Supporting Information

Towards ultra-stable aqueous Zinc-ion batteries via electrochemical polymerization of phthalimido anchored benzoquinone

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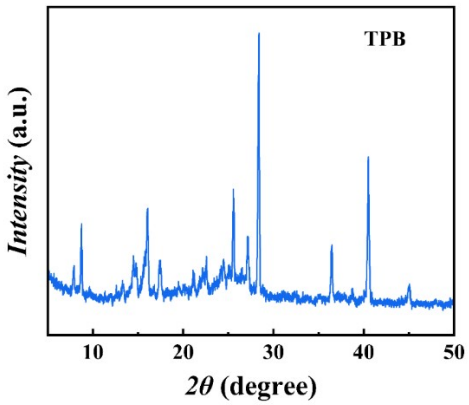

Fig.S1. X-ray diffraction pattern of TPB.

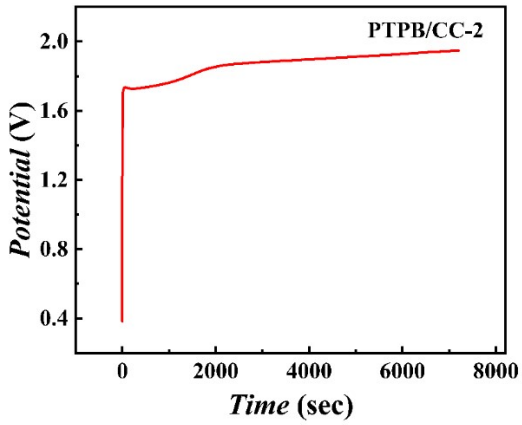

Fig. S2. The *E-t* curve for electropolymerization PTPB/CC-2.

(a) (b)

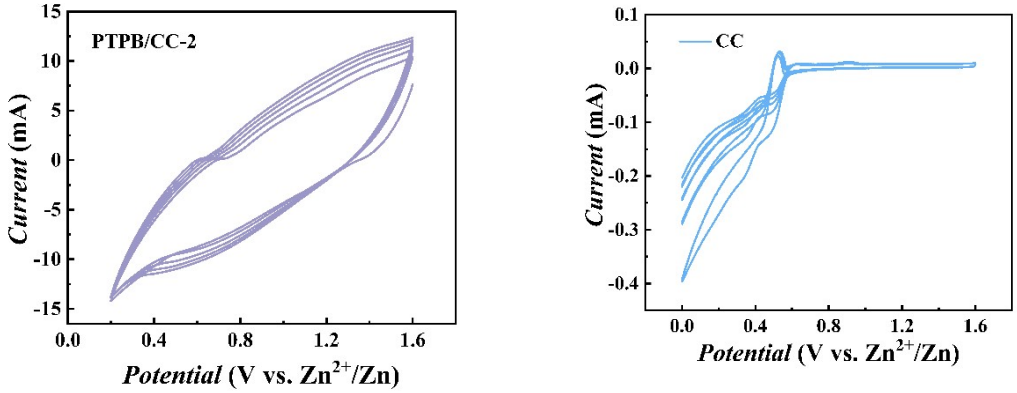

Fig. S3. (a) CV of PTPB/CC-2; (b) CV of CC.

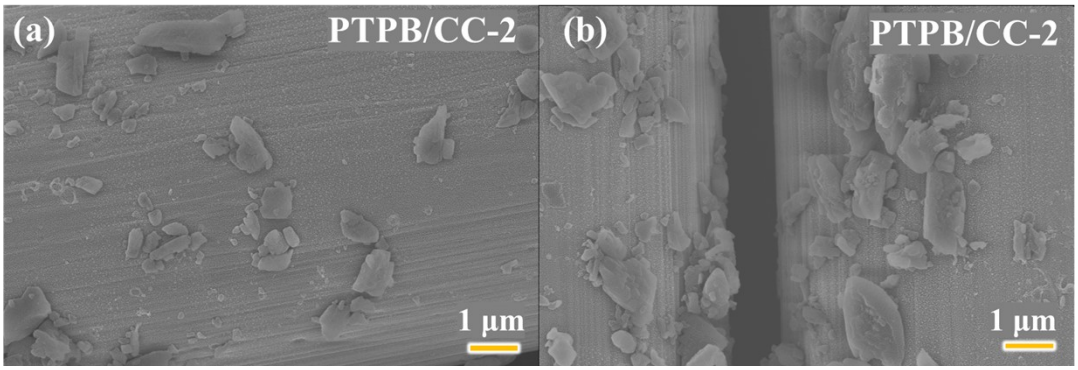

Fig. S4. (a) SEM images of the PTPB/CC-2.

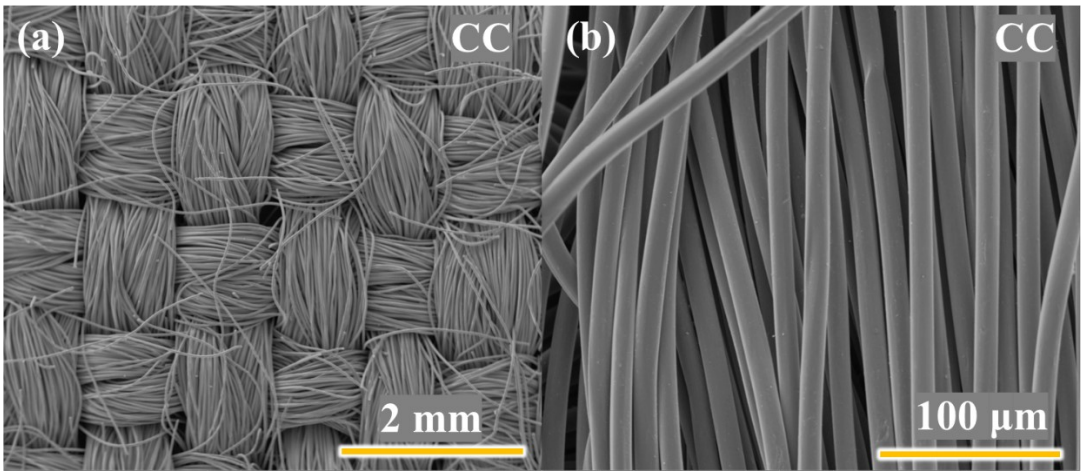

Fig. S5. (a) SEM images of the CC.

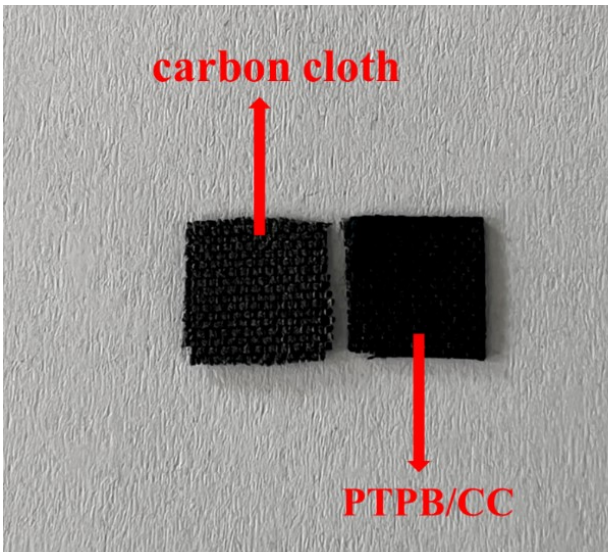

Fig. S6. The comparison between carbon cloth and PTPB/CC.

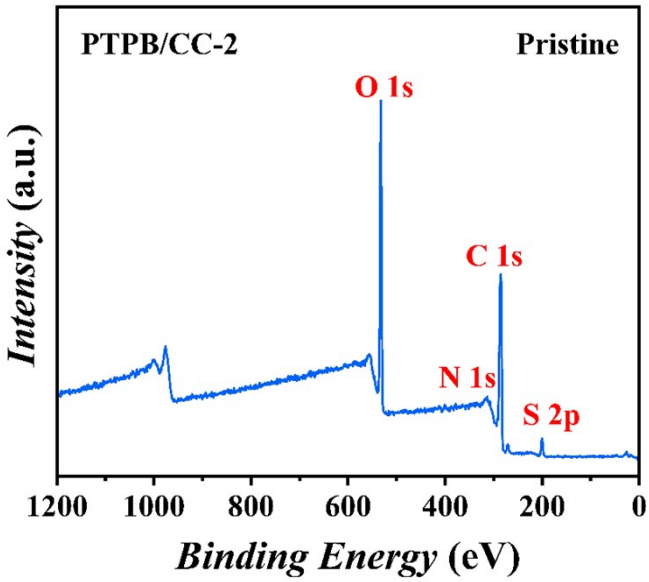

Fig. S7. XPS survey spectra of the PTPB/CC-2.

Fig. S8 shows the high-resolution XPS spectrum of the C 1s region for PTPB/CC-2, with peaks located at 284.8, 286.89, and 287.68 eV, which correspond to C–C, C-O/C-N and C=O/C=N, respectively.

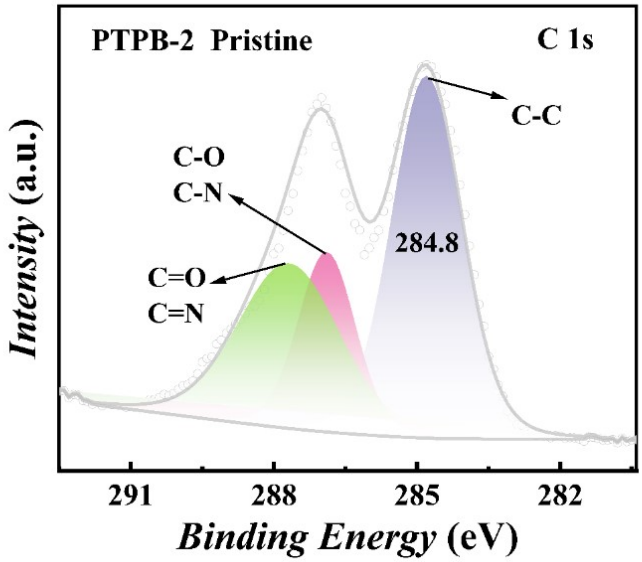

Fig. S8. C 1s XPS spectrum.

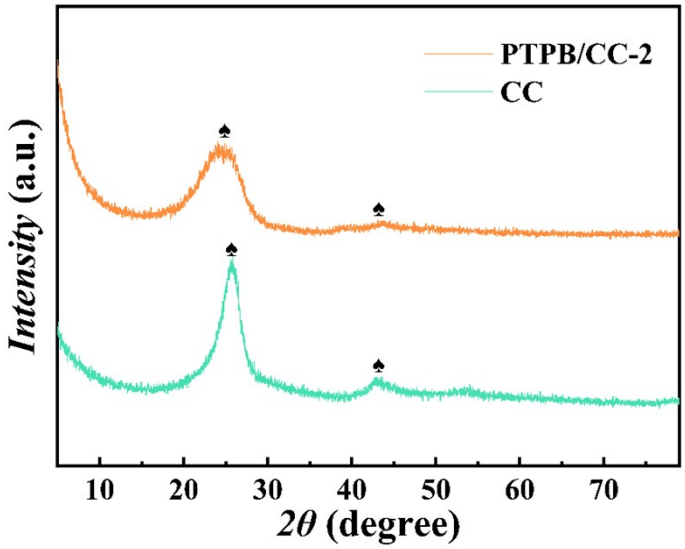

Fig. S9. XRD patterns of PTPB/CC.

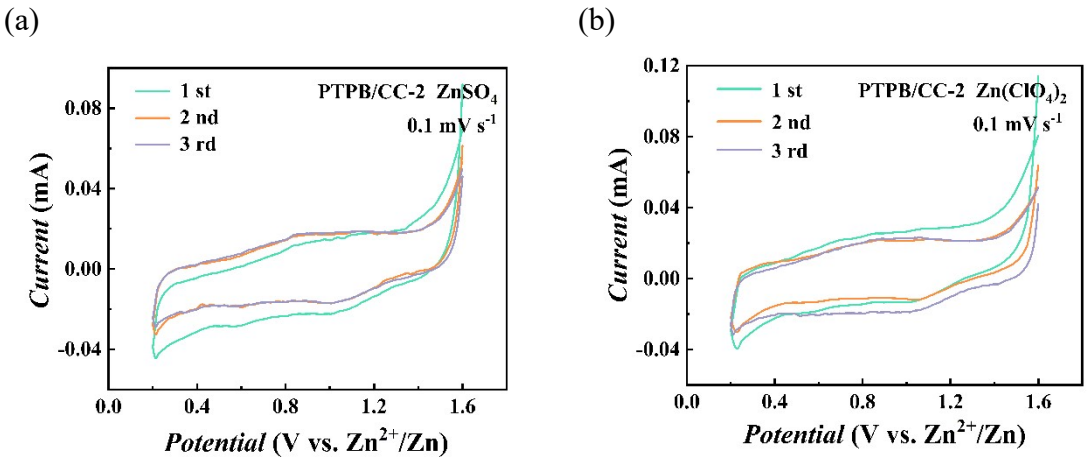

Fig. S10. CV of the ZIB with PTPB/CC-2 at 0.1 mV s^{-1} with electrolyte of (a) 2 M $ZnSO_4$ or (b) 2 M $Zn(ClO_4)_2$.

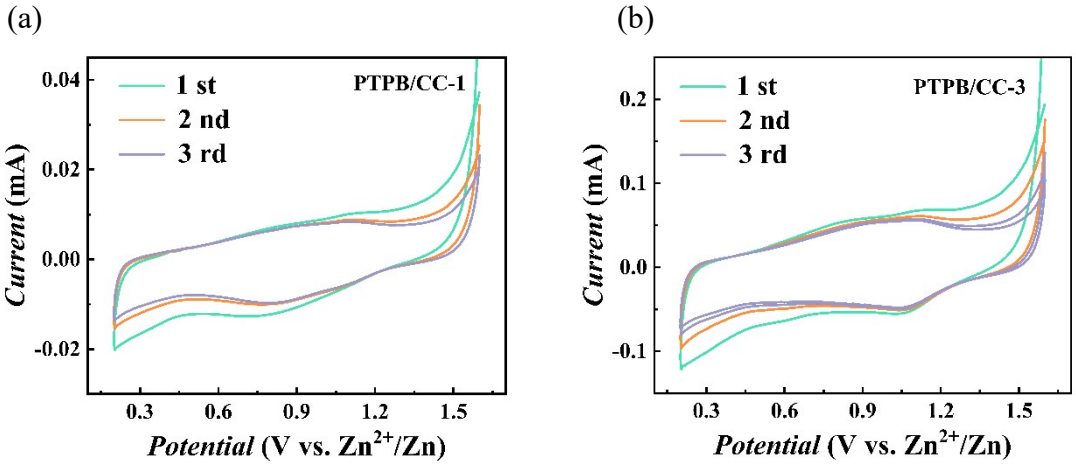

Fig. S11. Initial CV of ZIBs with (a) PTPB/CC-1 and (b) PTPB/CC-3 at 0.1 mV s^{-1}.

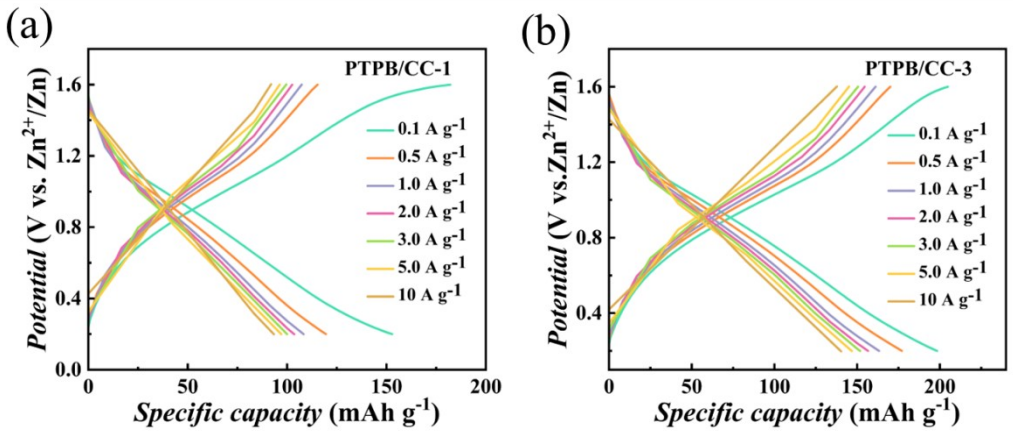

Fig. S12. GCD profiles at various current densities of ZIB with (a) PTPB/CC-1 and with (b) PTPB/CC-3.

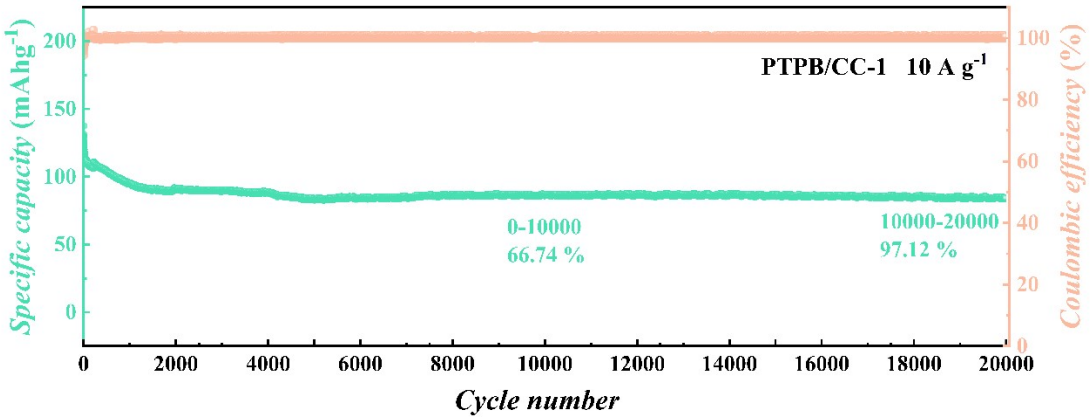

Fig. S13. Cycling performance of the ZIB with PTPB/CC-1 at 10 A g^{-1}.

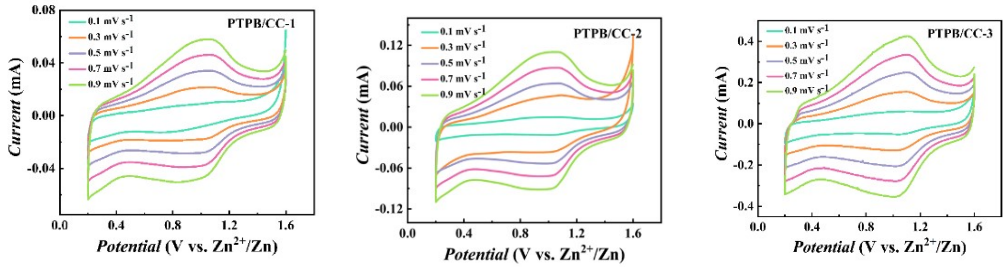

Fig. S14. CV at different scan rates of ZIB: (a) PTPB/CC-1; (b) PTPB/CC-2; (c) PTPB/CC-3.

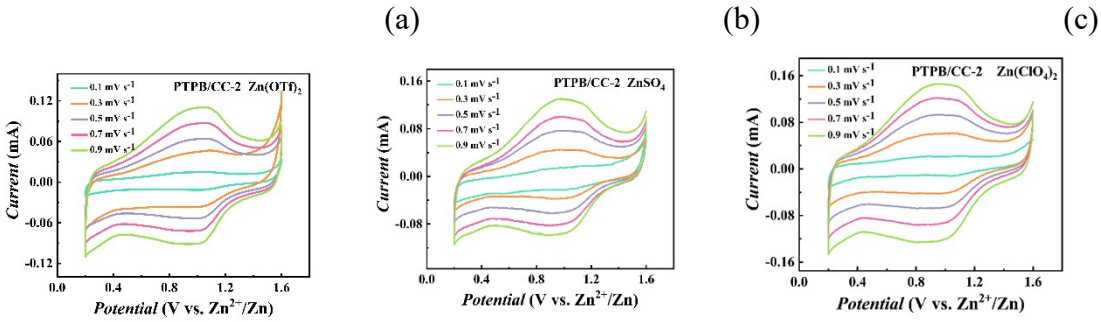

Fig. S15. (a) CV at different scan rates of ZIB with PTPB/CC-2:（a）2 M $Zn(OTf)_2$; (b) 2 M $ZnSO_4$; (c) 2 M $Zn(ClO_4)_2$.

The relationship between peak current (i) and scan rate (v) can be expressed as

$$i = av^b \qquad \textbf{Equation S(1)}$$

where b is a constant ranging from 0.5 to 1. When b = 0.5, the charge and discharge process is entirely governed by semi-infinite diffusion process. When b equals 1.0, surface capacitive process dominates the redox process. **Fig. S16a, b, c** illustrates the fitted curves of log i vs. log v for the ZIB with PTPB/CC. For the ZIB with PTPB/CC-2 **(Fig. S16b)**, the b values of the anodic and cathodic peaks are 0.9059 and 0.9318, respectively. For PTPB/CC-1 **(Fig. S16a)**, the slopes of the two characteristic peaks correspond to b values of 0.8038 and 0.7883. For PTPB/CC-3h **(Fig. S16c)**, the slopes of the two characteristic peaks correspond to b values of 0.8852 and 0.8801. These results indicate that both surface-capacitive controlled process and semi-infinite linear diffusion limited processes contribute to the charge storage process.

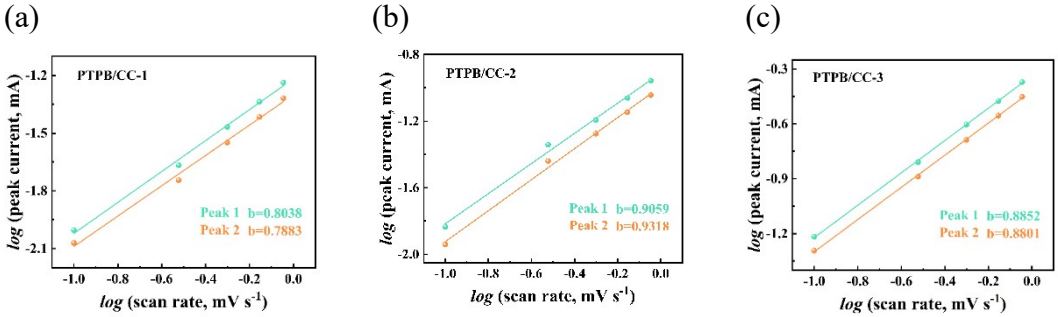

Fig. S16. log(current)–log(scan rate) plots for redox peaks currents: (a) PTPB/CC-1; (b) PTPB/CC-2; (c) PTPB/CC-3.

Fig. S17 depicts the relationship between peak current (i) and scan rate (v), showing that the total stored charge can be categorized into two components: a semi-infinite linear diffusion-limited process and a surface capacitance process. By assuming a linear combination of these two processes, the current can be modeled using the following equation:

$$i = k_1 v + k_2 v^{1/2} \qquad \textbf{Equation S(2)}$$

$$\frac{i}{v^{1/2}} = k_1 v^{1/2} + k_2 \qquad \textbf{Equation S(3)}$$

Where k_1 and k_2 indicate the contribution constants for the surface capacitance control process and the semi-infinite linear diffusion confinement process, respectively. For the ZIB with PTPB/CC-2**(Fig. S17 b)**. At a scan rate of 0.9 mV s^{-1}, the surface capacitance control process accounts for 85.83 % of the charge storage. For the PTPB/CC-1 and PTPB/CC-3 ZIBs, the contributions from the surface capacitance control process are 74.24 % and 85.77 %, respectively **(Fig. S17a and Fig. S17c)**.

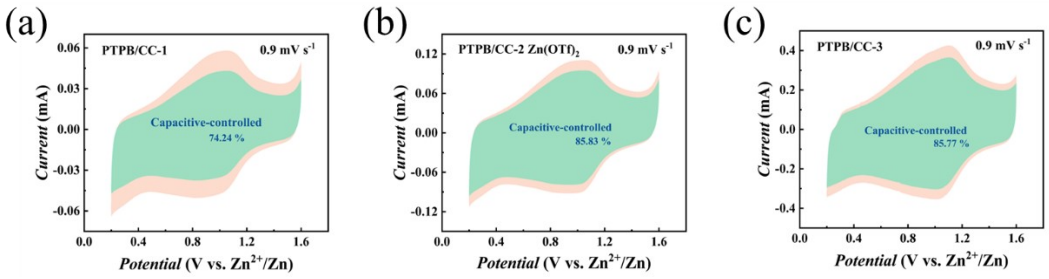

Fig. S17. Capacitive contribution and diffusion contribution at 0.9 mV s^{-1}: (a) PTPB/CC-1; (b) PTPB/CC-2; (c) PTPB/CC-3.

The charge storage contributions of the surface capacitance control process for PTPB/CC-2 at scan rates of 0.1, 0.3, 0.5, 0.7, and 0.9 mV s^{-1} are 69.08%, 71.73%, 82.05%, 84.42%, and 85.83%, respectively **(Fig. S18b)**. For PTPB/CC-1, the capacitive reaction contribution percentages at different scan rates **(Fig. S18a)** are 48.25%, 66.50%, 70.19%, 72.52%, and 74.24% at scan rates of 0.1, 0.3, 0.5, 0.7, and 0.9 mV

s^{-1}, respectively. PTPB/CC-3 shows capacitive reaction contribution percentages (**Fig. S18c**) of 66.79%, 78.33%, 81.36%, 84.66%, and 85.77% at scan rates of 0.1, 0.3, 0.5, 0.7, and 0.9 mV s^{-1}, respectively.

Notably, the contribution from the surface capacitance process increases with higher scan rates. At elevated scan rates, the diffusivity of the battery's cathode material typically declines due to the rapid electrochemical reactions, which shorten the migration time for Zn^{2+}, preventing them from diffusing adequately into the active regions of the cathode.

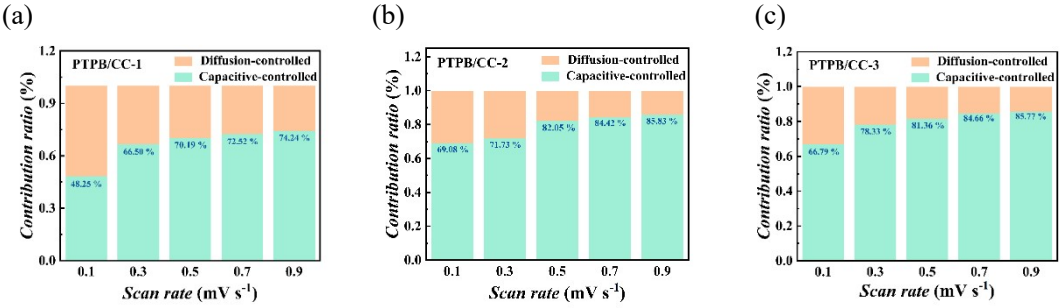

Fig. S18. Capacitive contribution ratios at corresponding scan rates: (a) PTPB/CC-1; (b) PTPB/CC-2; (c) PTPB/CC-3.

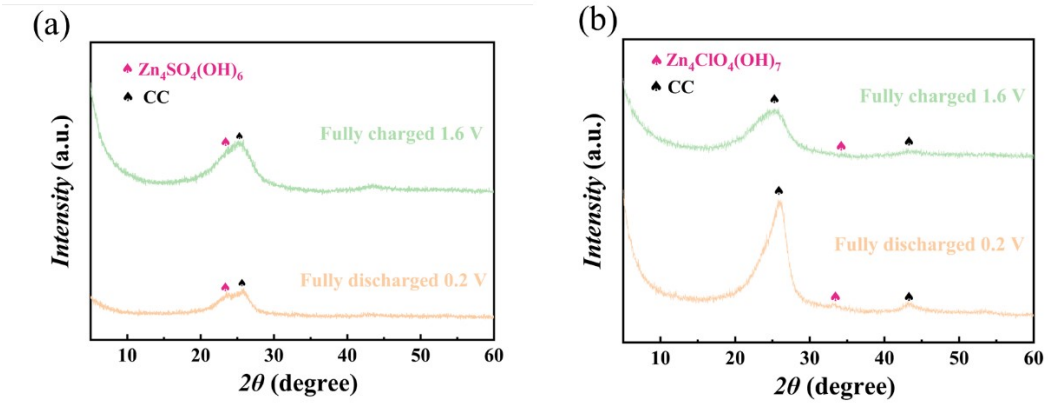

Fig. S19 PXRD patterns of PTPB/CC-2 at different states: a) ZnSO4; b) $Zn(ClO_4)_2$.

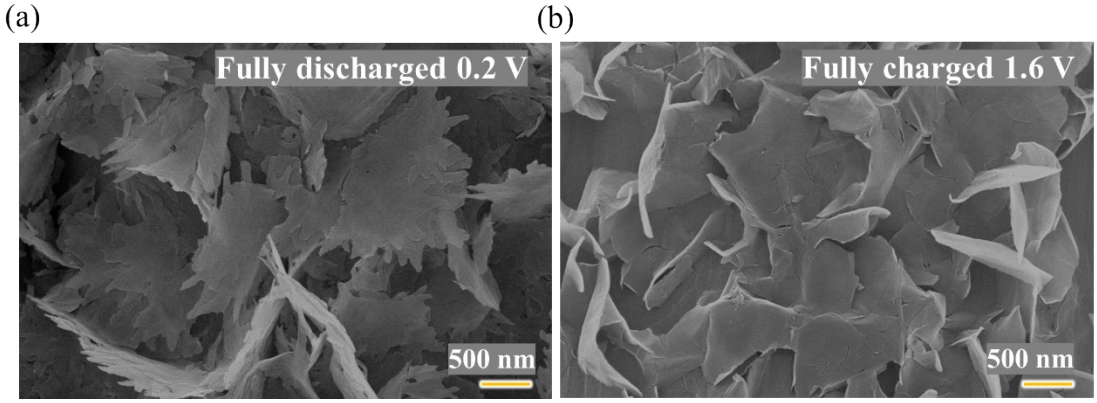

Fig. S20. SEM images of PTPB/CC-2: (a) Fully discharged state; (b) Fully charged state.

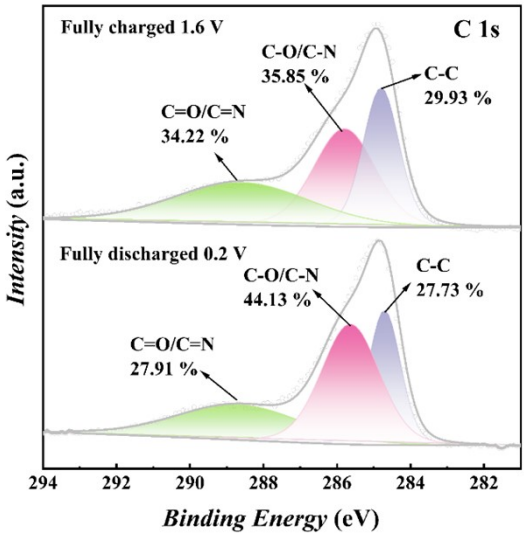

Fig. S21. C 1s XPS spectrum.

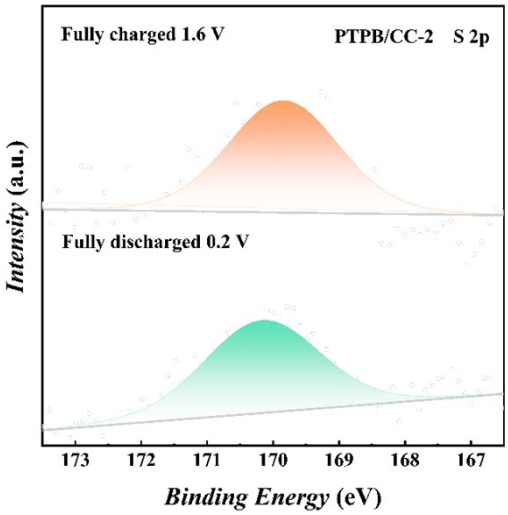

Fig. S22. S 2p XPS spectrum.

Table S1: Redox peak potentials of ZIBs.

	2 M $Zn(OTf)_2$		2 M $ZnSO_4$		2 M $Zn(ClO_4)_2$	
Scan rate mV s^{-1}	**Oxidation peak potential**	**Reduction peak potential**	**0xidation peak potential**	**Reduction peak potential**	**Oxidation peak potential**	**Reduction peak potential**
0.1	1.06 V	1.021V	1.038 V	1.017 V	1.031 V	1.023 V
0.3	1.063 V	1.02 V	1.012 V	0.997 V	1.025 V	1.017 V
0.5	1.068 V	1.017 V	1.005 V	0.967 V	0.993 V	0.979 V
0.7	1.068 V	1.004 V	0.982 V	0.965 V	0.951 V	0.937 V
0.9	1.06 V	1.002 V	0.981 V	0.972 V	0.949 V	0.921 V

Table S2: Performance Comparison of Polymer Organic Cathode Materials.

Cathode material	**Current density （A g^{-1})**	**Specifc capaciy mAh g^{-1}**	**Current density (A g^{-1})**	**Specific capacity mAh g^{-1}**	**Number of cycles**	**Capacity retention rate (%)**
1,8-DAN/AC[1]	0.2	450	20	272.4	50000	68.1
Poly(1,5-NAPD)[2]	0.05	134	5	50.6	1000	100
PPy[EMIm]TFS[3]	0.2	126	----	----	100	57.9
DA-CCP-2[4]	0.1	251.7	5	100	1000	84.5
Poly-(thionine) [5]	0.1	135	5	98	5000	66.3
PANI@CF[6]	0.35	235.9	3.5	90	10000	75.7
PANI-10[7]	0.1	178.4	10	102.8	10000	95.2
Q-PANI[8]	0.2	186	2	95	1500	88
PTA-O26[9]	0.05	283	1.6	50	240	92.2
m-PTPA[10]	0.5	210.7	6	107.5	1000	87.6
POLA/G[11]	0.1	224.3	10	145.5	3000	89.3
PDAP[12]	0.2	312	2.0	132	1000	65
rPOP[13]	0.1	120	2.0	40	30000	66
PTFHQ[14]	0.1	215	20	196	3400	92
PPPA[15]	0.1	191	5.0	130.3	20000	70.6
PTPB/CC-2	0.1	261	10	166	30000	74.9

Table S3. PTPB/CC-2 in the pristine, fully discharged and fully charged states deconvoluted O 1s XPS spectra components.

	532.3 eV	**533.2 eV**	**534.3 eV**
	C=O	**C-O**	**H_2O**
Pristine	62.6%	31.6%	5.8%
Fully discharged 0.2 V	23.6%	59.3%	17.1%
Fully charged 1.6 V	56.4%	34.5%	9.1%

Table S4. PTPB/CC-2 in the pristine, fully discharged and fully charged states deconstructed N 1s XPS spectral components.

	399.6 eV	**400.4 eV**	**401.3 eV**	**402.2 eV**
	-N=	**-NH-**	**$-NH^+-$**	**$-NH^+=$**
Pristine	25.4%	23.5%	33.9%	17.2%
Fully discharged 0.2 V	19.4%	56.2%	18.8%	5.7%
Fully charged 1.6 V	34.7%	28.8%	17.2%	19.3%

Table S5. The optimized Cartesian Coordinates (in Å) of species studied.

(a)

TPB	**Cartesian coordinates**			**TPB**	**Cartesian coordinates**		
C	1.276574	0.675733	-0.025026	C	-6.093567	-4.168592	-0.811650
C	1.276585	-0.675708	0.024782	C	-4.857560	-3.845276	-1.379146
C	0.000016	-1.446542	-0.000206	C	4.857499	3.845402	-1.379091
C	-1.276544	-0.675726	-0.025030	C	6.093517	4.168711	-0.811617
C	-1.276555	0.675712	0.024799	C	6.529396	3.559124	0.370412
C	0.000015	1.446547	-0.000156	C	5.742987	2.605898	1.023560
N	2.441752	1.436491	-0.036268	C	5.743048	-2.606032	-1.023372
N	-2.441738	1.436451	0.036131	C	6.529368	-3.559255	-0.370113
N	-2.441732	-1.436470	-0.036281	C	6.093375	-4.168764	0.811913
N	2.441757	-1.436464	0.036114	C	4.857323	-3.845380	1.379274
O	0.000001	2.653267	-0.000256	O	2.071973	-2.561475	2.041701
O	0.000032	-2.653262	-0.000224	O	3.500994	-0.585648	-1.848815
C	-3.485010	1.326821	-0.902998	O	3.500791	0.585543	1.848707
C	-4.517716	2.295284	-0.453722	O	2.072139	2.561657	-2.041795
C	-4.082951	2.902528	0.721533	O	-2.072027	2.561404	2.041767
C	-2.751834	2.349504	1.081872	O	-3.500926	0.585641	-1.848825
C	-3.484884	-1.326815	0.902966	O	-2.072211	-2.561530	-2.041887
C	-4.517677	-2.295243	0.453811	O	-3.500702	-0.585587	1.848761
C	-4.083041	-2.902533	-0.721468	H	-6.070271	2.119249	-1.944263
C	-2.751938	-2.349559	-1.081954	H	-7.501329	3.834004	-0.786251
C	2.751916	2.349630	-1.081910	H	-6.732677	4.909121	1.298231
C	4.083017	2.902611	-0.721437	H	-4.505754	4.309823	2.302545
C	4.517698	2.295275	0.453801	H	-6.070089	-2.119111	1.944486
C	3.484932	1.326812	0.902944	H	-7.501319	-3.833840	0.786643
C	3.485049	-1.326835	-0.902993	H	-6.732883	-4.909054	-1.297873
C	4.517725	-2.295333	-0.453723	H	-4.506035	-4.309860	-2.302403
C	4.082925	-2.902598	0.721507	H	4.505942	4.310020	-2.302318
C	2.751808	-2.349564	1.081827	H	6.732809	4.909204	-1.297826
C	-5.743035	2.605972	-1.023385	H	7.501319	3.833913	0.786623
C	-6.529386	3.559165	-0.370119	H	6.070153	2.119102	1.944426
C	-6.093426	4.168654	0.811931	H	6.070310	-2.119292	-1.944233
C	-4.857380	3.845279	1.379307	H	7.501313	-3.834104	-0.786234
C	-5.742955	-2.605872	1.023591	H	6.732602	-4.909255	1.298208
C	-6.529401	-3.559053	0.370420	H	4.505671	-4.309942	2.302492

(b)

TPB H^+ type I	Cartesian coordinates			TPB H^+ type II	Cartesian coordinates		
C	-1.235926	-0.685703	-0.186051	C	-1.487100	0.597250	0.132398
C	-1.271891	0.679311	-0.152879	C	-1.477255	-0.743618	0.119611
C	0.007754	1.475990	-0.196015	C	-0.174650	-1.478488	-0.050834
C	1.306143	0.732227	-0.141485	C	1.093675	-0.708779	0.030143
C	1.306963	-0.632608	-0.236952	C	1.071949	0.653407	0.018945
C	0.047771	-1.319888	-0.474778	C	-0.213322	1.385586	0.116462
N	-2.367385	-1.483012	0.056997	N	-2.635737	1.409557	0.267331
N	2.440478	-1.423656	-0.268584	N	2.203969	1.447427	0.013120
N	2.435719	1.485700	0.039659	N	2.245234	-1.467518	-0.035713
N	-2.428746	1.412249	-0.151863	N	-2.613587	-1.548871	0.084627
O	0.111183	-2.470925	-0.987213	O	-0.274491	2.585929	0.245040
O	-0.031532	2.675106	-0.237592	O	-0.203577	-2.644520	-0.355268
C	3.625245	-1.164125	-0.999762	C	3.320998	1.281280	0.866107
C	4.569369	-2.227680	-0.585907	C	4.301828	2.297305	0.418099
C	3.953572	-3.040756	0.368174	C	3.778573	2.981192	-0.679412
C	2.582548	-2.541106	0.604515	C	2.435589	2.438145	-0.987110
C	3.444522	1.185272	1.000512	C	3.323398	-1.257241	-0.927501
C	4.497680	2.198068	0.787120	C	4.332518	-2.277259	-0.560462
C	4.148215	3.001574	-0.298278	C	3.855653	-3.023187	0.517610
C	2.849521	2.552350	-0.843868	C	2.516577	-2.517655	0.895632
C	-2.816486	-2.549345	-0.707863	C	-2.799764	2.216555	1.489627
C	-4.157684	-2.902779	-0.238423	C	-3.696806	3.320497	1.087873
C	-4.464725	-2.084754	0.850816	C	-3.998078	3.176100	-0.271396
C	-3.336013	-1.159868	1.081953	C	-3.315828	1.982948	-0.748469
C	-3.535669	1.135565	-1.001284	C	-2.779350	-2.677433	0.982374
C	-4.542593	2.165790	-0.681641	C	-3.840537	-3.496837	0.356785
C	-4.065717	2.964219	0.358856	C	-4.226471	-2.891559	-0.842697
C	-2.723131	2.495093	0.763979	C	-3.433073	-1.668550	-1.022071
C	5.869721	-2.459197	-1.007162	C	5.559323	2.588397	0.924598
C	6.544216	-3.542296	-0.435090	C	6.286571	3.599123	0.289068
C	5.928374	-4.355595	0.522645	C	5.763296	4.283558	-0.813767
C	4.615979	-4.115544	0.941198	C	4.494900	3.981514	-1.318344
C	5.682201	2.389818	1.483654	C	5.574494	-2.526486	-1.124648
C	6.516134	3.424434	1.051893	C	6.335043	-3.557979	-0.566421
C	6.167788	4.228147	-0.040521	C	5.858188	-4.304535	0.517133
C	4.974067	4.025145	-0.738376	C	4.604590	-4.045818	1.079305
C	-5.028652	-3.885187	-0.684957	C	-4.225066	4.356170	1.836680
C	-6.243095	-4.012540	-0.002391	C	-5.060842	5.263019	1.169915
C	-6.551262	-3.193630	1.089052	C	-5.359329	5.119545	-0.188789
C	-5.658722	-2.213492	1.540106	C	-4.835007	4.061291	-0.937787
C	-5.789966	2.379575	-1.251045	C	-4.428061	-4.671617	0.795233
C	-6.553716	3.431426	-0.738328	C	-5.417975	-5.233219	-0.020007
C	-6.077477	4.229409	0.308993	C	-5.800977	-4.629277	-1.222454
C	-4.821374	4.004000	0.879430	C	-5.208705	-3.439117	-1.655684
O	-2.023049	2.833609	1.664841	O	-3.463335	-0.890385	-1.968557
O	-3.573812	0.229140	-1.789700	O	-2.168640	-2.802375	1.994791
O	-3.180762	-0.307849	1.902224	O	-3.375384	1.539129	-1.924886
O	-2.148697	-3.112844	-1.568557	O	-2.290917	1.927965	2.520254
O	1.718395	-2.918724	1.343526	O	1.675157	2.696039	-1.873987
O	3.768545	-0.255656	-1.770927	O	3.398245	0.467739	1.745605
O	2.255572	2.897973	-1.816722	O	1.781501	-2.838551	1.781616
O	3.380301	0.285442	1.791215	O	3.353006	-0.417199	-1.785508
H	6.340400	-1.817338	-1.754330	H	5.957649	2.044502	1.783277
H	7.570643	-3.758858	-0.739096	H	7.281570	3.859696	0.656546
H	6.484989	-5.192476	0.949995	H	6.359117	5.066596	-1.287922
H	4.127204	-4.742879	1.688920	H	4.078283	4.506123	-2.180200
H	5.944600	1.753423	2.330863	H	5.936035	-1.935382	-1.968248
H	7.457872	3.610482	1.572810	H	7.319628	-3.786432	-0.980358
H	6.843334	5.028104	-0.351322	H	6.478885	-5.102927	0.929752
H	4.693580	4.643303	-1.593176	H	4.223082	-4.619927	1.925744
H	-4.775759	-4.524148	-1.532946	H	-3.992665	4.462229	2.897949
H	-6.963359	-4.767681	-0.324006	H	-5.488625	6.102062	1.723080
H	-7.506890	-3.325515	1.601134	H	-6.014003	5.847287	-0.672501
H	-5.887378	-1.577041	2.396986	H	-5.065262	3.939718	-1.997795
H	-6.151491	1.749382	-2.065781	H	-4.121473	-5.138376	1.733199
H	-7.540011	3.636682	-1.160087	H	-5.900221	-6.164184	0.285998
H	-6.700389	5.044049	0.684808	H	-6.575430	-5.098086	-1.833109
H	-4.440349	4.619345	1.696591	H	-5.499505	-2.960961	-2.592844
H	-0.848705	-2.827879	-1.322621	H	-3.202548	0.498338	-1.995385

(c)

TPB-Zn^{2+} type I	Cartesian coordinates			TPB-Zn^{2+} type II	Cartesian coordinates		
C	-1.275193	-0.456229	0.320431	C	-1.265686	0.669560	1.265459
C	-1.316061	0.905035	0.142760	C	-1.265868	-0.678559	1.249206
C	-0.000009	1.606650	-0.114171	C	-0.000017	-1.451085	1.487727
C	1.316045	0.905047	0.142785	C	1.265831	-0.678550	1.249226
C	1.275189	-0.456218	0.320449	C	1.265630	0.669570	1.265461
C	-0.000001	-1.109249	0.550353	C	-0.000032	1.437728	1.517079
N	-2.403832	-1.286603	0.406314	N	-2.316159	1.421432	0.740282
N	2.403832	-1.286587	0.406334	N	2.316092	1.421460	0.740288
N	2.416634	1.675812	-0.028121	N	2.326593	-1.424248	0.737136
N	-2.416644	1.675807	-0.028155	N	-2.326619	-1.424261	0.737099
O	0.000004	-2.330752	0.871237	O	-0.000036	2.631361	1.646300
O	-0.000013	2.600089	-0.784461	O	-0.000016	-2.645324	1.610289
C	2.656156	-2.385245	-0.356242	C	3.357869	2.130057	1.474150
C	4.005257	-2.851640	-0.067850	C	4.029305	2.937144	0.429924
C	4.556668	-2.008582	0.906368	C	3.387413	2.728291	-0.800973
C	3.561213	-0.974251	1.242416	C	2.288335	1.790050	-0.585195
C	2.536591	3.007746	0.563337	C	2.291642	-1.856316	-0.568327
C	3.842712	3.499566	0.098816	C	3.418742	-2.766224	-0.758547
C	4.455510	2.522934	-0.694369	C	4.096437	-2.880643	0.465702
C	3.585366	1.341375	-0.783595	C	3.420406	-2.039026	1.479163
C	-2.656149	-2.385269	-0.356251	C	-3.357933	2.130037	1.474143
C	-4.005249	-2.851666	-0.067858	C	-4.029309	2.937192	0.429930
C	-4.556669	-2.008595	0.906344	C	-3.387488	2.728247	-0.800987
C	-3.561223	-0.974252	1.242377	C	-2.288446	1.789962	-0.585219
C	-3.585389	1.341395	-0.783626	C	-3.420501	-2.038959	1.479089
C	-4.455531	2.522952	-0.694347	C	-4.096423	-2.880704	0.465660
C	-3.842693	3.499583	0.098807	C	-3.418684	-2.766323	-0.758569
C	-2.536554	3.007759	0.563271	C	-2.291616	-1.856376	-0.568348
C	4.713717	-3.925359	-0.589787	C	5.114077	3.788540	0.542085
C	6.008139	-4.132634	-0.098630	C	5.543205	4.435915	-0.625674
C	6.554204	-3.295226	0.878034	C	4.903970	4.228785	-1.851627
C	5.831033	-2.212104	1.401675	C	3.808101	3.365633	-1.960685
C	4.458321	4.715236	0.359114	C	3.838246	-3.450838	-1.891285
C	5.713452	4.931083	-0.217454	C	4.968273	-4.265852	-1.761266
C	6.323457	3.957515	-1.019229	C	5.642543	-4.379566	-0.541939
C	5.700517	2.732574	-1.272210	C	5.215728	-3.683093	0.598107
C	-4.713700	-3.925397	-0.589781	C	-5.113993	3.788697	0.542115
C	-6.008125	-4.132669	-0.098629	C	-5.543121	4.436067	-0.625646
C	-6.554201	-3.295247	0.878018	C	-4.903964	4.228837	-1.851622
C	-5.831037	-2.212114	1.401645	C	-3.808173	3.365589	-1.960701
C	-5.700566	2.732593	-1.272128	C	-5.215672	-3.683212	0.598070
C	-6.323489	3.957538	-1.019124	C	-5.642410	-4.379768	-0.541954
C	-5.713441	4.931108	-0.217383	C	-4.968103	-4.266085	-1.761263
C	-4.458284	4.715258	0.359127	C	-3.838112	-3.451020	-1.891285
O	-1.721571	3.470720	1.295172	O	-1.434746	-1.492508	-1.384048
O	-3.730403	0.300767	-1.366473	O	-3.627719	-1.828914	2.627940
O	-3.576317	-0.052627	1.993897	O	-1.452398	1.369848	-1.396008
O	-1.863209	-2.916118	-1.178663	O	-3.535998	2.002076	2.639600
O	3.576291	-0.052656	1.993972	O	1.452269	1.369959	-1.395978
O	1.863222	-2.916087	-1.178665	O	3.536080	2.001917	2.639566
O	3.730339	0.300755	-1.366467	O	3.627631	-1.828953	2.628009
O	1.721650	3.470705	1.295286	O	1.434811	-1.492414	-1.384054
H	4.285565	-4.575849	-1.354562	H	5.609036	3.950378	1.501806
H	6.602669	-4.963346	-0.484484	H	6.393947	5.119305	-0.576385
H	7.566144	-3.488605	1.241020	H	5.266179	4.752490	-2.738776
H	6.253925	-1.558243	2.166920	H	3.304488	3.202875	-2.915315
H	3.974441	5.469565	0.982398	H	3.307201	-3.361134	-2.840694
H	6.229147	5.877954	-0.043081	H	5.329782	-4.825564	-2.626442
H	7.304745	4.162184	-1.452806	H	6.519868	-5.026966	-0.475767
H	6.169404	1.968858	-1.895411	H	5.739032	-3.770924	1.552402
H	-4.285541	-4.575898	-1.354542	H	-5.608899	3.950604	1.501852
H	-6.602650	-4.963389	-0.484473	H	-6.393802	5.119532	-0.576341
H	-7.566142	-3.488623	1.240999	H	-5.266165	4.752547	-2.738771
H	-6.253938	-1.558241	2.166876	H	-3.304609	3.202766	-2.915346
H	-6.169484	1.968878	-1.895307	H	-5.739012	-3.771011	1.552348
H	-7.304795	4.162210	-1.452657	H	-6.519704	-5.027209	-0.475779
H	-6.229124	5.877982	-0.042991	H	-5.329549	-4.825866	-2.626421
H	-3.974371	5.469588	0.982384	H	-3.307030	-3.361350	-2.840676
Zn	0.000008	-3.122613	-0.953145	Zn	-0.000011	-0.051325	-1.340845

(d)

TPB-Zn1	Cartesian coordinates			TPB-Zn2	Cartesian coordinates		

C	-1.193951	0.668872	1.278418	C	-1.196886	0.703214	0.521069
C	-1.187394	-0.729697	1.122288	C	-1.196894	-0.703113	0.521193
C	-0.000361	-1.559690	1.227872	C	0.000002	-1.512097	0.515295
C	1.186758	-0.729828	1.122322	C	1.196907	-0.703127	0.521125
C	1.193513	0.668788	1.278439	C	1.196914	0.703204	0.521001
C	-0.000178	1.469990	1.438319	C	0.000019	1.512184	0.515018
N	-2.272120	1.405274	0.734367	N	-2.403480	1.442035	0.479217
N	2.271846	1.404995	0.734524	N	2.403513	1.442013	0.479077
N	2.324918	-1.423102	0.651616	N	2.403502	-1.441951	0.479356
N	-2.325634	-1.422850	0.651600	N	-2.403497	-1.441929	0.479483
O	-0.000205	2.715752	1.377019	O	0.000022	2.759955	0.476426
O	-0.000419	-2.799324	1.121475	O	-0.000009	-2.759875	0.476946
C	3.169966	2.244891	1.446934	C	2.910704	2.185614	1.587501
C	3.816244	3.086825	0.396780	C	3.930309	3.101424	1.000313
C	3.252453	2.763730	-0.838216	C	3.956693	2.901877	-0.379692
C	2.227078	1.730424	-0.596493	C	2.948339	1.872215	-0.698685
C	2.311384	-1.934158	-0.624470	C	2.948390	-1.872319	-0.698312
C	3.460704	-2.851796	-0.745389	C	3.956758	-2.901905	-0.379118
C	4.099652	-2.888593	0.494795	C	3.930320	-3.101239	1.000917
C	3.359430	-1.996650	1.435141	C	2.910673	-2.185357	1.587921
C	-3.169531	2.246073	1.446714	C	-2.910570	2.185682	1.587660
C	-3.815281	3.088239	0.396398	C	-3.930233	3.101463	1.000527
C	-3.251755	2.764485	-0.838557	C	-3.956752	2.901849	-0.379466
C	-2.227025	1.730591	-0.596597	C	-2.948422	1.872180	-0.698508
C	-3.360186	-1.996277	1.435158	C	-2.910627	-2.185306	1.588086
C	-4.100316	-2.888365	0.494902	C	-3.930265	-3.101233	1.001139
C	-3.461194	-2.851925	-0.745203	C	-3.956734	-2.901957	-0.378903
C	-2.311887	-1.934246	-0.624367	C	-2.948397	-1.872360	-0.698160
C	4.807040	4.046799	0.506948	C	4.764122	4.021505	1.612198
C	5.219450	4.683350	-0.669481	C	5.632478	4.747914	0.789488
C	4.652269	4.359877	-1.906136	C	5.656899	4.548064	-0.594580
C	3.651954	3.387906	-2.009642	C	4.813250	3.614264	-1.204561
C	3.919055	-3.590373	-1.824840	C	4.813365	-3.614401	-1.203841
C	5.054189	-4.381889	-1.621447	C	5.657010	-4.548088	-0.593680
C	5.695254	-4.419741	-0.379254	C	5.632534	-4.747723	0.790419
C	5.224467	-3.667845	0.703395	C	4.764127	-4.021207	1.612979
C	-4.805410	4.048919	0.506376	C	-4.763988	4.021572	1.612448
C	-5.217406	4.685513	-0.670176	C	-5.632426	4.747939	0.789789
C	-4.650487	4.361381	-1.906776	C	-5.656983	4.548023	-0.594267
C	-3.650846	3.388696	-2.010099	C	-4.813391	3.614195	-1.204286
C	-5.225245	-3.667459	0.703505	C	-4.764039	-4.021196	1.613255
C	-5.695920	-4.419588	-0.379024	C	-5.632446	-4.747765	0.790742
C	-5.054653	-4.382111	-1.621128	C	-5.656954	-4.548186	-0.593364
C	-3.919441	-3.590716	-1.824549	C	-4.813342	-3.614504	-1.203580
O	-1.495024	-1.632490	-1.490454	O	-2.646400	-1.449993	-1.814225
O	-3.562641	-1.770031	2.590232	O	-2.579950	-2.040055	2.724475
O	-1.458784	1.231818	-1.419134	O	-2.646457	1.449550	-1.814484
O	-3.354246	2.225368	2.625361	O	-2.579863	2.040696	2.724074
O	1.458814	1.232026	-1.419188	O	2.646271	1.449629	-1.814647
O	3.354692	2.223942	2.625592	O	2.580102	2.040581	2.723940
O	3.561641	-1.770796	2.590331	O	2.580023	-2.040151	2.724323
O	1.494605	-1.632302	-1.490615	O	2.646358	-1.449916	-1.814356
H	5.237964	4.294409	1.479061	H	4.732496	4.170526	2.693293
H	5.996314	5.450021	-0.622943	H	6.302975	5.487195	1.233757
H	4.995631	4.878178	-2.804233	H	6.345574	5.133804	-1.207585
H	3.197828	3.129310	-2.968026	H	4.820253	3.450810	-2.283842
H	3.407010	-3.554795	-2.788185	H	4.820410	-3.451115	-2.283147
H	5.446543	-4.983378	-2.444455	H	6.345724	-5.133906	-1.206565
H	6.578083	-5.050745	-0.253236	H	6.303030	-5.486920	1.234830
H	5.714218	-3.691119	1.678929	H	4.732460	-4.170061	2.694096
H	-5.236110	4.297058	1.478454	H	-4.732256	4.170645	2.693533
H	-5.993716	5.452752	-0.623789	H	-6.302882	5.487239	1.234088
H	-4.993535	4.879723	-2.804970	H	-6.345720	5.133730	-1.207233
H	-3.196946	3.129559	-2.968444	H	-4.820499	3.450689	-2.283559
H	-5.715160	-3.690454	1.678965	H	-4.732347	-4.170005	2.694378
H	-6.578823	-5.050481	-0.252982	H	-6.302916	-5.486959	1.235196
H	-5.446917	-4.983786	-2.444043	H	-6.345667	-5.134045	-1.206212
H	-3.407237	-3.555410	-2.787819	H	-4.820412	-3.451263	-2.282893
Zn	-0.000001	-0.218640	-0.961971	Zn	-1.162775	-0.000202	-2.022891
				Zn	1.162639	-0.000221	-2.022920

(e)

TPB-Zn3	**Cartesian coordinates**			**TPB-Zn4**	**Cartesian coordinates**		
C	1.193983	-0.522965	0.328972	C	1.206182	0.698978	-0.195434

C	1.210801	0.872046	0.419129	C	1.206095	-0.699270	-0.195181
C	0.000011	1.672710	0.489866	C	-0.000030	-1.438466	-0.153943
C	-1.210783	0.872051	0.419131	C	-1.206074	-0.699100	-0.195042
C	-1.193972	-0.522960	0.328975	C	-1.206006	0.699123	-0.195405
C	0.000004	-1.253339	0.171500	C	0.000142	1.438384	-0.154644
N	2.359053	-1.295314	0.234668	N	2.361999	1.495200	-0.197938
N	-2.359045	-1.295304	0.234670	N	-2.361743	1.495437	-0.197890
N	-2.418810	1.599749	0.468443	N	-2.361838	-1.495383	-0.197834
N	2.418833	1.599736	0.468439	N	2.361754	-1.495689	-0.198080
O	0.000001	-2.553470	-0.045903	O	0.000220	2.738142	-0.175421
O	0.000014	2.907951	0.570293	O	-0.000116	-2.738320	-0.174590
C	-2.613697	-2.396684	1.066304	C	-2.614531	2.421290	-1.230278
C	-3.695027	-3.102652	0.446565	C	-3.605250	3.321831	-0.711195
C	-4.008208	-2.451936	-0.783671	C	-3.845526	2.985019	0.647744
C	-3.091097	-1.352131	-0.942961	C	-2.967231	1.885816	0.991008
C	-2.850421	2.336789	-0.610602	C	-2.967785	-1.885712	0.990811
C	-3.908543	3.245744	-0.124812	C	-3.845950	-2.984812	0.647220
C	-4.046050	3.040835	1.248292	C	-3.605288	-3.321502	-0.711792
C	-3.063272	2.002743	1.669138	C	-2.614542	-2.421038	-1.230420
C	2.613701	-2.396694	1.066303	C	2.614771	2.421100	-1.230423
C	3.695028	-3.102668	0.446565	C	3.605409	3.321649	-0.711312
C	4.008212	-2.451953	-0.783671	C	3.845868	2.984711	0.647583
C	3.091107	-1.352144	-0.942962	C	2.967658	1.885417	0.990826
C	3.063317	2.002704	1.669131	C	2.614095	-2.421578	-1.230622
C	4.046030	3.040864	1.248303	C	3.604841	-3.322108	-0.711993
C	3.908546	3.245752	-0.124808	C	3.845717	-2.985349	0.646944
C	2.850447	2.336775	-0.610605	C	2.967668	-1.886152	0.990545
C	-4.391804	-4.253259	0.836186	C	-4.255296	4.413157	-1.297472
C	-5.390904	-4.730169	-0.000419	C	-5.148331	5.136826	-0.517484
C	-5.702671	-4.081769	-1.216065	C	-5.394981	4.792378	0.827649
C	-5.013671	-2.945043	-1.618818	C	-4.741291	3.719325	1.423850
C	-4.692829	4.161682	-0.807779	C	-4.742008	-3.719165	1.422965
C	-5.630983	4.881590	-0.061086	C	-5.395638	-4.792087	0.826510
C	-5.769602	4.677168	1.315470	C	-5.148647	-5.136410	-0.518634
C	-4.975218	3.746223	1.994020	C	-4.255359	-4.412787	-1.298296
C	4.391800	-4.253277	0.836187	C	4.255410	4.413061	-1.297528
C	5.390899	-4.730192	-0.000417	C	5.148538	5.136625	-0.517558
C	5.702669	-4.081794	-1.216064	C	5.395357	4.792036	0.827506
C	5.013674	-2.945065	-1.618818	C	4.741717	3.718916	1.423660
C	4.975139	3.746313	1.994047	C	4.254676	-4.413497	-1.298529
C	5.769507	4.677277	1.315503	C	5.147995	-5.137176	-0.518939
C	5.630920	4.881667	-0.061062	C	5.395205	-4.792789	0.826138
C	4.692815	4.161709	-0.807768	C	4.741784	-3.719750	1.422624
O	2.434404	2.214051	-1.756193	O	2.702367	-1.384769	2.099325
O	2.833214	1.559770	2.754906	O	1.972892	-2.438053	-2.314376
O	2.877593	-0.589912	-1.917737	O	2.702319	1.383939	2.099517
O	1.945163	-2.657582	2.112209	O	1.974162	2.437561	-2.314328
O	-2.877579	-0.589899	-1.917735	O	-2.701621	1.384517	2.099646
O	-1.945160	-2.657575	2.112210	O	-1.974070	2.437805	-2.314269
O	-2.833227	1.559754	2.754902	O	-1.973547	-2.437434	-2.314428
O	-2.434380	2.214062	-1.756190	O	-2.702552	-1.384253	2.099605
H	-4.148635	-4.754509	1.775332	H	-4.062079	4.679066	-2.338701
H	-5.948602	-5.625930	0.282646	H	-5.671485	5.992124	-0.951522
H	-6.496378	-4.485837	-1.848282	H	-6.106399	5.383252	1.408617
H	-5.243526	-2.444187	-2.561601	H	-4.914814	3.454480	2.468868
H	-4.574236	4.311678	-1.882455	H	-4.915774	-3.454408	2.467968
H	-6.266544	5.617138	-0.559193	H	-6.107259	-5.382961	1.407224
H	-6.511509	5.257164	1.869153	H	-5.671773	-5.991610	-0.952905
H	-5.073319	3.578010	3.068271	H	-4.061951	-4.678638	-2.339506
H	4.148628	-4.754525	1.775333	H	4.062093	4.679103	-2.338705
H	5.948592	-5.625955	0.282649	H	5.671649	5.991969	-0.951563
H	6.496375	-4.485866	-1.848280	H	6.106852	5.382842	1.408446
H	5.243532	-2.444211	-2.561601	H	4.915339	3.453949	2.468631
H	5.073222	3.578116	3.068302	H	4.061084	-4.679400	-2.339690
H	6.511376	5.257311	1.869196	H	5.670963	-5.992462	-0.953229
H	6.266462	5.617235	-0.559163	H	6.106839	-5.383699	1.406800
H	4.574238	4.311690	-1.882448	H	4.915725	-3.454960	2.467587
Zn	0.000001	-3.021385	1.849927	Zn	0.000154	2.990258	-2.170882
Zn	1.188737	0.535984	-2.179643	Zn	-0.000621	-2.988295	-2.169654
Zn	-1.188717	0.535992	-2.179639	Zn	1.206874	-0.000515	2.441750
				Zn	-1.206300	-0.000449	2.441777

(f)

TPB-Zn5	Cartesian coordinates			TPB-Zn5	Cartesian coordinates		
C	1.444522	-0.787221	-0.201666	C	7.066132	-2.624447	-0.780558

C	0.162403	-1.341045	-0.127333	C	6.912921	-2.979818	0.576428
C	-0.988459	-0.528227	-0.015595	C	5.697380	-2.807888	1.228662
C	-0.795170	0.870691	-0.078325	C	-2.132796	-5.599864	-1.084780
C	0.484920	1.425252	-0.161297	C	-2.391707	-6.710840	-0.290031
C	1.643820	0.613182	-0.173410	C	-1.890687	-6.804915	1.023596
N	2.633473	-1.530293	-0.259261	C	-1.123889	-5.782024	1.574214
N	0.753171	2.802239	-0.186211	O	0.247065	-2.982159	2.163351
N	-1.984260	1.612429	-0.035921	O	-1.301642	-2.719278	-2.140784
N	-0.116264	-2.717587	-0.115633	O	2.774225	-1.869910	2.037905
O	2.834705	1.130830	-0.253827	O	3.239717	-0.808484	-2.412518
O	-2.174605	-1.048946	0.057884	O	0.600995	3.087681	2.115430
C	1.457048	3.397928	-1.250694	O	1.683243	2.814500	-2.342878
C	1.901895	4.672677	-0.758604	O	-2.723538	0.888596	-2.134093
C	1.549008	4.768303	0.613546	O	-1.940448	1.975588	2.261317
C	0.910009	3.523595	0.992264	H	2.892578	5.625176	-2.434843
C	-2.543020	2.035382	1.165497	H	3.494230	7.641144	-1.087908
C	-3.888845	2.436479	0.851211	H	2.853988	7.812854	1.297444
C	-4.147608	2.081266	-0.507260	H	1.614652	5.951747	2.422915
C	-2.951226	1.487265	-1.049889	H	-4.690309	3.256699	2.688208
C	3.533468	-1.398130	-1.336534	H	-6.906892	3.753382	1.648524
C	4.776761	-1.941067	-0.872451	H	-7.318511	3.258926	-0.748890
C	4.628664	-2.287425	0.498690	H	-5.567494	2.174826	-2.150626
C	3.289175	-1.920876	0.902848	H	6.127272	-1.825842	-2.564896
C	-0.951161	-3.301683	-1.088003	H	8.038307	-2.762924	-1.259493
C	-1.350572	-4.576083	-0.544252	H	7.766237	-3.390066	1.120807
C	-0.854347	-4.669187	0.780869	H	5.573930	-3.065820	2.282520
C	-0.165741	-3.426780	1.080803	H	-2.522886	-5.521801	-2.101603
C	2.612177	5.703459	-1.382500	H	-2.997221	-7.528342	-0.688174
C	2.941900	6.820241	-0.624607	H	-2.113939	-7.693388	1.618199
C	2.579825	6.918017	0.734526	H	-0.743619	-5.840100	2.596100
C	1.886994	5.890995	1.367249	Zn	2.962921	1.212315	-2.254580
C	-4.888105	3.016666	1.641353	Zn	-2.698175	-1.204031	-1.905286
C	-6.114566	3.290725	1.056188	Zn	0.942095	-1.030750	2.464495
C	-6.350392	3.003384	-0.311756	Zn	-0.074811	1.161972	2.506476
C	-5.384321	2.402999	-1.098073	Zn	-4.994638	-0.918557	-0.753910
C	6.009817	-2.102625	-1.515201				

Preparation of TPB Batteries

A CR2032 coin type TPB//Zn cell was assembled. The TPB monomer electrode was synthesized from 70 wt% TPB powder, 20 wt% carbon black and 10 wt% polyvinylidene fluoride coated on a 12 mm titanium foil with an active material loading mass of about 0.4 mg cm^{-2}. The cell anode was made of pure Zn foil (12 mm), the electrolyte was 2 M $Zn(OTf)_2$, and the diaphragm was made of 16 mm fiberglass membrane (GF/A1820).A CR2032 coin-type TPB//Zn cell was assembled and subjected to a constant-current charge/discharge (GCD) test using a battery test system (LAND MTI-5 V 10 mA) with cutoff voltages set at 0.2 V and 1.6 V to evaluate the charge/discharge performance of the cells. All electrochemical tests were performed at room temperature.

The diffusion coefficient (D) is obtained from the following equation:

$$D = \frac{4L^2}{\pi\tau}\left(\frac{\Delta Es}{\Delta Et}\right)^2$$

where τ (s) is the constant current pulse time. The L is diffusion length (cm) of Zn^{2+}, which is equal to thickness of electrode. The ΔEs is the steady-state voltage change caused by the current pulse. The ΔEt are voltage changes during the constant current pulse.

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