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

A novel aqueous ammonium dual-ion battery based on organic polymers

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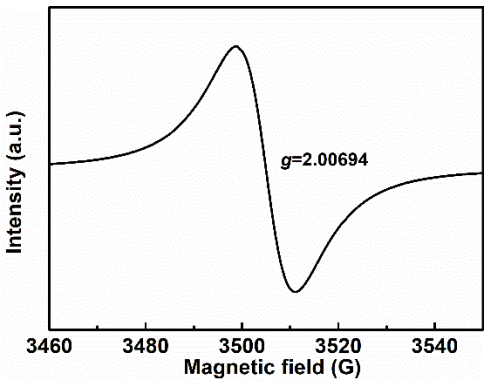

Fig. S1 ESR spectrum of the powder sample of PTMA.

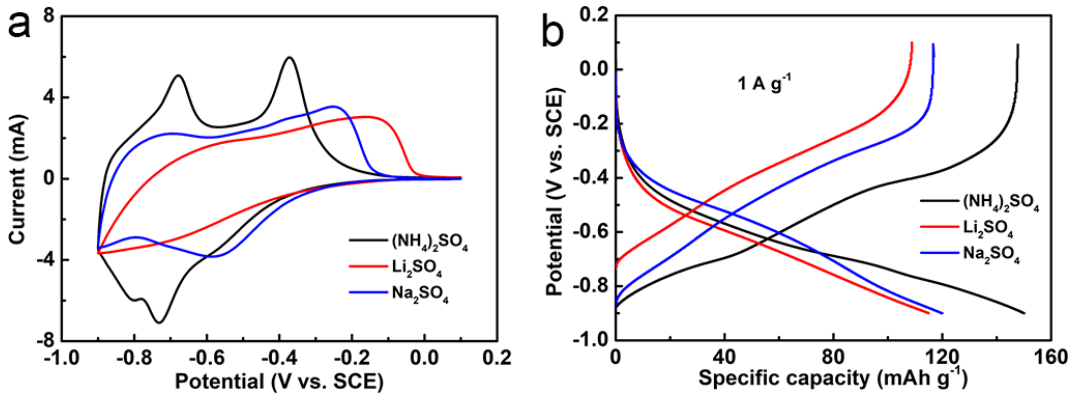

Fig. S2. (a) CV curves of PI anode in different electrolytes with a scan rate of 2 mV s^{-1}, and (b) charge-discharge curves of PI anode in different electrolytes with a current density of 1 A g^{-1}.

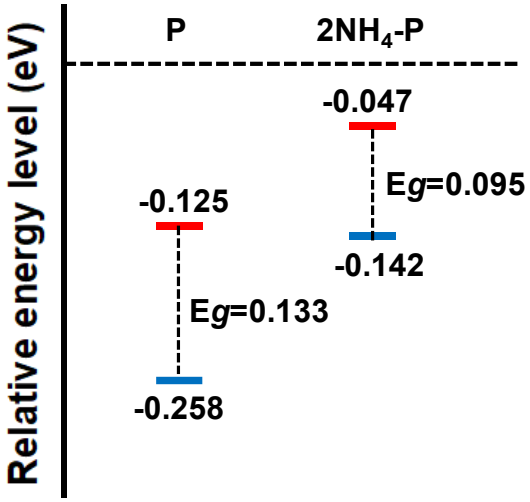

Fig. S3. The HOMO-LUMO gap for P and $2NH_4$-P.

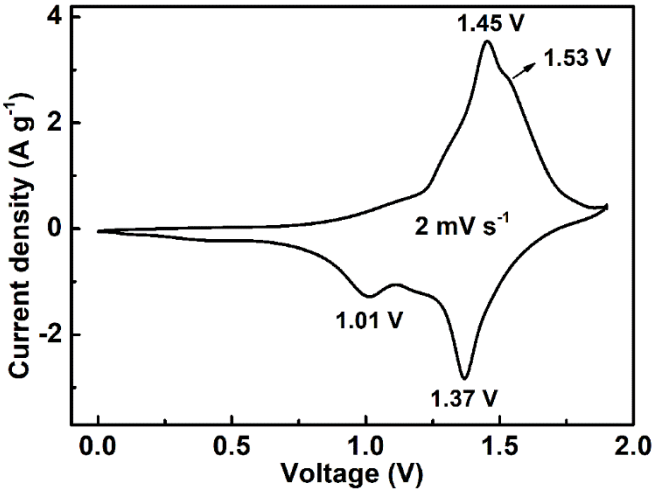

Fig. S4. CV curve of PI//PTMA ADIB at a scan rate of 2 mV s^{-1}.

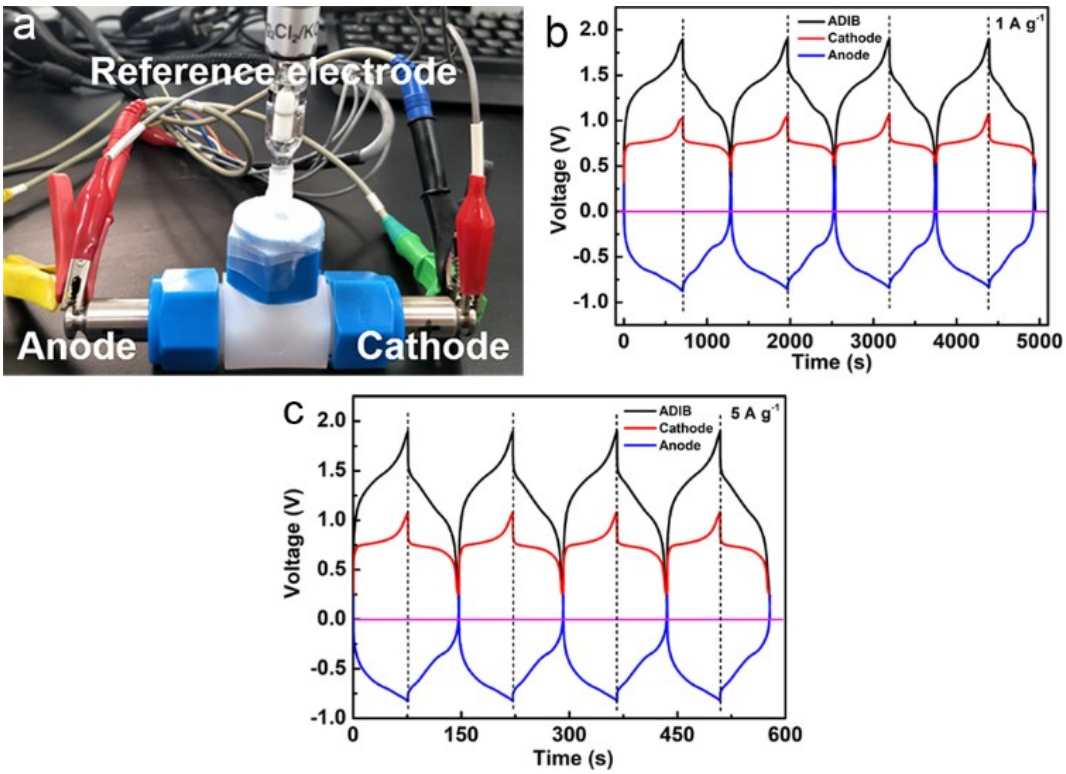

Fig. S5. (a) Photograph of SwagelokTM T-cell for the real-time investigation of voltage, and (b, c) the relationship between voltages of PI anode, PTMA cathode and full ADIB and test time at current densities of 1 A g^{-1} and 5 A g^{-1}, respectively.

Table S1. Cartesian coordinates (in Å) for optimized structures of P, NH_4^+ and $2NH_4$-P at M06/6-31+G(d, p).

P:

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.40375	1.23647	1.10E-05
2	6	0	0.71046	0.00189	4.00E-06
3	6	0	-0.71046	-0.00189	6.00E-06
4	6	0	-1.4091	1.22921	0
5	6	0	-0.71018	2.42569	1.00E-06
6	6	0	0.69771	2.42918	1.10E-05
7	6	0	1.4091	-1.22921	1.00E-05
8	6	0	0.71018	-2.42569	7.00E-06
9	6	0	-0.69771	-2.42918	-5.00E-06
10	6	0	-1.40375	-1.23647	-4.00E-06
11	6	0	-2.89173	-1.25924	-5.00E-06

12	7	0	-3.53722	-0.01067	8.00E-06
13	6	0	-2.89552	1.23624	-1.00E-06
14	6	0	2.89173	1.25924	8.00E-06
15	7	0	3.53722	0.01067	-7.00E-06
16	6	0	2.89552	-1.23624	1.70E-05
17	8	0	-3.55004	2.26812	-3.00E-05
18	8	0	-3.52417	-2.30457	-1.90E-05
19	8	0	3.52417	2.30457	1.10E-05
20	8	0	3.55004	-2.26812	1.30E-05
21	6	0	5.00546	-0.0182	-3.80E-05
22	6	0	-5.00546	0.01819	1.90E-05
23	1	0	-1.26964	3.35513	-5.00E-06
24	1	0	1.25208	3.36153	1.70E-05
25	1	0	1.26964	-3.35513	1.30E-05
26	1	0	-1.25208	-3.36153	-1.40E-05
27	1	0	5.35677	1.01082	-1.38E-04
28	1	0	5.36372	-0.54747	0.88598
29	1	0	5.36365	-0.54765	-0.88597
30	1	0	-5.35677	-1.01083	1.04E-04
31	1	0	-5.36367	0.54763	0.88595
32	1	0	-5.36371	0.54748	-0.886
1	6	0	1.40375	1.23647	1.10E-05

NH_4^+:

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	7	0	9E-6	8E-6	4E-6
2	1	0	0.13318	-0.7729	-0.6634
3	1	0	-0.32727	0.8324	-0.50519
4	1	0	-0.69778	-0.26954	0.70402
5	1	0	0.89181	0.20999	0.46453

$2NH_4$-P:

Center number	Atomic number	Atomic type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.92787	1.61172	0.19627
2	6	0	-0.67215	0.24968	-0.03088
3	6	0	0.67811	-0.24453	0.03919
4	6	0	1.7392	0.67346	0.3405
5	6	0	1.42286	2.0461	0.63864
6	6	0	0.13965	2.49664	0.55691
7	6	0	-1.73313	-0.66876	-0.33111
8	6	0	-1.41658	-2.04093	-0.62995
9	6	0	-0.13302	-2.49086	-0.55053

10	6	0	0.93425	-1.60611	-0.18961
11	6	0	2.27835	-2.1342	-0.09716
12	7	0	3.29129	-1.16021	0.1601
13	6	0	3.04337	0.17251	0.33873
14	6	0	-2.27092	2.14039	0.10059
15	7	0	-3.28481	1.16563	-0.15263
16	6	0	-3.03742	-0.16702	-0.32922
17	8	0	2.58765	-3.32069	-0.24224
18	8	0	-4.13526	-0.91233	-0.50948
19	8	0	-2.58041	3.32702	0.24294
20	8	0	4.13949	0.91938	0.52365
21	6	0	4.67984	-1.63283	0.202
22	6	0	-4.6734	1.63853	-0.191
23	1	0	-5.25843	1.1536	0.59442
24	1	0	-5.12562	1.40322	-1.15721
25	1	0	-4.63837	2.71475	-0.03555
26	1	0	5.12438	-1.41237	1.17541
27	1	0	5.27059	-1.13503	-0.57079
28	1	0	4.64679	-2.70662	0.03013
29	1	0	-2.20771	-2.70161	-0.96819
30	1	0	2.21447	2.70593	0.97814
31	1	0	0.12721	-3.51771	-0.78332
32	1	0	-0.12014	3.52412	0.7875
33	7	0	-4.04838	-3.25356	0.89107
34	1	0	-3.09436	-3.44795	1.19445
35	1	0	-4.61266	-3.1217	1.72937
36	1	0	-4.39227	-4.09494	0.43008
37	1	0	-4.03959	-1.82326	-0.08032
38	7	0	4.00571	3.21242	-0.94873
39	1	0	4.57413	3.10432	-1.78767
40	1	0	4.05432	1.81748	0.06452
41	1	0	3.0386	3.33661	-1.2476
42	1	0	4.29352	4.08145	-0.50128
1	6	0	-0.92787	1.61172	0.19627

Table S2. The comparation of oxidation and reduction peaks of anode, cathode and full ADIB at a scan rate of 2 mV s^{-1}.

	Oxidation peaks (V)		Reduction peaks (V)	
Anode	-0.67	-0.37	-0.70	-0.79

Cathode	0.78		0.68	
Theoretical ADIB	1.48	1.57	1.35	1.05
Practical ADIB	1.45	1.53	1.37	1.01
Difference values	0.03	0.04	-0.02	0.04

Table S3. A summary of some aqueous storage systems based on Li^+, Na^+ Mg^{2+} and NH_4^+.

System	Cell voltage (V)	Energy density (Wh kg^{-1})	Power density (kW kg^{-1})	Cycle stability (%)/cycle number	Ref.
PNFE//$LiMn_2O_4$	2.4	76.1	12. 610	65.5/1000	1
$NaTi_2(PO_4)_3$//$K_{0.27}MnO_2$	1.6	---	---	83/100	2
PNTCDA//PTPAn	2.1	52.8	32.0	85/700	3
PI/AC//$LiMn_2O_4$	1.75	51	---	89/450	4
PBN//polyimide	1.55	45	---	60/5000	5
PNTCDA//I^-/I_3^-	1.6 1.6	65.3 63.8	--- ---	70/50 000 70/50 000	6
Polyimide//$LiMn_2O_4$	2.5	48.93	10.217	98/1000	7
PTCDI//$(NH_4)_{1.47}Ni[Fe(CN)_6]_{0.88}$	1.9	43	---	67/1000	8
Mo_6S_8// $LiMn_2O_4$	2.3	84	---	68/1000	9
PI//PTMA	1.9	51.3	15.8	86.3/10 000	This

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