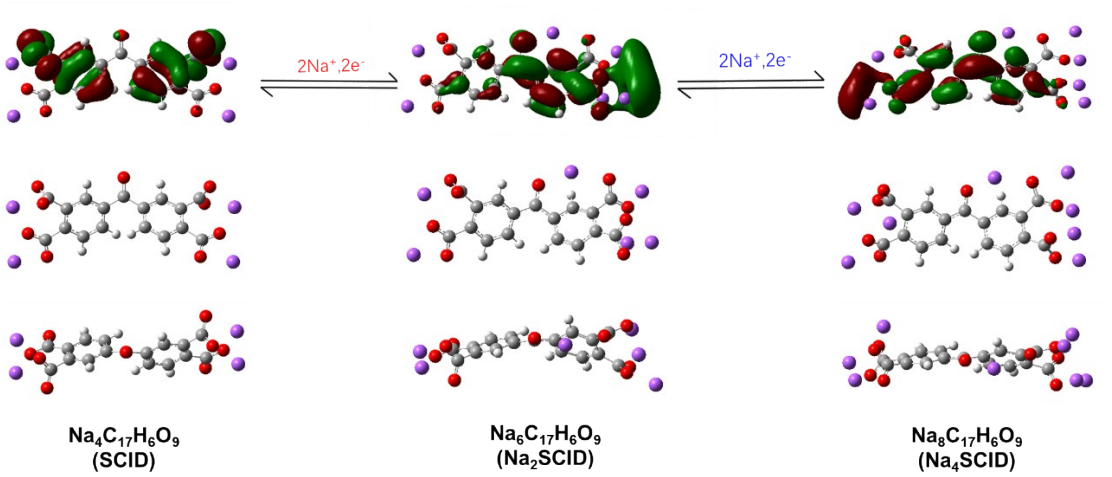


Figure S2. Calculated HOMO plots and spatial structure of molecule SCID with different uptake amounts of sodium.

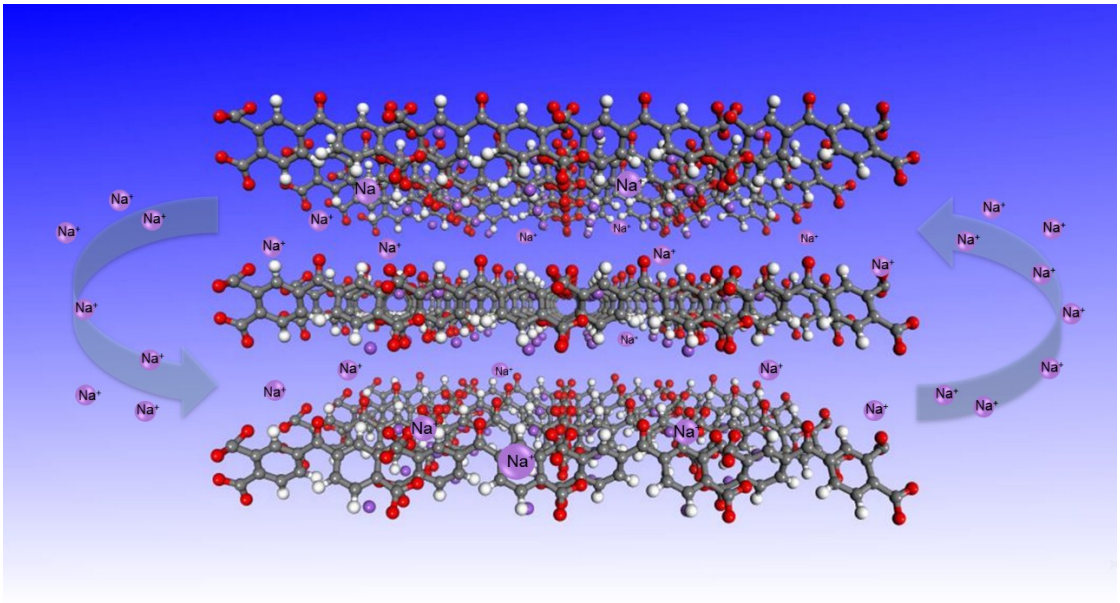


Figure S3. Spatial structure of SCID after recrystallization and sodium ion transfer process

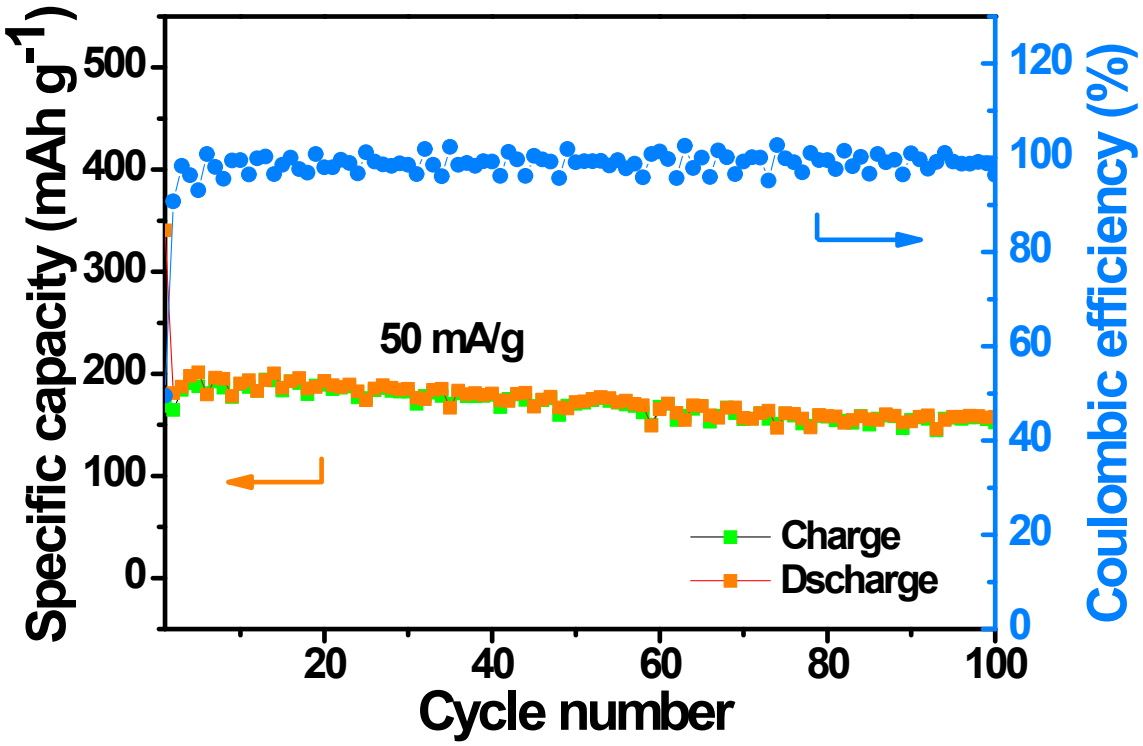


Figure S4. Cycling performance of SCID at a current density of 50 mA g^{-1}

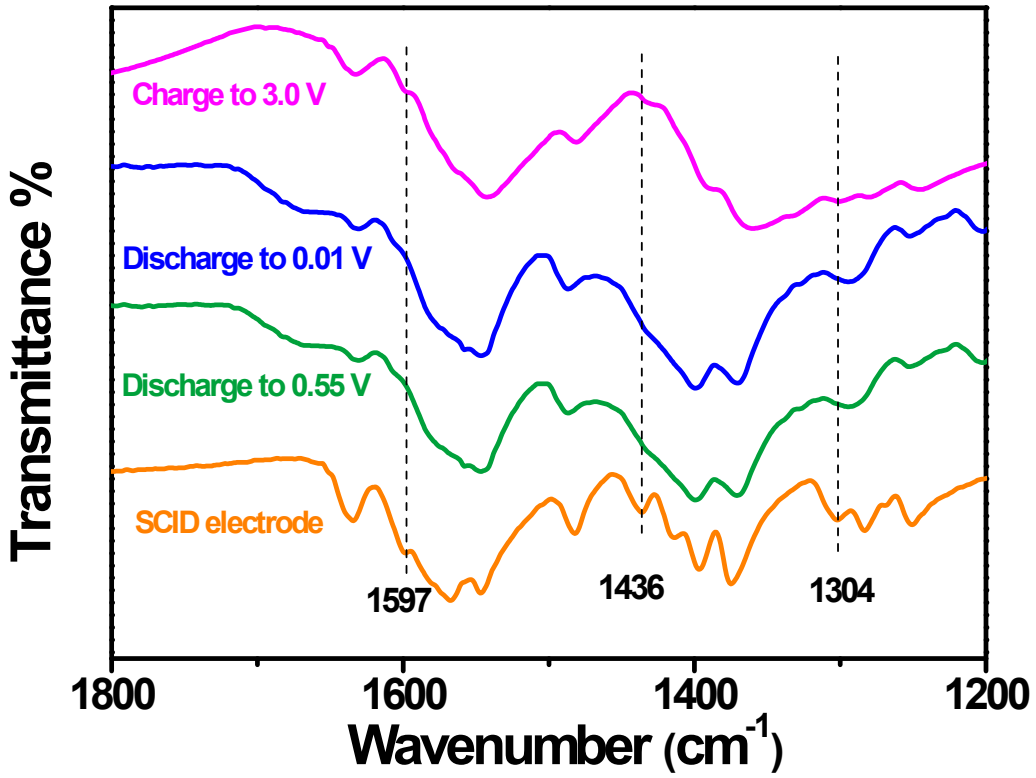


Figure S5. ATR-FTIR spectrum of pure SCID, discharged to 0.5V, 0.01 V and charged to 3.0 V

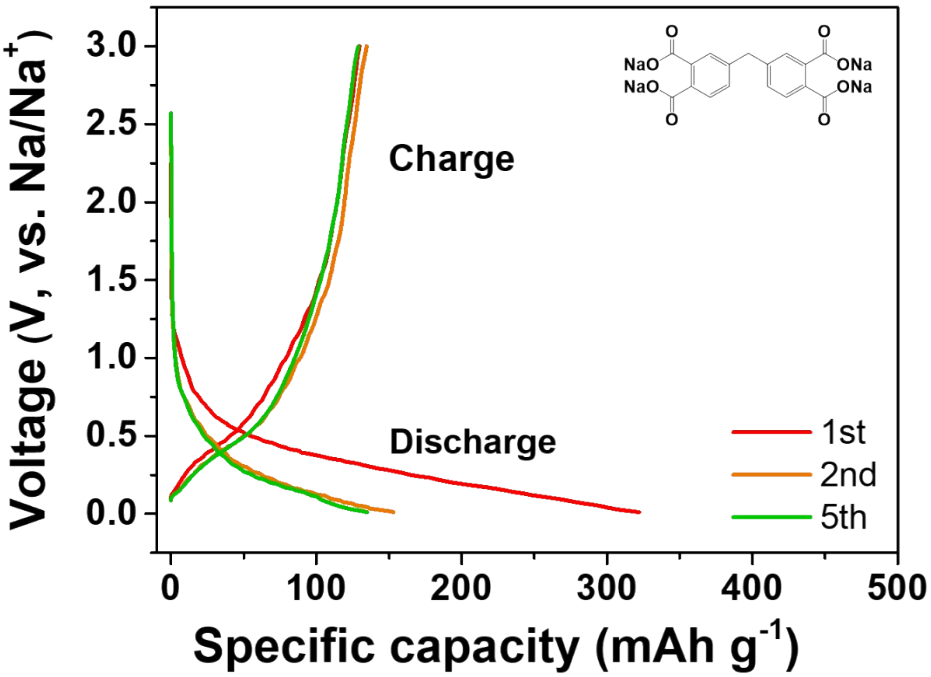


Figure S6. Galvanostatic discharge/charge profiles of SDTC at a current density of 50 mA g^{-1}:

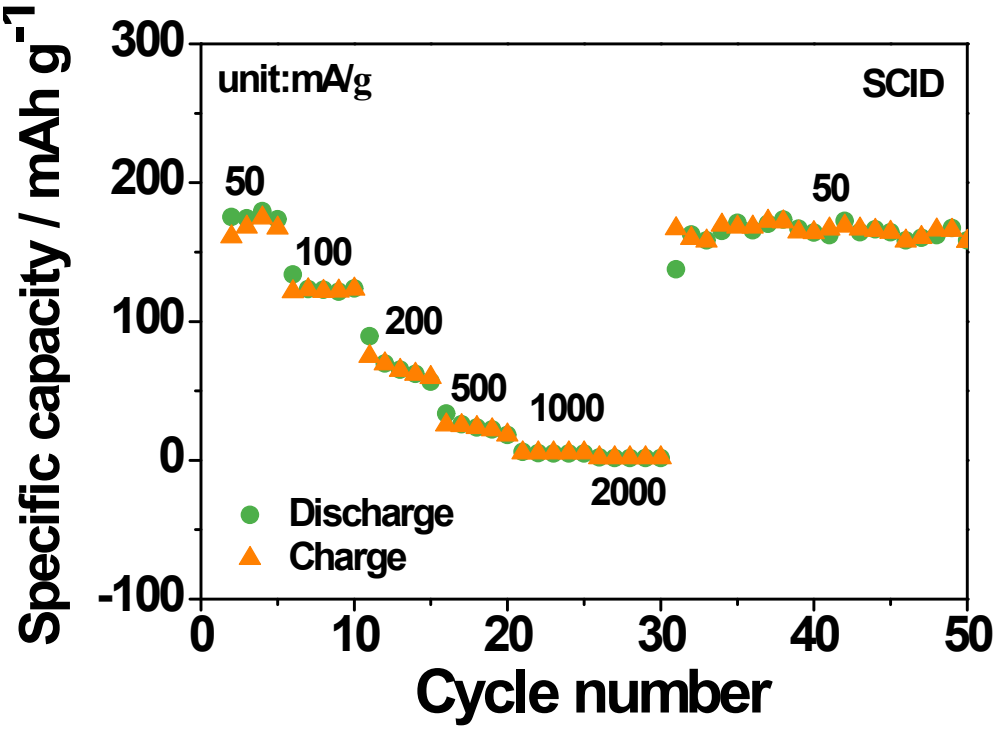


Figure S7. the rate capabilities of SCID

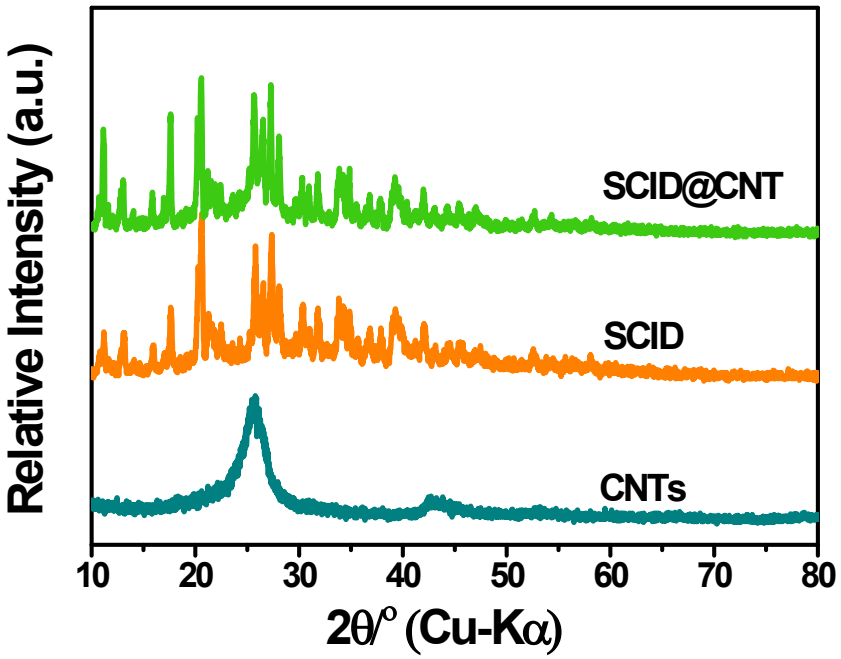


Figure S8. X-ray diffraction patterns of SCID@CNT, SCID, and CNT.

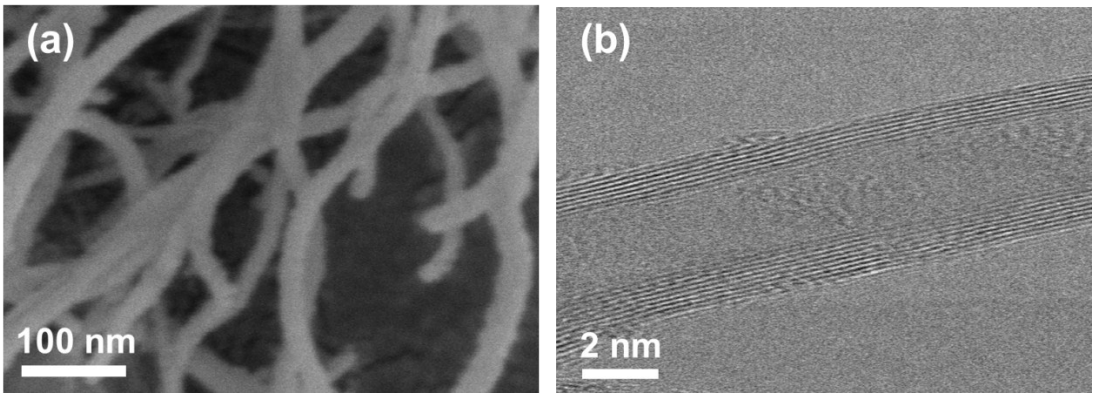


Figure S9. (a) SEM and (b) TEM images of MWCNTs,

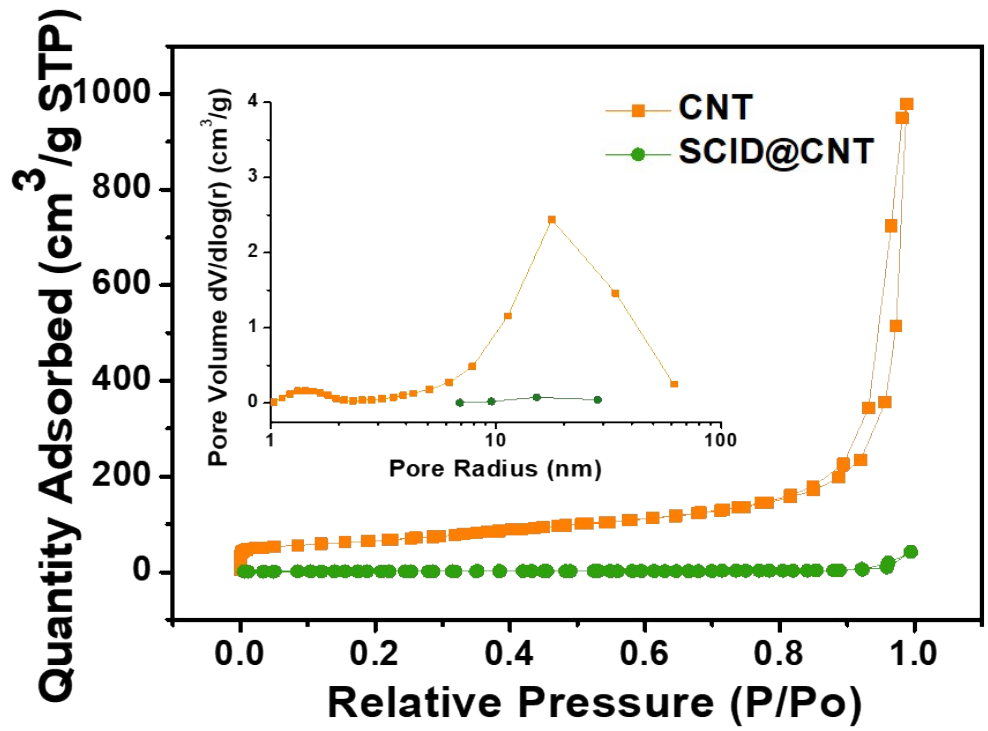


Figure S10. N_2 adsorption/desorption isotherms and pore size distribution of CNT and SCID@CNT.

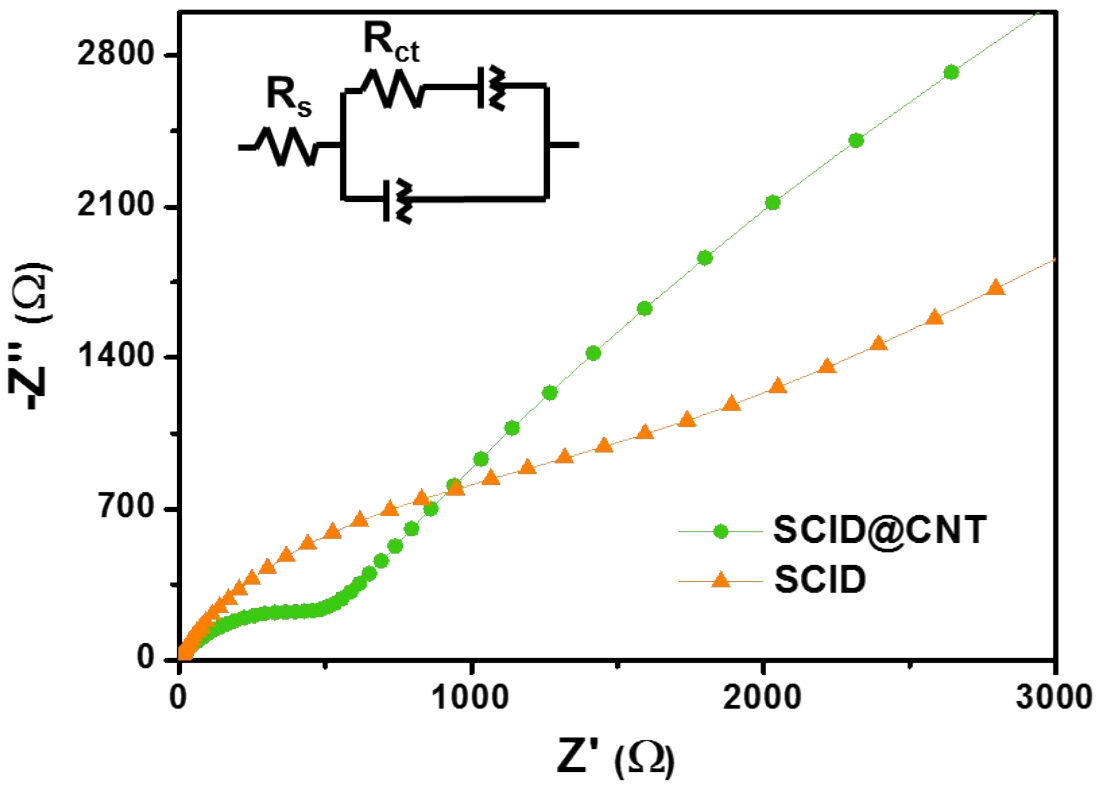
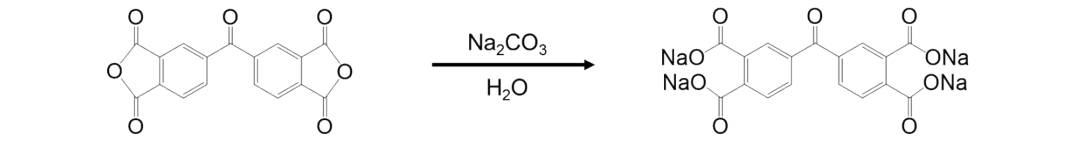


Figure S11. Electrochemical impedance spectrum and equivalent circuit diagram of the SCID@CNT and SCID electrodes after first cycling



5,5'-Carbonylbis(isobenzofuran-1,3-dione)
CID

Sodium 5,5'-Carbonylbis(isobenzofuran-1,3-dione)
SCID

Figure S12. Synthesis route diagram of the SCID

Table S1. Voltage under different sodium-insertion conditions

Insertion conditions	Vacuum	Organic solvents (DMSO)	Inorganic solvents (H_2O)
Insertion voltage (Na_4SCID)	0.97 V	0.33 V	0.33 V
Insertion voltage (Na_2SCID)	1.05 V	1.42 V	1.44 V

Table S2 Electrochemical performances of SCID@CNT compared to references of organic-based active materials and composites.

Materials	Carbon additives [wt%]	Discharge capacity 1st/2nd (mAh g^{-1})	Rates	Capacity (mAh g^{-1})/ Cycle number	Ref.
GO-CADs	20% CB	293	20 mA g^{-1}	~130/100	1
$(COONa)_2$ Na_2BDC	35% SP	305/160	20 mA g^{-1}	130/20	2
ALD20	10% CB	285	0.1 C	225/100	3
SSDC	40% SP	247	1000 mA g^{-1}	112/400	4
SPT	50% AB	242	20 mA g^{-1}	68/50	5
BDT-G	40% AB	217	0.2 C	175/70	6
HA	10% SP	163	40 mA g^{-1}	133/200	7
Na_2PDS	30% SP	309/224.9	100 mA g^{-1}	183/150	8
Na_2DBQ	30% CB	398/265	0.1 C	231/50	9
PTCDA	20% SP	135/145	200 mA g^{-1}	100/200	10
PI	30% SP	120/122	50 mA g^{-1}	86/100	11
SCID@CNT	20% SP	476/252	50 mA g^{-1}	182/100	This work

GO-CAD: graphene oxide-croconic acid disodium salt

$(COONa)_2Na_2BDC$: 1,2,4,5-tetrasodiumterephthalate

ALD20: Disodium terephthalate electrode was coated through the atomic layer deposition (ALD) method for 20 cycles

SSDC: sodium 4,4'-stilbene-dicarboxylate

SPT: sulfur-containing dithiin ring, dibenzo[b,i]thianthrene-5,7,12,14-tetrone

BDT-G: 4,8-dihydrobenzo[1,2-b:4,5-b0] dithiophene-4,8-dione-graphene

HA: Humic acid

Na_2PDS: poly (2,5-dihydroxy-p-benzoquinonyl sulfide)

Na_2DBQ: Disodium 2,5-dihydroxy-1,4-benzoquinone

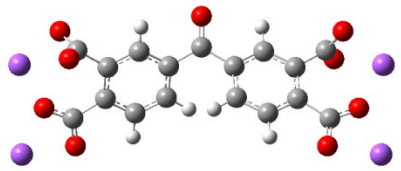
PTCDA: 3,4,9,10-perylene-tetracarboxylicacid-dianhydride

PI: polyimide

S13. Coordinates of molecular structures

All coordinates are reported as XYZ Cartesian coordinates. Converged geometries and the thermochemistriy were also obtained from M06/6-31+G(d,p) level of theory. They are stated in Hartrees units. All energies reported were calculated using the GAUSSIAN 09 Revision-D.01 computational chemistry package.

(a)



Standard orientation

Center Number	Element Symbol	Coordinates (Angstroms)		
		X	Y	Z
1	C	-3.79629	-0.50445	-0.41317
2	C	-3.70387	0.735007	0.26166
3	C	-2.46072	1.36218	0.380895
4	C	-1.29406	0.776363	-0.12427
5	C	-2.62193	-1.07386	-0.93828
6	C	1.294062	0.776354	0.124121
7	C	1.384517	-0.45758	0.788728
8	C	2.621879	-1.07389	0.938172
9	C	3.796269	-0.50448	0.413116
10	C	3.703884	0.73498	-0.26172
11	C	2.460743	1.362166	-0.38099
12	C	-5.07418	-1.2841	-0.63304
13	C	-4.91831	1.404639	0.861288
14	C	4.918356	1.404599	-0.8613
15	C	5.07414	-1.28414	0.633044
16	O	-6.2189	-0.87212	-0.19671
17	O	-5.23416	1.07125	2.04142
18	O	5.234349	1.071087	-2.04135
19	O	4.980381	-2.37544	1.275225
20	O	5.594568	2.163205	-0.10779
21	Na	7.193057	0.835184	-0.96536
22	O	6.218915	-0.87207	0.196925

23	Na	7.102103	-2.71161	1.145885
24	O	-5.59465	2.163117	0.10777
25	Na	-7.19296	0.835084	0.965701
26	O	-4.98048	-2.37531	-1.27539
27	Na	-7.10218	-2.71155	-1.14583
28	H	-2.38982	2.325065	0.876058
29	H	-2.70453	-2.01609	-1.46664
30	H	0.497931	-0.92026	1.20919
31	H	2.704453	-2.01612	1.466523
32	H	2.389874	2.325057	-0.87615
33	C	0.000004	1.528771	-0.0001
34	O	0.000004	2.755585	-5.3E-05
35	C	-1.38456	-0.45757	-0.78888
36	H	-0.49799	-0.92025	-1.20939

Zero-point Energy correction= 0.205630
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Thermal correction to Enthalpy= 0.234525
Thermal correction to Free Energy= 0.141745
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Electronic Energy (EE) + Thermal Energy Correction= -1977.788399
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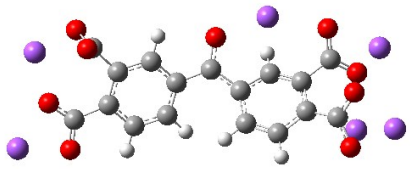
(b)



Standard orientation

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4	C	1.129643	-1.40433	-0.06528
5	C	0.902512	-0.10862	-0.64876

6	C	2.087573	0.568792	-1.07796
7	C	-0.26712	0.733473	-0.60024
8	O	-0.08204	2.014053	-0.60549
9	C	4.484466	1.140758	-0.96983
10	C	4.780672	-1.16514	0.907639
11	O	5.551536	0.610342	-1.43564
12	O	5.438271	-0.17528	1.439228
13	O	5.290948	-2.35984	0.919685
14	Na	5.517927	-1.67794	-1.40203
15	O	4.380521	2.375539	-0.66886
16	Na	6.451366	1.601864	0.460321
17	H	2.541137	-2.75197	0.80966
18	H	0.291818	-2.04466	0.189084
19	H	1.97629	1.372239	-1.80563
20	Na	7.062013	-1.6248	2.088099
21	Na	1.987132	2.830598	-0.09729
22	C	-1.64343	0.214903	-0.49465
23	C	-2.01415	-1.08019	-0.91616
24	C	-2.65465	1.056752	0.003492
25	C	-3.33004	-1.50415	-0.81048
26	H	-1.27779	-1.73789	-1.36553
27	C	-3.97907	0.636655	0.120723
28	H	-2.38198	2.06211	0.304536
29	C	-4.34182	-0.67188	-0.2855
30	H	-3.61278	-2.49534	-1.14533
31	C	-4.99406	1.601572	0.686743
32	C	-5.72345	-1.2572	-0.21886
33	O	-5.20596	1.556615	1.935796
34	O	-5.64414	2.313918	-0.13501
35	O	-5.87415	-2.45074	-0.63662
36	O	-6.74028	-0.59519	0.242045
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38	Na	-7.29206	1.42367	1.105881

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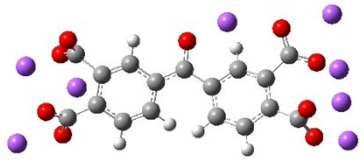
Electronic Energy (EE) + Thermal Free Energy Correction= -2302.520993

(c)



Standard orientation

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5	C	-0.82095	-0.10235	0.235106
6	C	-1.98846	0.609706	0.601439
7	C	0.38695	0.722436	0.102815
8	O	0.174622	2.006591	-0.07315
9	C	-4.36697	1.176278	0.527538
10	C	-4.84249	-1.66218	-0.50983
11	O	-5.55549	0.792947	0.84139
12	O	-5.42501	-1.19711	-1.54499
13	O	-5.39737	-2.54197	0.237499
14	Na	-6.46178	-1.08582	1.707943
15	O	-4.0986	2.408387	0.333428
16	Na	-6.91829	0.531491	-1.28405
17	H	-2.46996	-2.96799	-0.67
18	H	-0.21521	-2.07457	-0.47121
19	H	-1.85749	1.546637	1.130351
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21	Na	-1.79327	2.820368	-0.62112
22	C	1.716602	0.202128	0.12138
23	C	2.0806	-1.1114	0.572459
24	C	2.802877	1.075112	-0.22314
25	C	3.388828	-1.54873	0.547049
26	H	1.321644	-1.77241	0.976675
27	C	4.109129	0.637836	-0.25488
28	H	2.573774	2.116877	-0.41825
29	C	4.443943	-0.72382	0.056713
30	H	3.629604	-2.55633	0.876138

31	C	5.248514	1.617286	-0.37452
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33	O	5.40674	2.309917	-1.40819
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Electronic Energy (EE) + Thermal Enthalpy Correction= -2627.047694
Electronic Energy (EE) + Thermal Free Energy Correction= -2627.157469

References

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