Supporting Information

High-Performance Rechargeable Aqueous Zn-Ion Batteries with Poly(Benzoquinonyl Sulfide) Cathode

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Calculations Methods

Density functional theory (DFT) calculations were performed with Gaussian 16 software package.[1]

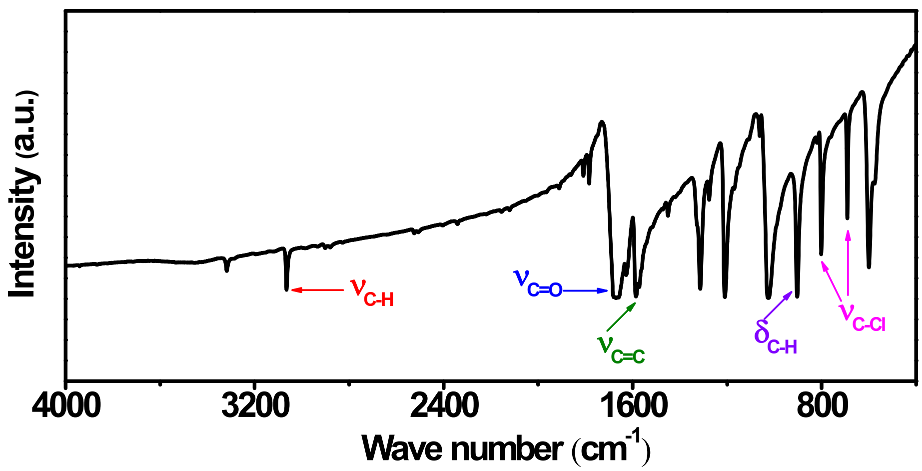

Fig. S1 IR spectrum of 2,5-dichloro-1,4-benzoquinone (DCBQ).

The IR spectrum of 2,5-dichloro-1,4-benzoquinone indicates a high purity of the starting materials.

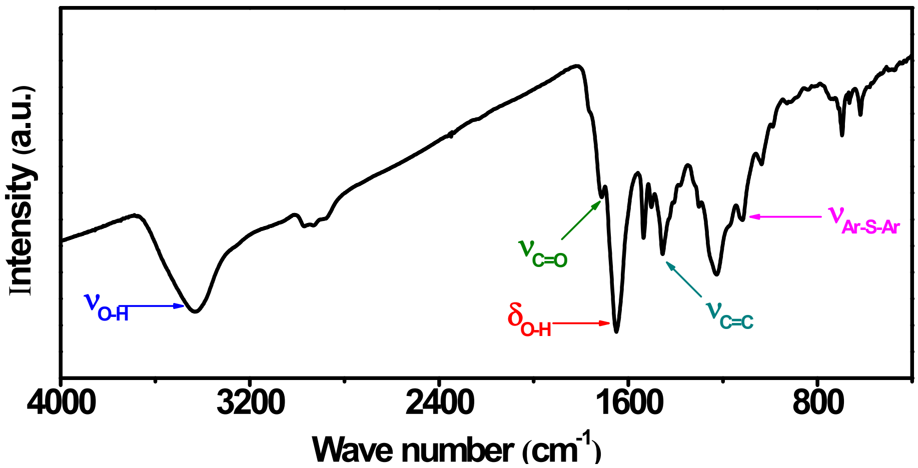

Fig. S2 The IR spectra of PBQS from 4000 to 400 cm^{-1}.

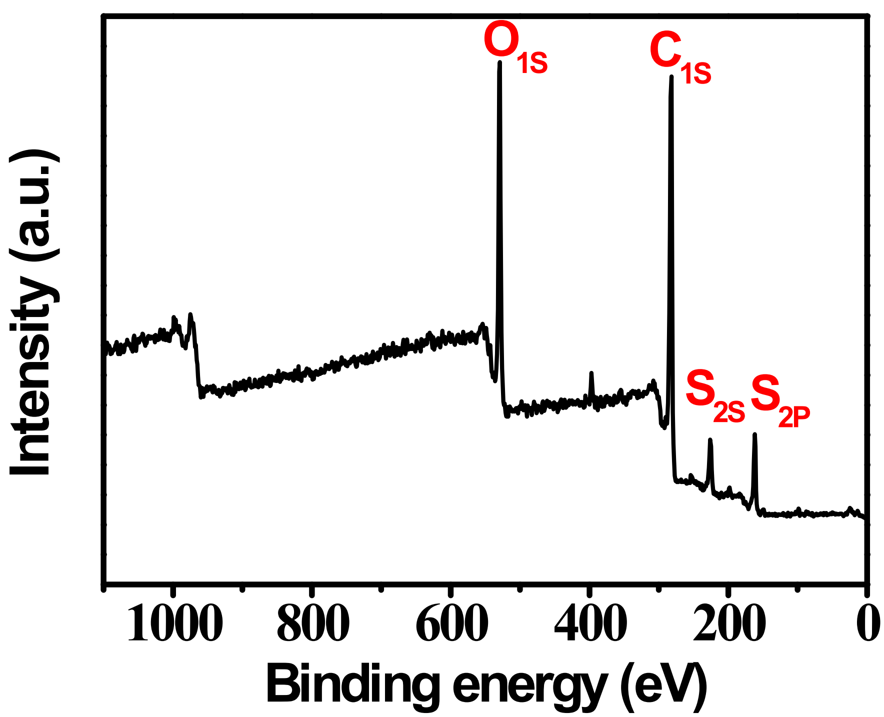

Fig. S3 Overall XPS spectra of PBQS.

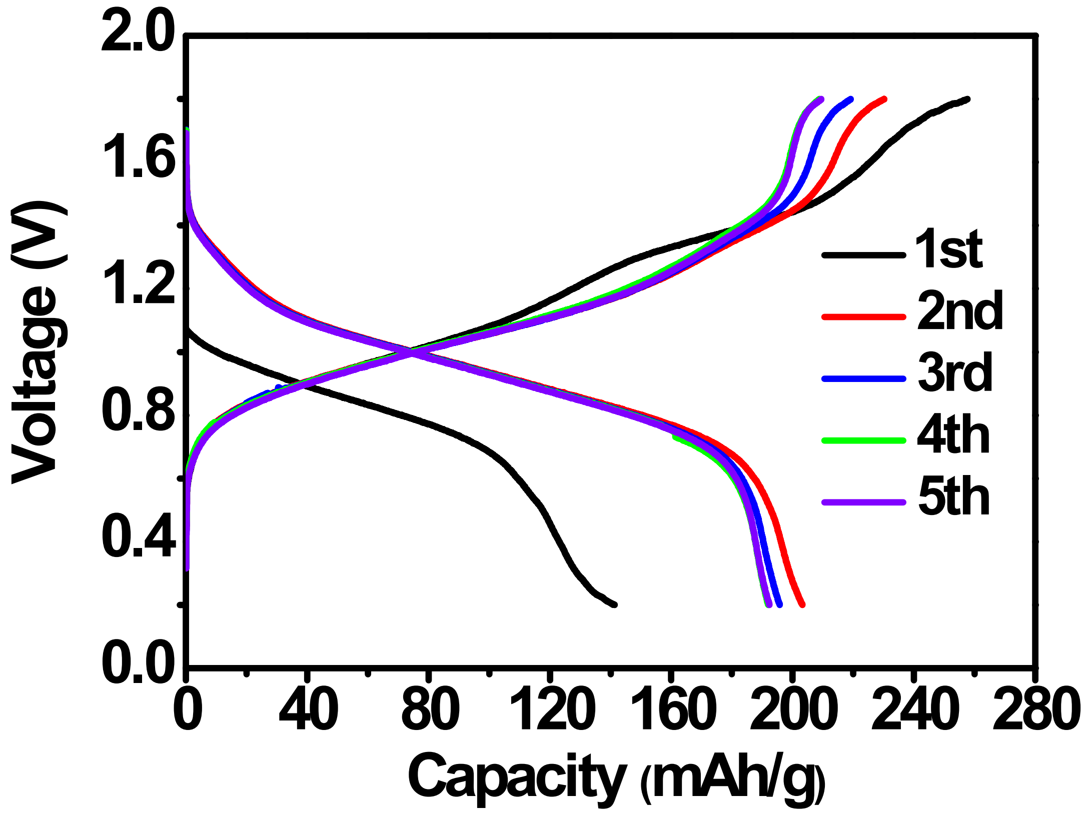

Fig. S4 Typical discharge/charge curves of Zn-PBQS batteries at 0.1 C rate for the first 5 cycles.

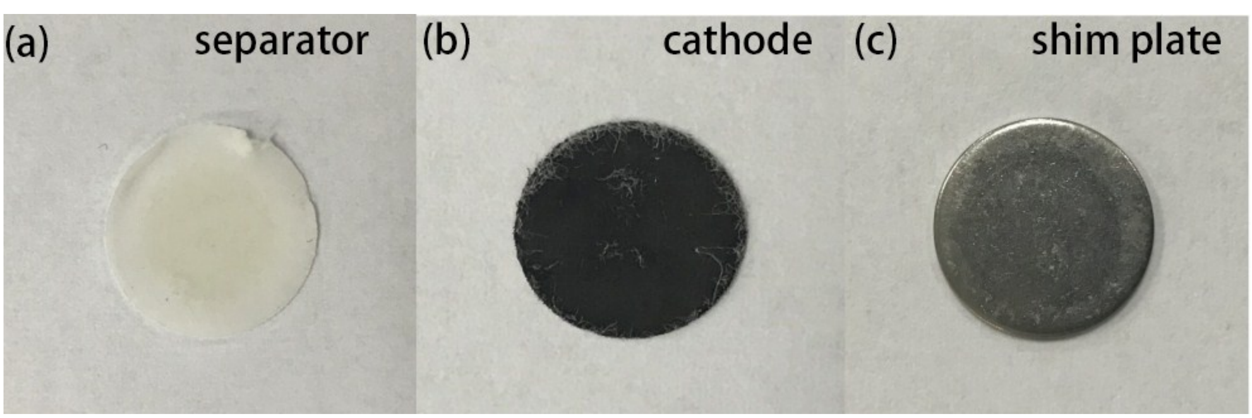

Fig. S5 Digital photographs of disassembled cell after 50 discharge/charge cycles.

The digital photographs were taken from the disassembled cell after 50 discharge/charge cycles. The separator became light yellow, indicating the slight dissolution of the electrode materials in the electrolyte. The surface of the Shim plate and the electrode were clean, further reflecting the slight dissolution of the electrode materials in the electrolyte.

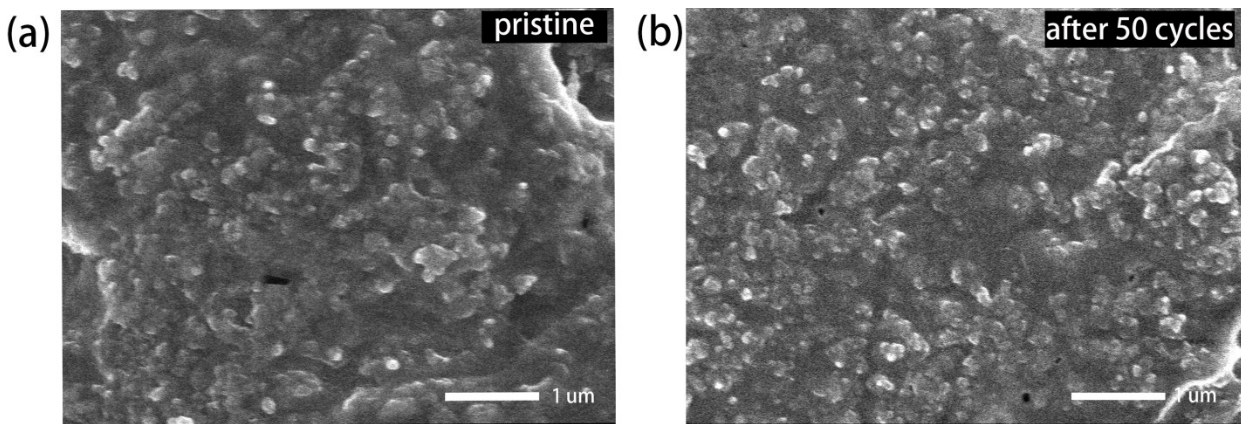

Fig. S6 SEM images of (a) fresh PBQS composite electrode and (b) PBQS composite electrode after 50 cycles.

The morphology of PBQS composite electrode remains almost unchanged after 50 cycles, indicating the stability of PBQS during the long discharge/charge cycles.

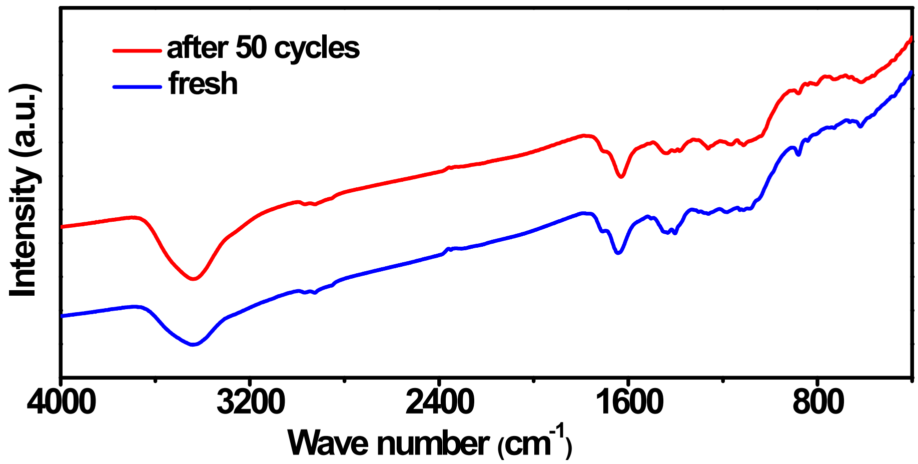

Fig. S7 IR spectra of fresh and cycled PBQS composite electrodes.

We have characterized the fresh and cycled PBQS composite electrodes (PBQS: Super P: PVDF= 6: 3: 1) respectively. The fresh electrode was tested as prepared. The cycled electrode was taken from the disassembled cell after 50 discharge/charge cycles. Before FTIR tests, the cycled electrode was rinsed with deionized water and dried in vacuum oven overnight. We have observed that the two spectra are almost the same, this result proves that the PBQS composite electrode is stable during the long discharge/charge cycles.

Table S1 Comparison of electrochemical performance of this work versus other related aqueous ZIBs with polymer cathode materials.

Polymers	Electrolyte	Capacity (mA h g^{-1})$^{\alpha}$	Voltage (V)	Energy density (W h kg^{-1})$^{\alpha}$	Ref.
PAnFc	0.5 M Na_2SO_4	124.0 (0.5 mA cm^{-2})	1.0	126.2	2
poly(aniline-co-*o*-aminophenol)	2.5 M $ZnCl_2$ + 3.0 M NH_4Cl	103.0 (0.5 mA cm^{-2})	-	120.4	3
PANI/Zn^{2+}	1.0 M $ZnCl_2$ + 2.0 M NH_4Cl	90.8 (25 mA g^{-1})	-	-	4
PANAB	2.0 M $ZnCl_2$+ 3.0 M NH_4Cl	134.0 (120 mA g^{-1})	1.08	144.1	5
poly(acetylene)-based polymer with exTTF moieties	1 M $Zn(BF_4)_2 \cdot 6H_2O$	128 (20 C)	1.1	140.8	6
PBQS	3M $Zn(CF_3SO_3)_2$	203 (0.1 C)	0.95	192.8	This work

$^{\alpha}$ Based on the active electrode materials.

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