Supporting Information

Conjugated porous polyimide poly(2,6-diaminoanthraquinone) benzamide with good stability and high-performance as cathode for sodium ion batteries

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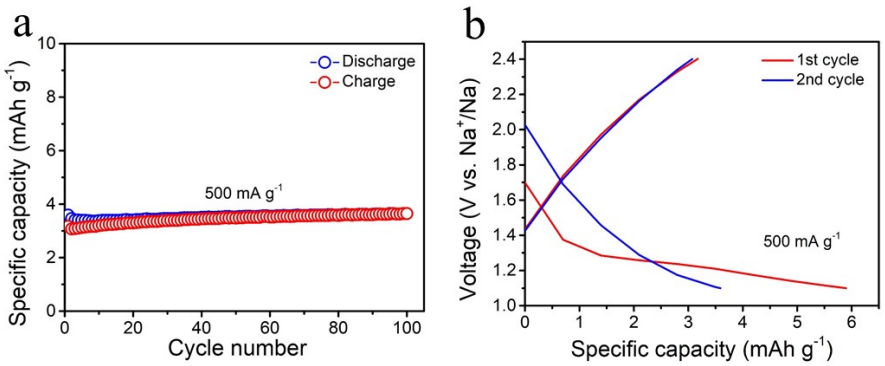

Fig. S1 Electrochemical properties of PMDA monomer cathode for Na-ion storage at 0.5 A g^{-1}. (a) The cycling performance, and (b) charge-discharge voltage profiles for the selected cycles.

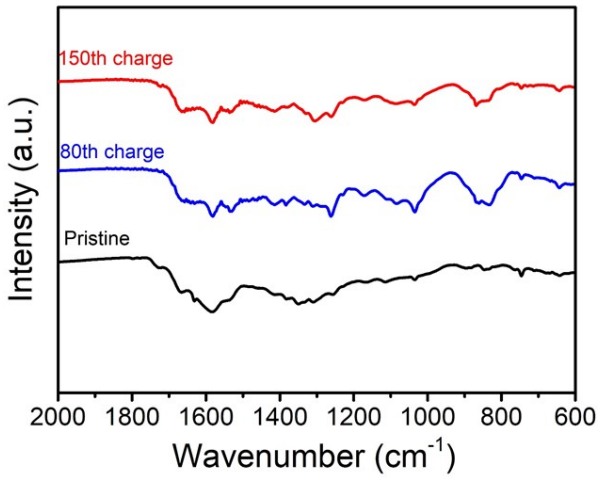

Fig. S2 *Ex-situ* FT-IR spectra of CP-PDAB electrodes after 80 and 150 cycles.

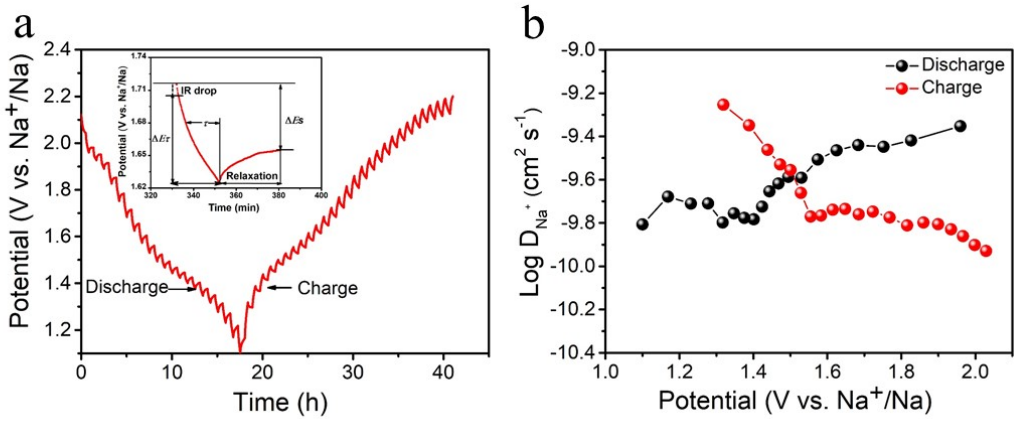

Fig. S3 (a) GITT curve of CP-PDAB for sodification/desodification process after 10 cycles in SIBs (the inset shows the schematic diagram of calculating the diffusion coefficient of Na^+). (b) Diffusion coefficients at different potential during sodification and desodification for CP-PDAB.

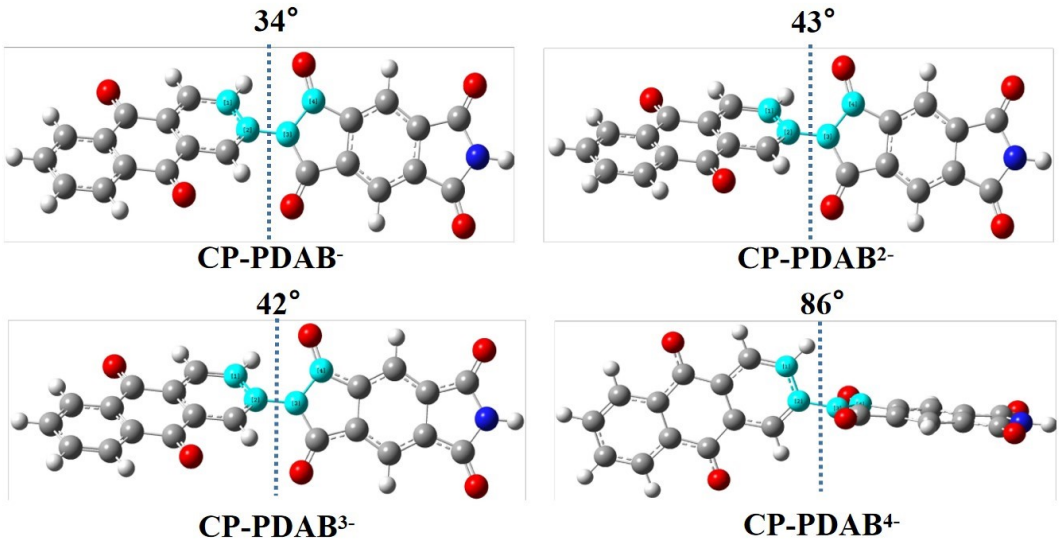

Fig. S4 The optimized structures of CP-PDAB anions and the related dihedral angles between PMDA and AQ moieties by B3LYP/6-31+G(d,p).

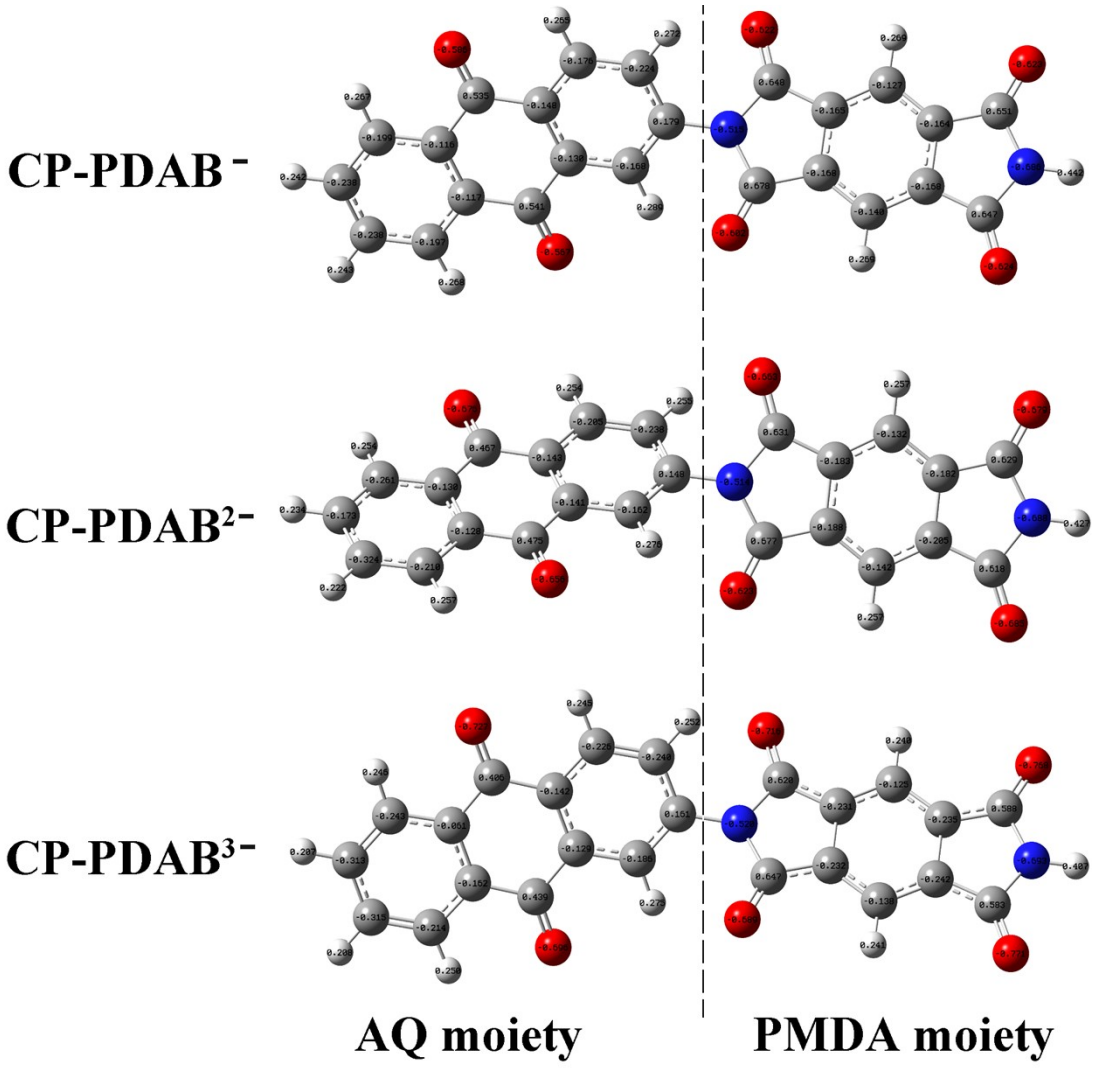

Fig. S5 The Natural Bond Orbital (NBO) analysis of CP-PDAB by B3LYP/6-31+G(d,p).

Table S1 The Natural Bond Orbital charge distribution of CP-PDAB about every moiety.

	CP-PDAB (45°)	CP-PDAB^{-} (34°)	CP-PDAB^{2-} (43°)	CP-PDAB^{3-} (42°)
PMDA moiety	-0.227	-1	-1.388	-2.034
AQ moiety	0.227	0	-0.612	-0.966

Table S2 Cartesian coordinates of CP-PDAB$^-$ (34^o).

Element	x	y	z
C	-5.25819	-0.89636	0.223827
C	-5.44369	0.433892	-0.28381
C	-4.37443	1.291135	-0.50821
C	-3.10308	0.792685	-0.20909
C	-2.91844	-0.53373	0.292358
C	-3.9905	-1.39465	0.516488
C	-1.80388	1.436381	-0.33921
N	-0.84682	0.459715	0.092087
C	-1.48968	-0.75857	0.500456
C	-6.57552	-1.53215	0.346095
N	-7.48802	-0.55274	-0.09396
C	-6.88635	0.653193	-0.48722
O	-0.90373	-1.73862	0.946278
O	-1.5156	2.564066	-0.74064
O	-6.89679	-2.65431	0.734105
O	-7.49684	1.636786	-0.90141
C	0.545034	0.678775	0.153281
C	1.046354	1.940667	0.534977
C	2.416404	2.152209	0.606029
C	3.325131	1.12586	0.30696
C	2.820783	-0.13764	-0.08526
C	1.439963	-0.35171	-0.16096
C	4.776701	1.386169	0.41135
C	5.699174	0.259627	0.085441
C	5.203415	-0.9974	-0.32122
C	3.737231	-1.25229	-0.44031
C	7.084639	0.459056	0.18327
C	7.967802	-0.57435	-0.11655
C	7.474644	-1.82457	-0.52105
C	6.101895	-2.03193	-0.623
O	5.223446	2.486369	0.75509
O	3.319148	-2.3469	-0.82288
H	-4.51686	2.296488	-0.89225
H	-3.84403	-2.40048	0.897876
H	0.354267	2.741909	0.758141
H	2.8107	3.118154	0.903387
H	1.079558	-1.32836	-0.45501
H	7.439321	1.435383	0.496907
H	9.039417	-0.41209	-0.03774
H	8.163817	-2.63154	-0.75476
H	5.694361	-2.9883	-0.9339

H	-8.48621	-0.70495	-0.12175

Table S3 Cartesian coordinates of CP-PDAB^{2-} (43°).

Element	x	y	z
C	-5.29316	-0.86474	0.275271
C	-5.44405	0.438402	-0.3442
C	-4.34725	1.247496	-0.61907
C	-3.0866	0.7595	-0.26294
C	-2.93596	-0.5359	0.347676
C	-4.02603	-1.35268	0.61709
C	-1.7751	1.355469	-0.43894
N	-0.84724	0.39784	0.07086
C	-1.51275	-0.7628	0.588394
C	-6.60878	-1.45513	0.429736
N	-7.49633	-0.48803	-0.10214
C	-6.86821	0.672011	-0.58143
O	-0.94431	-1.70508	1.1372
O	-1.45163	2.445434	-0.93219
O	-6.99083	-2.5406	0.901126
O	-7.47489	1.633773	-1.0808
C	0.553125	0.616022	0.159699
C	1.037078	1.859034	0.635188
C	2.399872	2.075297	0.739044
C	3.335891	1.081495	0.382384
C	2.846622	-0.16847	-0.10471
C	1.456062	-0.37757	-0.20598
C	4.768941	1.360377	0.520919
C	5.686217	0.280052	0.121068
C	5.204053	-0.96583	-0.3792
C	3.762237	-1.24209	-0.52294
C	7.079099	0.479661	0.231211
C	7.978528	-0.5105	-0.13675
C	7.500634	-1.74537	-0.63266
C	6.134618	-1.95971	-0.74913
O	5.203677	2.45817	0.956583
O	3.353747	-2.33469	-0.98362
H	-4.46351	2.221196	-1.08664
H	-3.8991	-2.32942	1.075572
H	0.329772	2.636779	0.897139
H	2.785788	3.022428	1.103052
H	1.107718	-1.33696	-0.56811
H	7.415425	1.438482	0.614727
H	9.049151	-0.33745	-0.04462

H	8.202276	-2.52538	-0.92198
H	5.737227	-2.8971	-1.12706
H	-8.49648	-0.62148	-0.12804

Table S4 Cartesian coordinates of CP-PDAB^{3-} (42°).

Element	x	y	z
C	-5.31965	-0.87007	0.273711
C	-5.46793	0.469254	-0.34069
C	-4.34536	1.255484	-0.6102
C	-3.08453	0.75415	-0.28571
C	-2.93626	-0.57207	0.313822
C	-4.04612	-1.36483	0.587092
C	-1.78202	1.3392	-0.4477
N	-0.8532	0.357657	0.051004
C	-1.53264	-0.82092	0.537857
C	-6.62469	-1.43939	0.438285
N	-7.50137	-0.44816	-0.07142
C	-6.86887	0.71909	-0.55107
O	-0.94571	-1.78789	1.053713
O	-1.43	2.441601	-0.92109
O	-7.05078	-2.53503	0.90302
O	-7.51611	1.691628	-1.03226
C	0.546364	0.572524	0.143618
C	1.028264	1.823115	0.614452
C	2.386212	2.052354	0.729092
C	3.343051	1.068526	0.383611
C	2.864327	-0.19012	-0.10118
C	1.468607	-0.41115	-0.20553
C	4.768934	1.369057	0.530364
C	5.690533	0.309615	0.138801
C	5.221012	-0.95275	-0.36711
C	3.795811	-1.25092	-0.51481
C	7.088078	0.518153	0.249626
C	8.002259	-0.45646	-0.115
C	7.538352	-1.70442	-0.61582
C	6.176387	-1.93149	-0.73387
O	5.187635	2.487734	0.972804
O	3.40188	-2.35974	-0.98238
H	-4.45041	2.241335	-1.05903
H	-3.92598	-2.34925	1.035193
H	0.31176	2.597516	0.861612
H	2.759933	3.005859	1.0911

H	1.131425	-1.37796	-0.55757
H	7.410146	1.482362	0.634746
H	9.072004	-0.26883	-0.01971
H	8.250634	-2.47741	-0.90439
H	5.789686	-2.87394	-1.11305
H	-8.50322	-0.56825	-0.08639

Table S5 Cartesian coordinates of CP-PDAB^{4-} (86^{o}).

Element	x	y	z
C	5.433351	-0.00972	0.758471
C	5.429688	-0.30344	-0.70421
C	4.210366	-0.34545	-1.40729
C	3.025907	-0.11337	-0.72131
C	3.029562	0.174776	0.712433
C	4.217606	0.224645	1.429054
C	1.651904	-0.07045	-1.18957
N	0.852967	0.214529	-0.03583
C	1.657959	0.396272	1.13435
C	6.784391	-0.01639	1.216483
N	7.536979	-0.3069	0.052111
C	6.778468	-0.48786	-1.13054
O	1.20002	0.693332	2.253631
O	1.188435	-0.22654	-2.33462
O	7.348276	0.172233	2.348149
O	7.336773	-0.75163	-2.24989
C	-0.5678	0.472972	-0.08263
C	-1.0146	1.804287	-0.31767
C	-2.36491	2.088493	-0.36859
C	-3.3636	1.089149	-0.19299
C	-2.91566	-0.26808	0.046351
C	-1.51134	-0.52383	0.091976
C	-4.76777	1.468328	-0.26012
C	-5.69119	0.384555	-0.0682
C	-5.24859	-0.99537	0.175346
C	-3.85421	-1.37013	0.241086
C	-7.09297	0.631865	-0.11002
C	-8.03923	-0.36414	0.066895
C	-7.60649	-1.71322	0.304464
C	-6.2476	-1.98877	0.351605
O	-5.14943	2.695292	-0.47718
O	-3.46936	-2.58584	0.455974
H	4.195527	-0.55432	-2.47625
H	4.207941	0.446306	2.495495

H	-0.27195	2.588335	-0.45437
H	-2.71972	3.101007	-0.54723
H	-1.20294	-1.54917	0.272193
H	-7.38934	1.664144	-0.29137
H	-9.10593	-0.1263	0.026522
H	-8.33909	-2.51198	0.446495
H	-5.88517	-3.00022	0.530049
H	8.543677	-0.37675	0.06365