

Supplementary information

Molecule Chemistry Inducing Crystallographic Reorientation and Smart Interface to Boost Zinc-Iodine Battery Capacity

Ming Zhao^{1,2}, Yanqun Lv², Zhenhao Wang¹, Jun Qi¹, Yadong Du¹, Yangjun Ma¹, Qi Yang¹, Jieshan Qiu^{1,*}, Shimou Chen^{1,*}

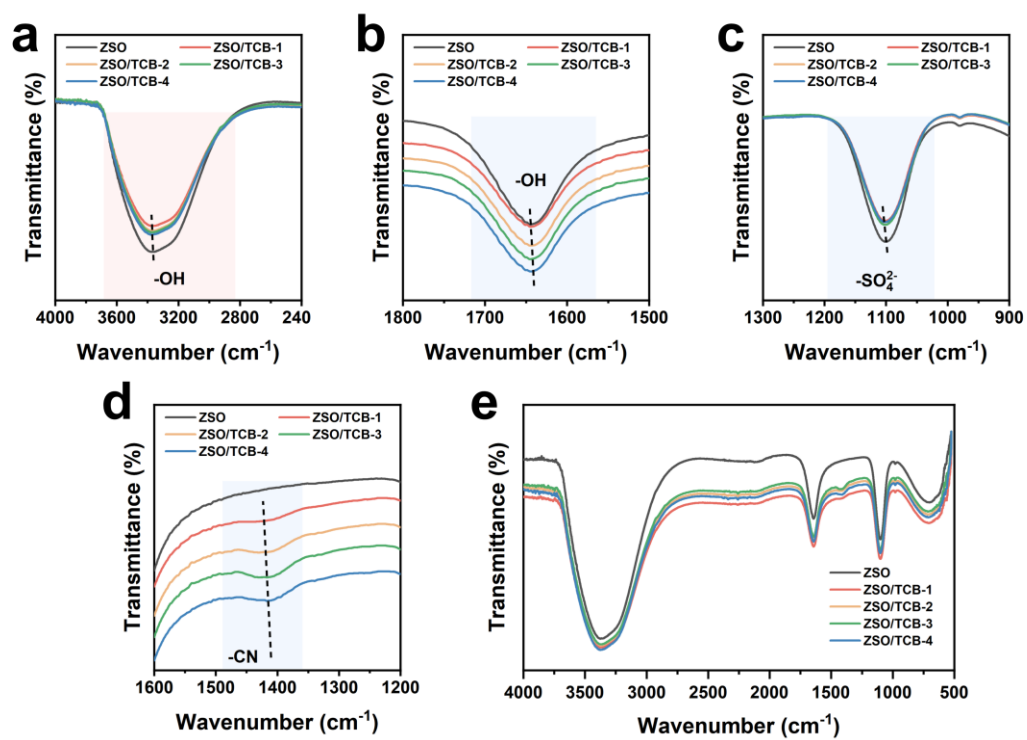
¹State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, P.R. China

²College of Chemical and Biological Engineering, Zhejiang University, Hangzhou 310058, P.R. China

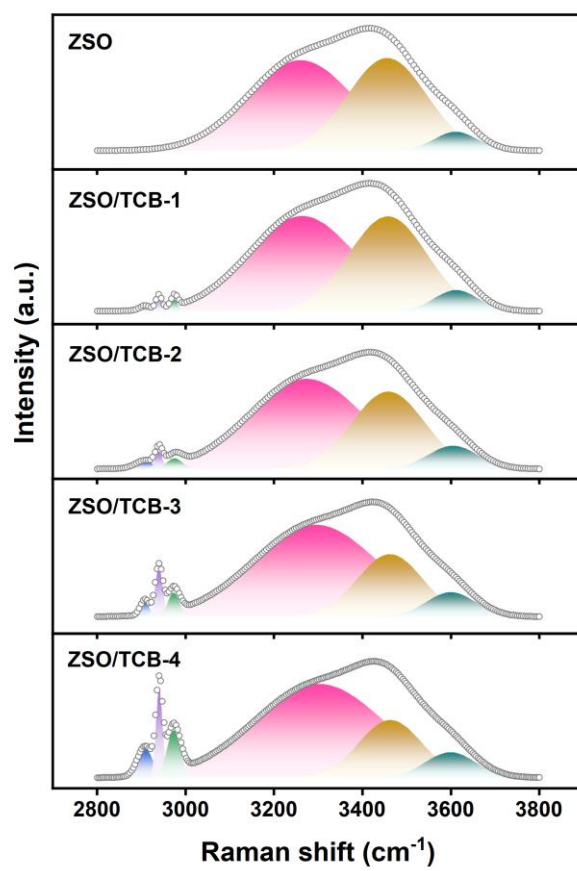
Corresponding author:

Jieshan Qiu (qiujs@mail.buct.edu.cn);

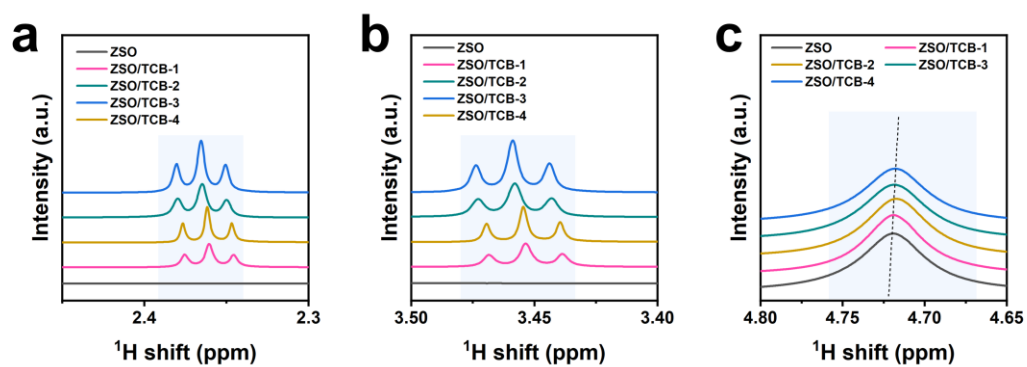
Shimou Chen (chensm@mail.buct.edu.cn)



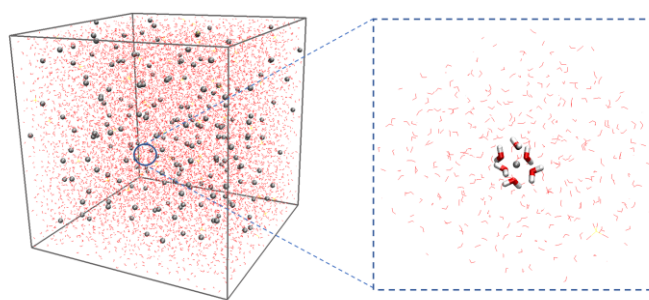
Supplementary Fig. 1 | FTIR spectra of the different electrolytes.



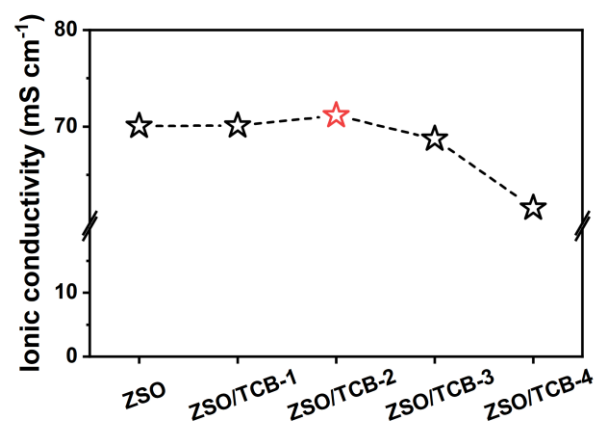
Supplementary Fig. 2 | Raman spectra of the different electrolytes.



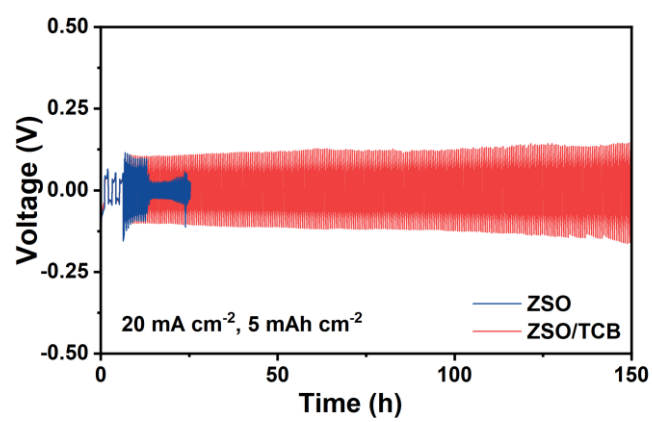
Supplementary Fig. 3 | H^1 NMR spectra of the different electrolytes.



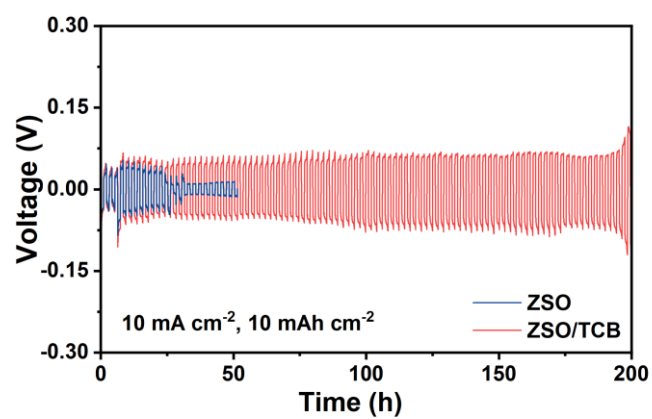
Supplementary Fig. 4 | 3D snapshot of the bare ZSO electrolyte system obtained MD simulation and a locally enlarged view of the Zn²⁺ solvation structure.



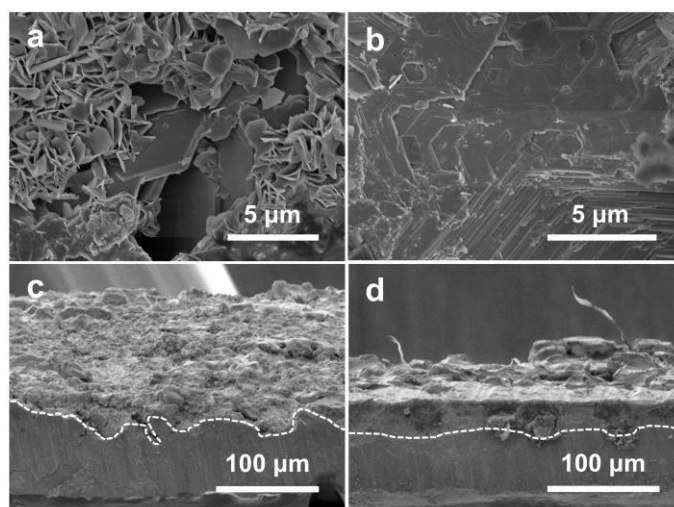
Supplementary Fig. 5 | Ionic conductivity of the different electrolytes.



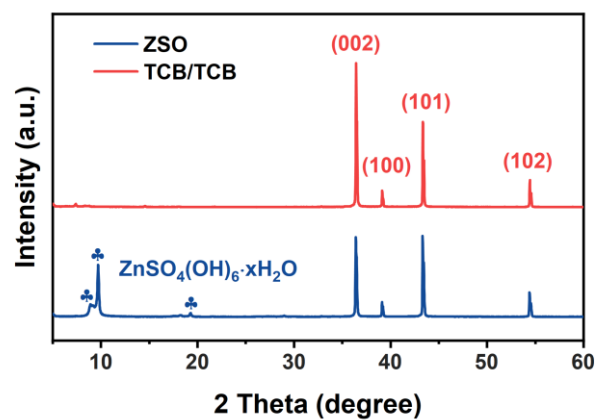
Supplementary Fig. 6 | Cycling performance of Zn symmetric batteries at 20 mA cm⁻² and 5 mAh cm⁻².



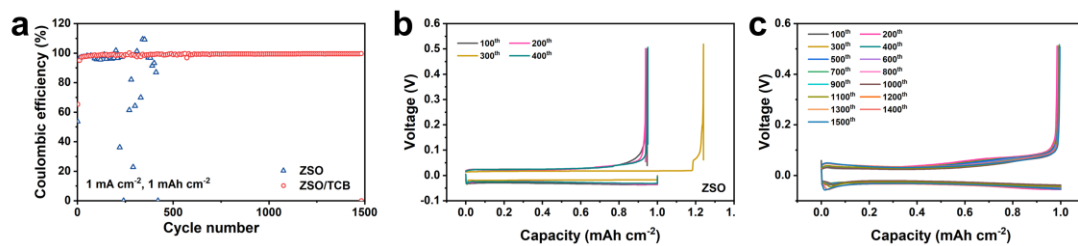
Supplementary Fig. 7 | Cycling performance of Zn symmetric batteries at 20 mA cm⁻² and 5 mAh cm⁻².



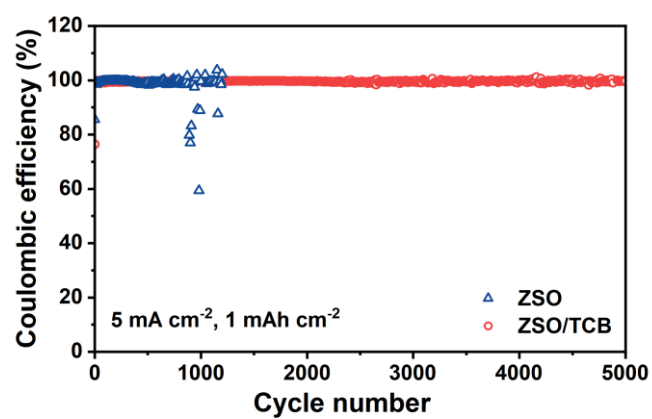
Supplementary Fig. 8 | SEM images of Zn anode after cycles.



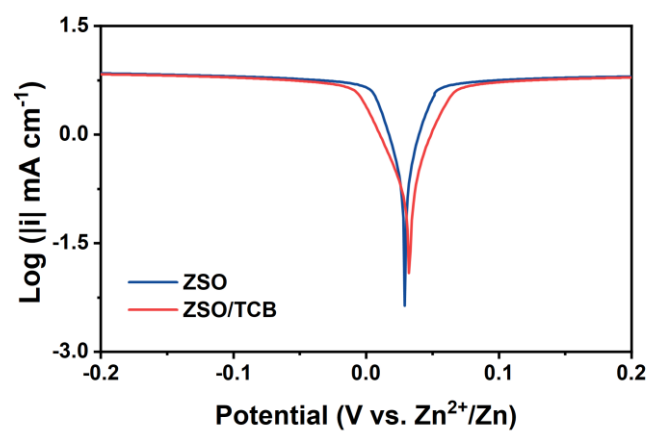
Supplementary Fig. 9 | XRD patterns of Zn anode after cycles.



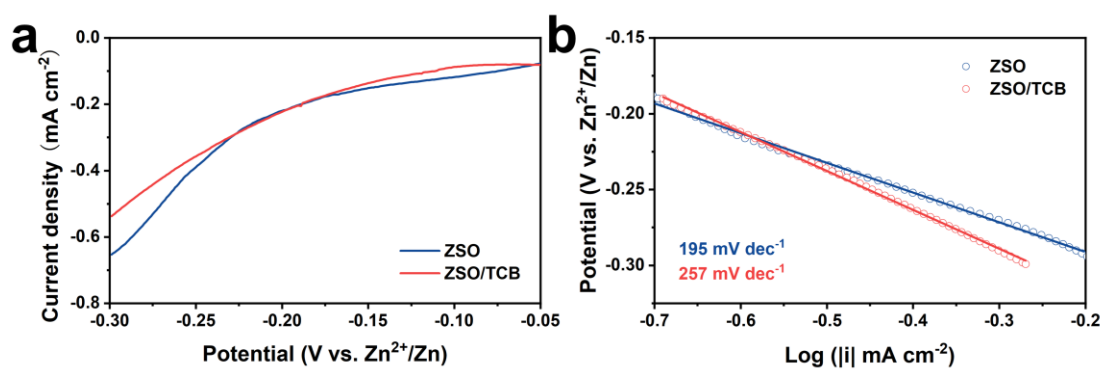
Supplementary Fig. 10 | a) The cycling performance of Zn//Cu batteries and b-c) corresponding voltage curves at 1 mA cm^{-2} and 1 mAh cm^{-2} .



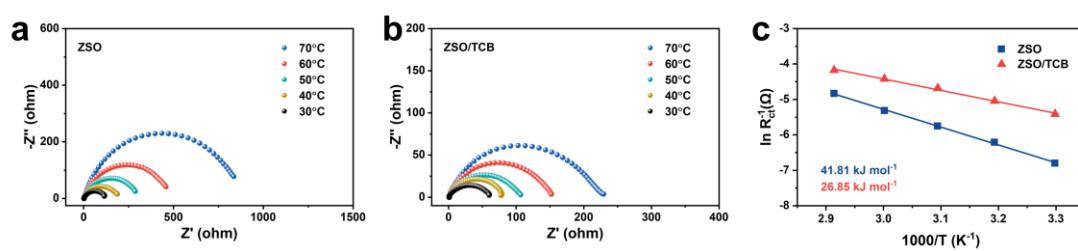
Supplementary Fig. 11 | The cycle performance of Zn//Cu batteries in different electrolytes.



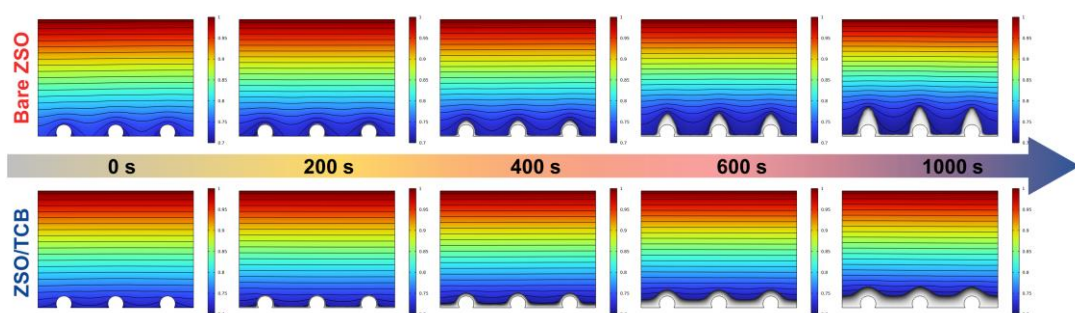
Supplementary Fig. 12 | The linear polarization curves of zinc anodes in different electrolytes.



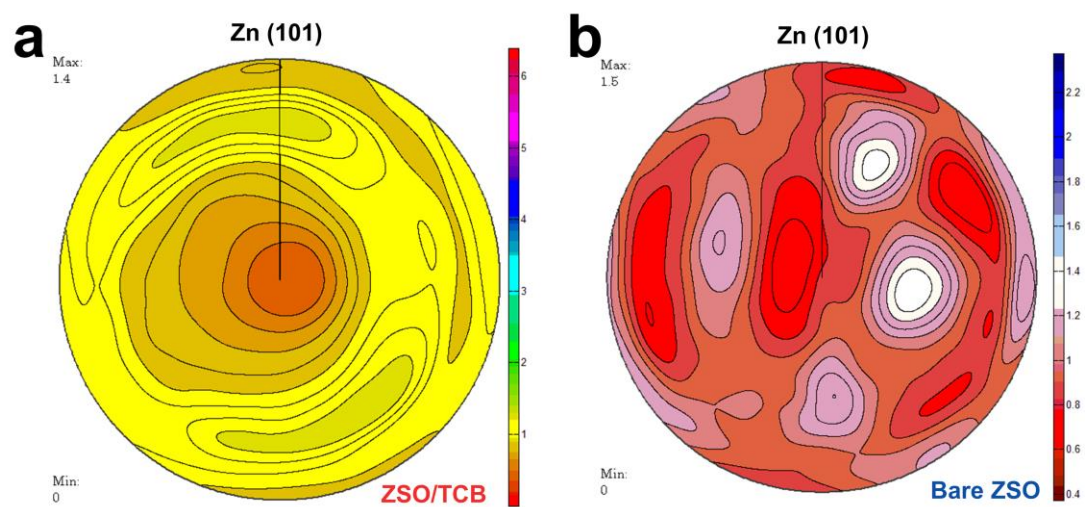
Supplementary Fig. 13 | a) HER analysis of the different electrolytes and b) corresponding Tafel curves.



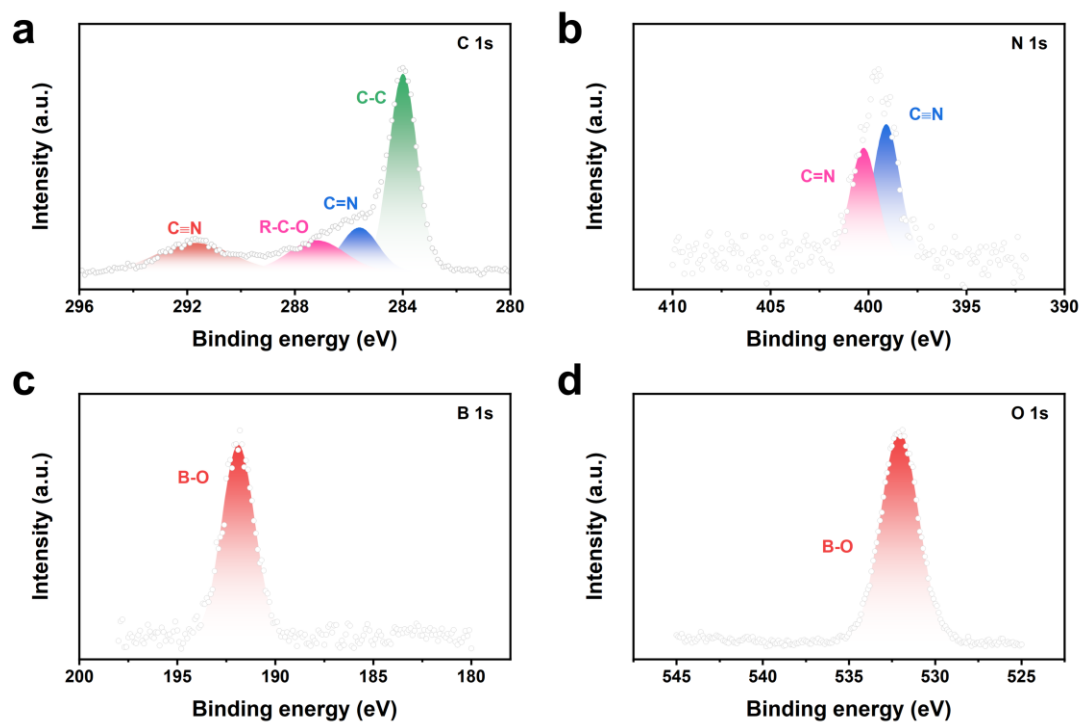
Supplementary Fig. 14 | a-b) Interface impedance of Zn symmetric batteries and c) the corresponding activation energies in different electrolytes.



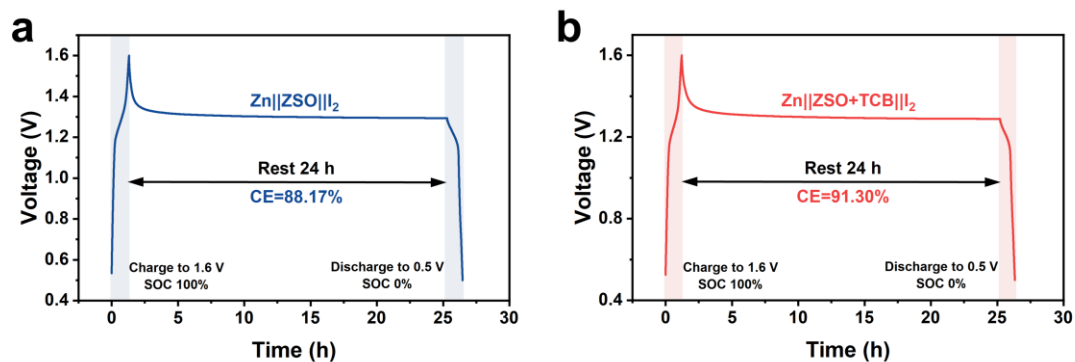
Supplementary Fig. 15 | Zn²⁺ concentration variation at Zn anode/electrolytes interface during Zn²⁺ deposition process by COMSOL simulation.



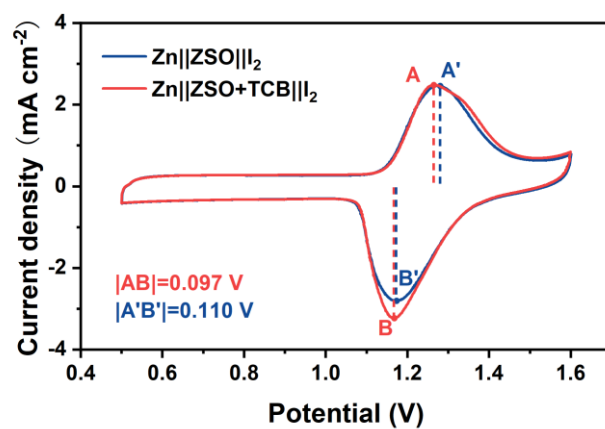
Supplementary Fig. 16 | Pore figures with (101) planes of Zn anodes in different electrolytes.



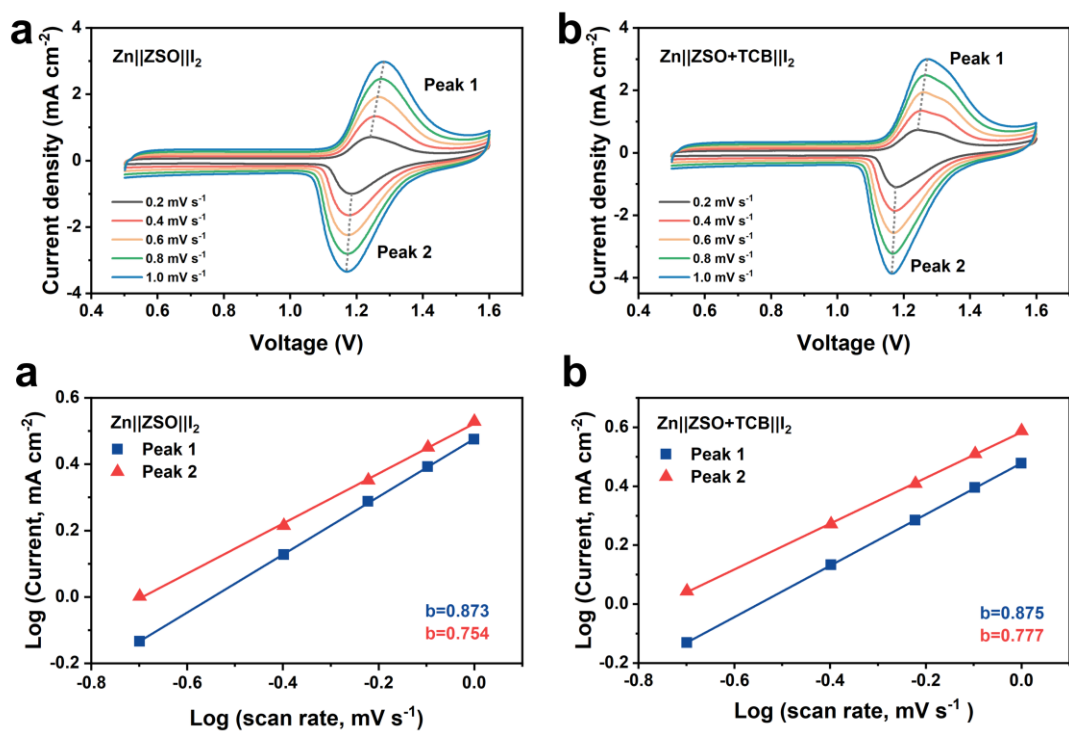
Supplementary Fig. 17 | XPS spectra of cathode surface after cycles.



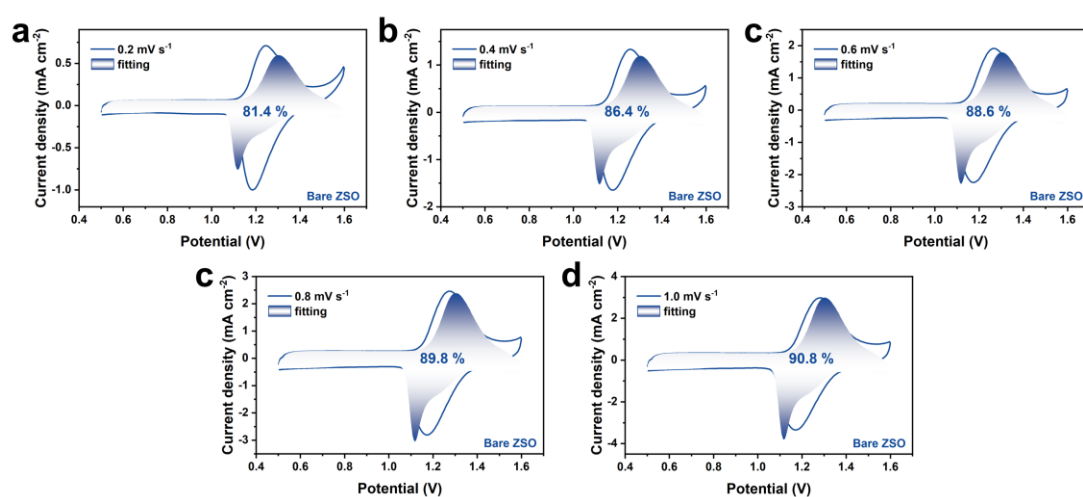
Supplementary Fig. 18 | Self-charge analysis of Zn//I₂ full battery in different electrolytes.



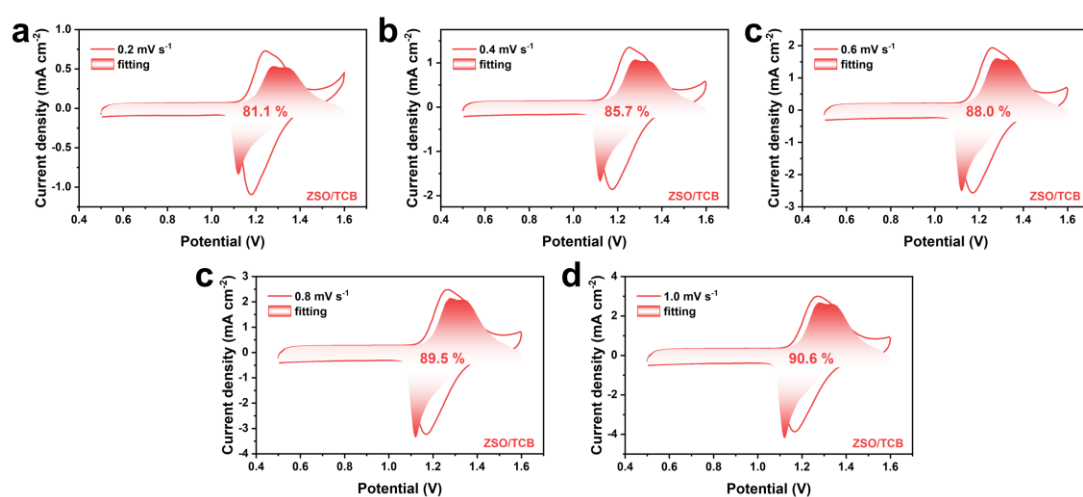
Supplementary Fig. 19 | CV curves of Zn//I₂ batteries in different electrolytes.



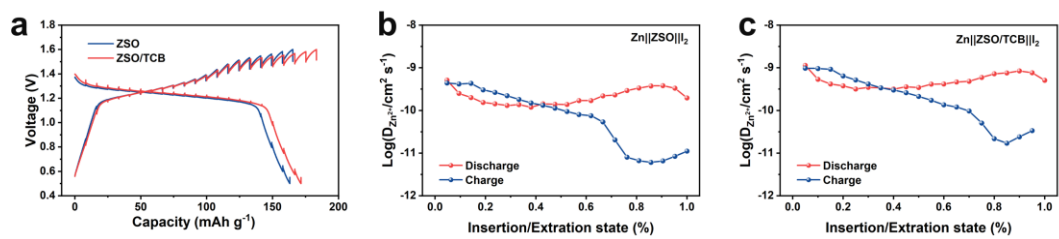
Supplementary Fig. 20 | (a-b) The CV curves of the full batteries at a scan rate from 0.2 mV s^{-1} to 1 mV s^{-1} . (c-d) Log (i) versus log (v) plots at specific peak currents of different full cells in different electrolytes.



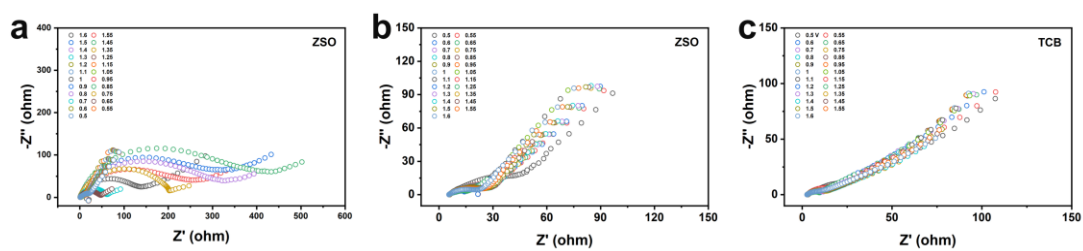
Supplementary Fig. 21 | The separation of the capacitive and diffusion-controlled current contribution at different currents in bare ZSO electrolytes.



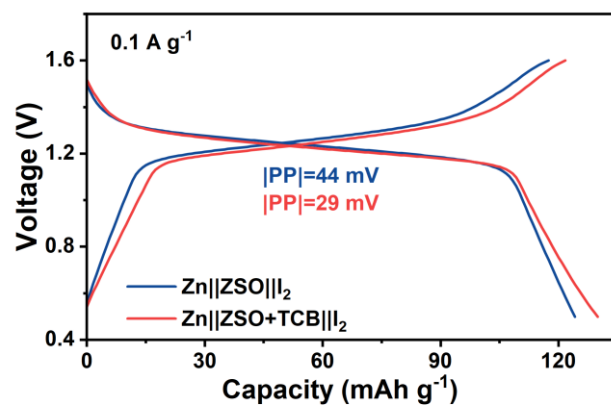
Supplementary Fig. 22 | The separation of the capacitive and diffusion-controlled current contribution at different currents in ZSO/TCB electrolytes.



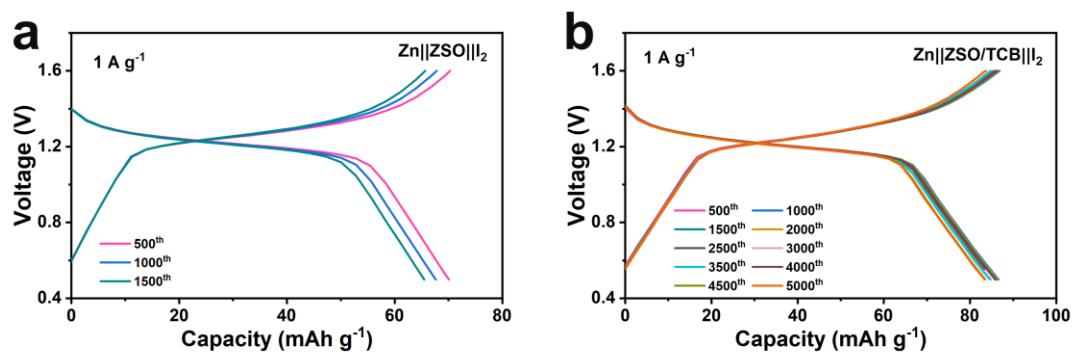
Supplementary Fig. 23 | (a) The GITT curves and (b-c) the corresponding diffusion coefficient of Zn//I₂ batteries in different electrolytes.



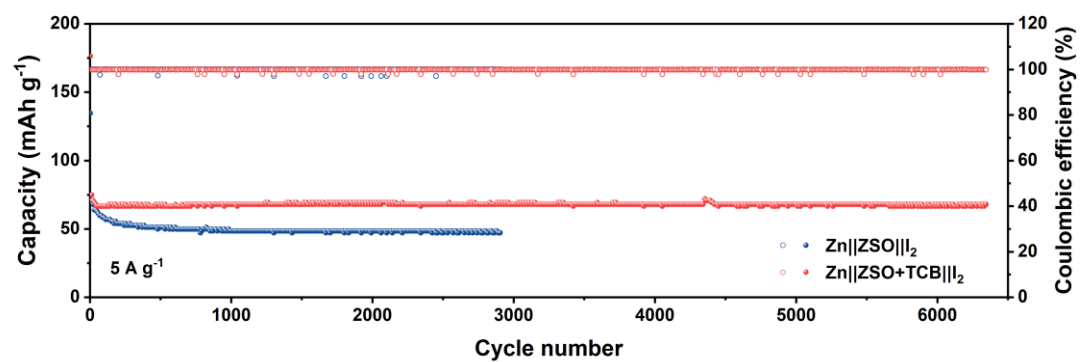
Supplementary Fig. 24 | EIS analysis of Zn/I₂ batteries during the charge-discharge process in (a-b) bare ZSO electrolytes and (c) ZSO/TCB electrolytes.



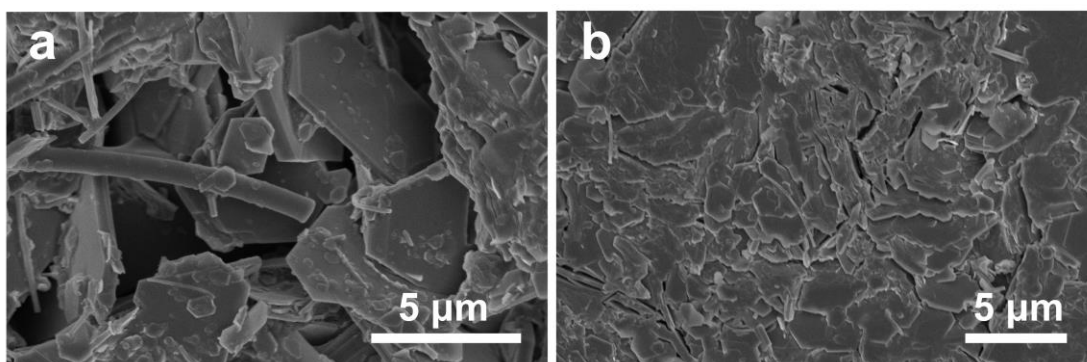
Supplementary Fig. 25 | The charge-discharge curves of Zn//I₂ batteries in different electrolytes.



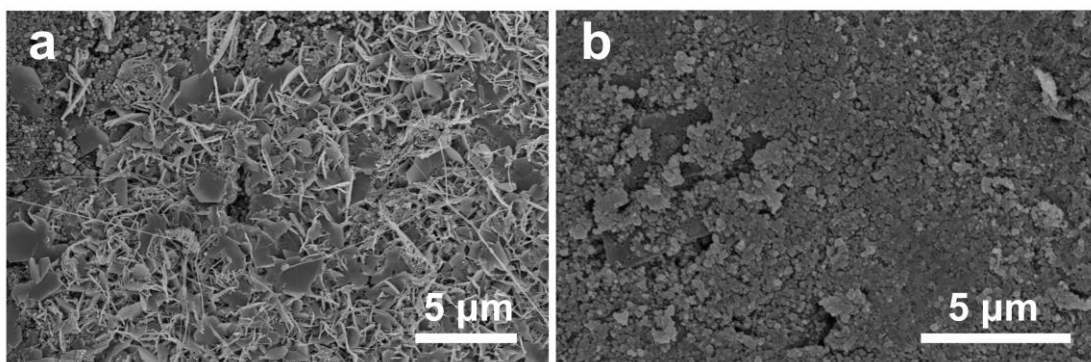
Supplementary Fig. 26 | The charge-discharge curves of $\text{Zn}||\text{I}_2$ batteries in different electrolytes.



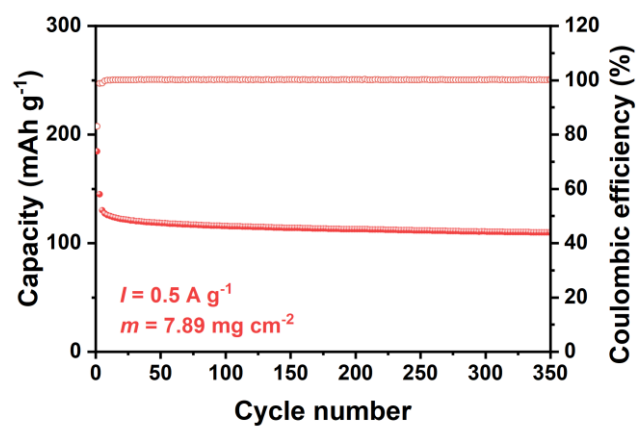
Supplementary Fig. 27 | The cycle performance of Zn//I₂ batteries in different electrolytes at 5 A g⁻¹.



Supplementary Fig. 28 | SEM images of Zn anode after cycles in (a) bare ZSO and (b) ZSO/TCB electrolytes.



Supplementary Fig. 29 | SEM images of I_2 cathode after cycles in (a) bare ZSO and (b) ZSO/TCB electrolytes.



Supplementary Fig. 30 | Cycle performance of Zn//I₂ battery in ZSO/TCB electrolyte at 0.5 A g⁻¹.