Supporting Information

Performance improvement of aqueous zinc batteries by zinc oxide and Ketjen Black co-modifying glass fiber separators

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In this study, all calculations were employed with spin-polarized DFT framework and implemented by the DMol^3 mode in Materials Studio software[1, 2]. The generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerh (PBE) functional was adopted to depict the electronic exchange-correlation effects [3, 4]. The double numerical plus polarization (DNP) was chosen as the atomic orbital basis set. During the geometry optimization, the energy, force, and displacement convergence criteria were set to 2×10^{-5} Ha, 4×10^{-3} Ha Å^{-1}, and 5×10^{-3} Å, respectively. A $2 \times 2 \times 1$ Monkhorst-Pack grid was employed to execute the Brillouin-zone integrations. The (400) facets of ZnO and (100) facets of Zn were used during simulating. The adsorption energy (E_{ads}) was calculated by the following equation:

$$E_{ads} = E_{total} - E_{sub} - E_{Zn}$$

E_{total} represents the total energy of Zn(100) and ZnO(400) substrates combined with zinc atom. E_{sub} and E_{Zn} represent the energy of the substrate and the energy of zinc atom, respectively.

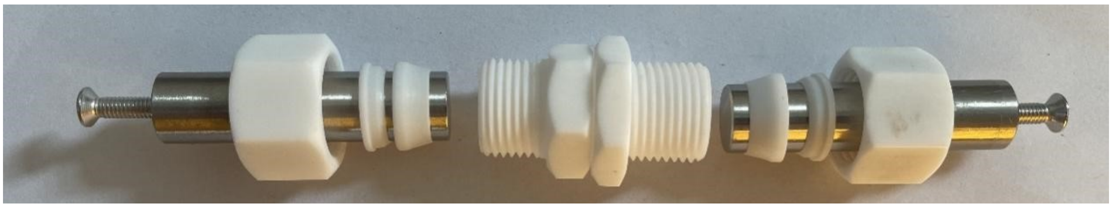

Fig. S1 The digital picture of the battery testing device used in this study.

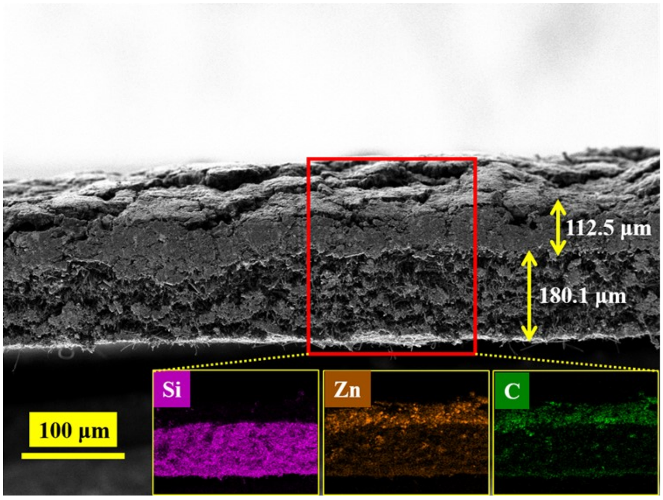

Fig.S2 the cross-section SEM image of the modified separator.

A cross-sectional SEM diagram of the modified separator has been added as requested by the reviewer, in Fig.S2. And this is described in the supporting information: The modified separator was put into the battery test device and sealed for 30 min, and then the cross-sectional SEM and EDS analysis were performed. The Si element belongs to glass fiber, and Zn and C belong to modified materials. It can be seen from the figure that a small amount of ZnO was found in the separator, but didn't penetrate through it, which is why the separator didn't cause a short circuit. According to the EDS results, the modified separator can be divided into two parts: 1) the separator with some ZnO and KB, with a thickness of 180.1 μm; 2) the modified layer of ZnO and KB not penetrated into the separator, with a thickness of 112.5 μm.

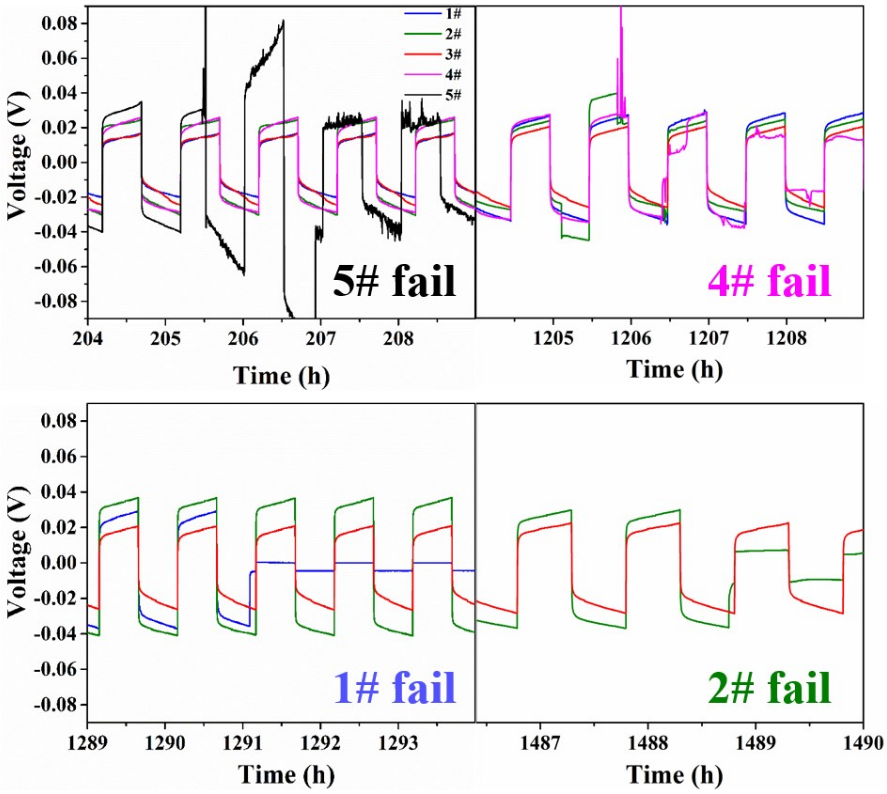

Fig. S3 The overpotential of 5#, 4#, 1# and 2# failed.

Table S1. The fitting results of EIS for different cells.

	R_e (Ω)	R_s (Ω)	R_{ct} (Ω)
Bare	0.792	3.9	226.8
ZnO	1.246	5.352	265.1
KB	0.353	0.7255	121.4
Zn//ZnO-KB//Zn (3#)	2.043	0.89	197.2

Table S2 The EIS fitting results of Bare Zn//MnO2 and Modified Zn//MnO_2

	Re(Ω)	Rct(Ω)
Bare Zn//MnO_2	1.15	96
Modified Zn//MnO_2	0.468	2.557

References

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4. J. P. Perdew and W. Yue, *Physical review. B, Condensed matter*, 1992, **45**, 13244-13249.