

Supplementary Materials

Multifunctional organic molecules as electron-buffering layers for stabilizing Zn anodes

Qu Yue^{1,2}, Junhui He¹, Yuhang Chen¹, Huaipu Zhu¹, Taotao Gao^{1,3}, Dan Xiao⁴,
Lu Qiu^{5,*}, Xiaoqin Li^{5,*}

¹School of Mechanical Engineering, Chengdu University, Chengdu 610106, Sichuan, China.

²Institute for Advanced Study, Chengdu University, Chengdu 610106, Sichuan, China.

³Key Laboratory of Fruit Waste Treatment and Resource Recycling of the Sichuan Provincial College, Neijiang Normal University, Neijiang 641100, Sichuan, China.

⁴College of Chemical Engineering, Sichuan University, Chengdu 610064, Sichuan, China.

⁵College of Food and Biological Engineering, Chengdu University, Chengdu 610106, Sichuan, China.

***Correspondence to:** Prof. Lu Qiu, Xiaoqin Li, College of Food and Biological Engineering, Chengdu University, Chengdu 610106, Sichuan, China. E-mail: qiulu@cdu.edu.cn; lixiaoqin@cdu.edu.cn

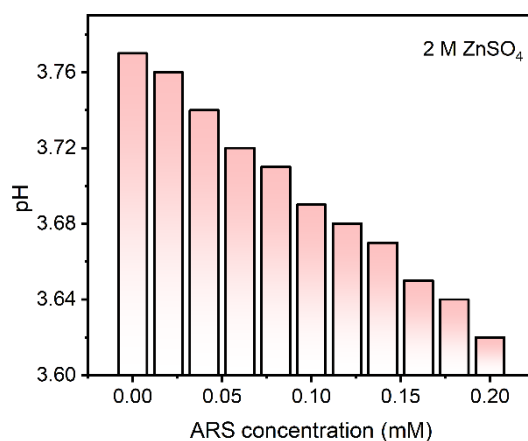


Figure S1. pH values of ZnSO₄ solution with different concentrations of ARS (0 ~ 0.2 mM).

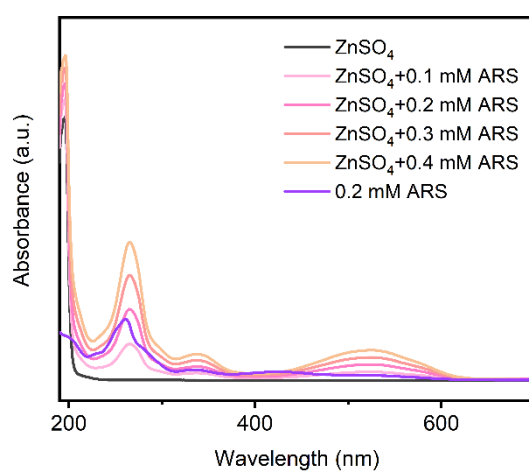


Figure S2. UV-Vis spectra of ZnSO₄ solution with different concentrations of ARS.

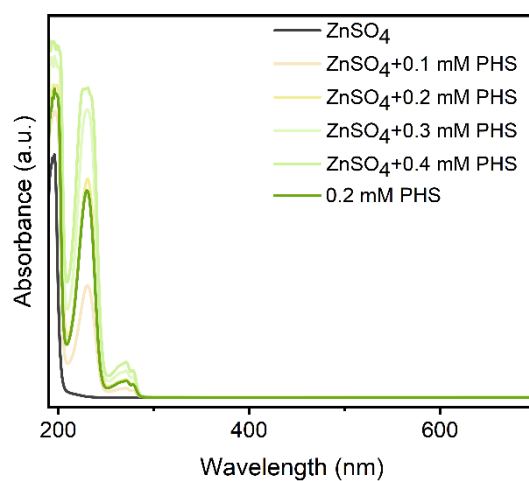


Figure S3. UV-Vis spectra of ZnSO₄ solution with different concentrations of PHS.

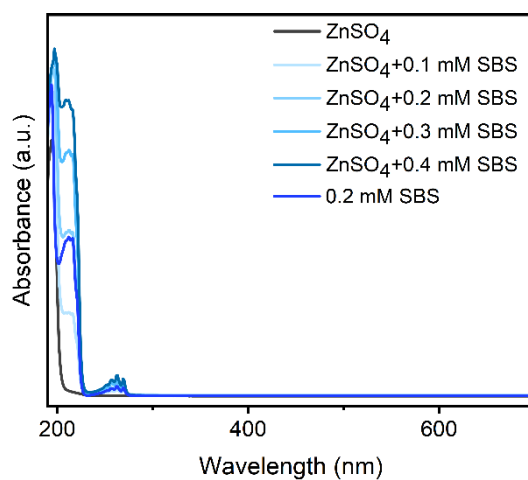


Figure S4. UV-Vis spectra of ZnSO_4 solution with different concentrations of SBS.

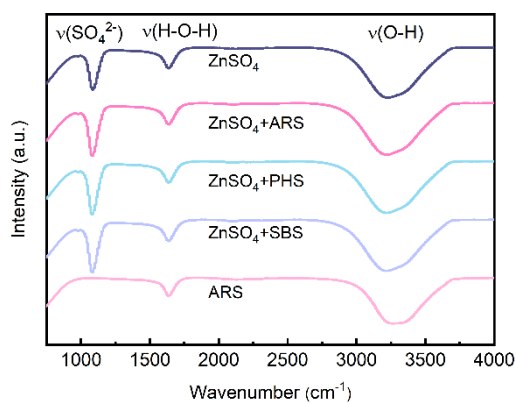


Figure S5. FTIR spectra of ZnSO_4 , $\text{ZnSO}_4 + \text{ARS}$, $\text{ZnSO}_4 + \text{PHS}$, and $\text{ZnSO}_4 + \text{SBS}$ electrolytes, respectively.

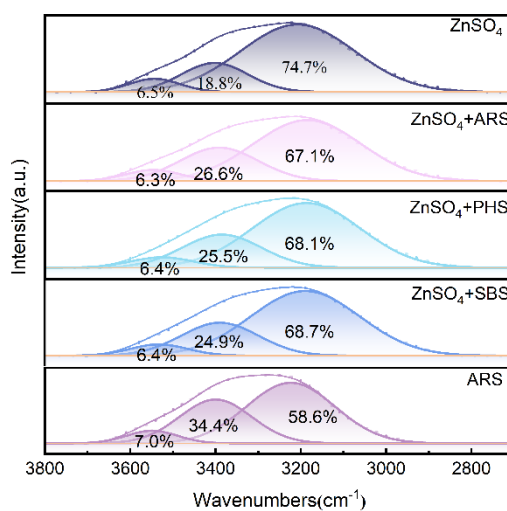


Figure S6. The proportion of strong, medium, and weak hydrogen bonding in ZnSO_4 , $\text{ZnSO}_4 + \text{ARS}$, $\text{ZnSO}_4 + \text{PHS}$, $\text{ZnSO}_4 + \text{SBS}$, and ARS electrolytes.

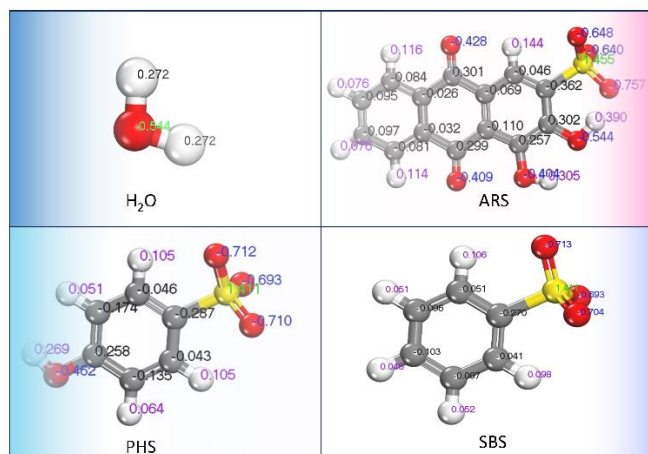


Figure S7. The charge distributions of the H₂O, ARS, PHS, and SBS molecules.

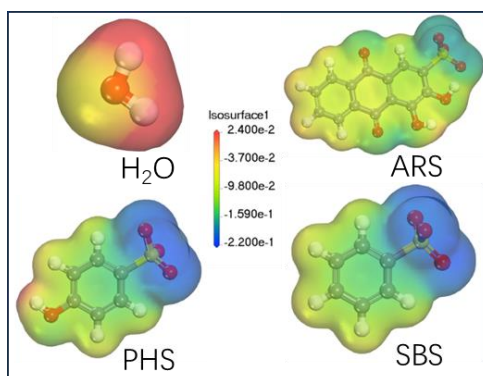


Figure S8. The electrostatic potential of the H₂O, ARS, PHS, and SBS molecules.

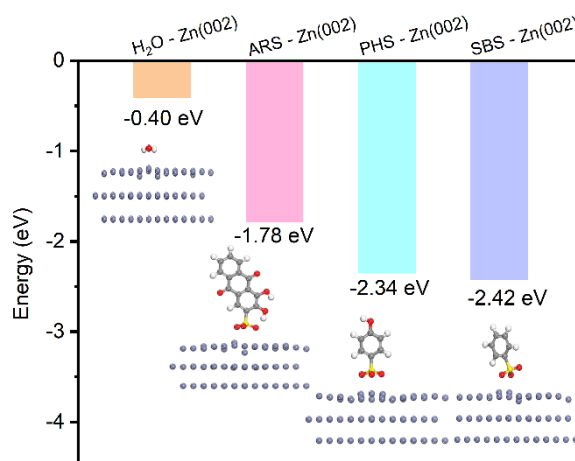


Figure S9. The adsorption energy of H₂O, ARS, PHS, and SBS molecules placed vertically on the Zn (002) surface, respectively.

Energy Materials

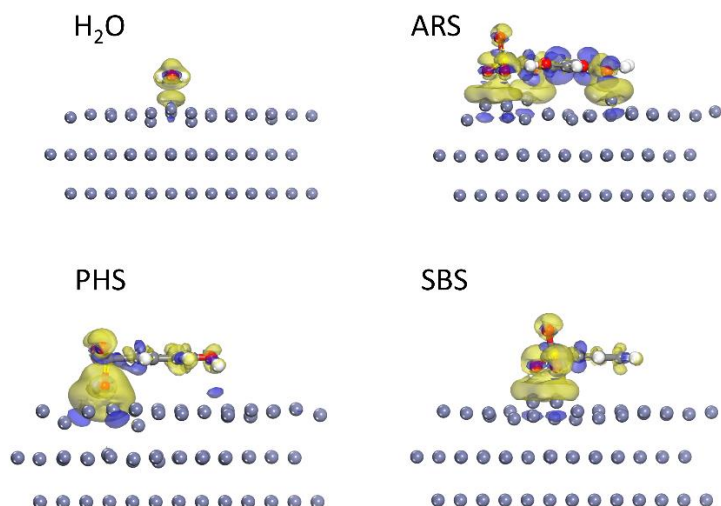


Figure S10. The charge density difference value of the Zn (002) surface with H₂O, ARS, PHS, and SBS molecules placed horizontally and the corresponding isosurface (yellow and cyan semi-transparent clusters represent the increase and decrease of electron density, respectively).

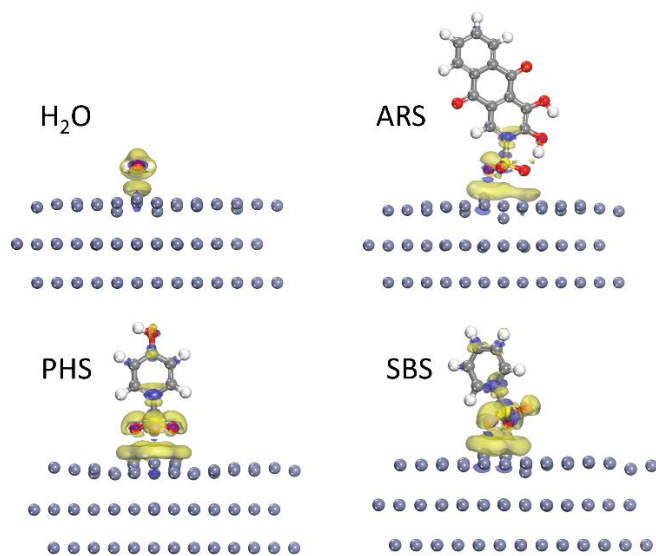


Figure S11. The charge density difference value of the Zn (002) surface with H₂O, ARS, PHS, and SBS molecules and the corresponding isosurface.

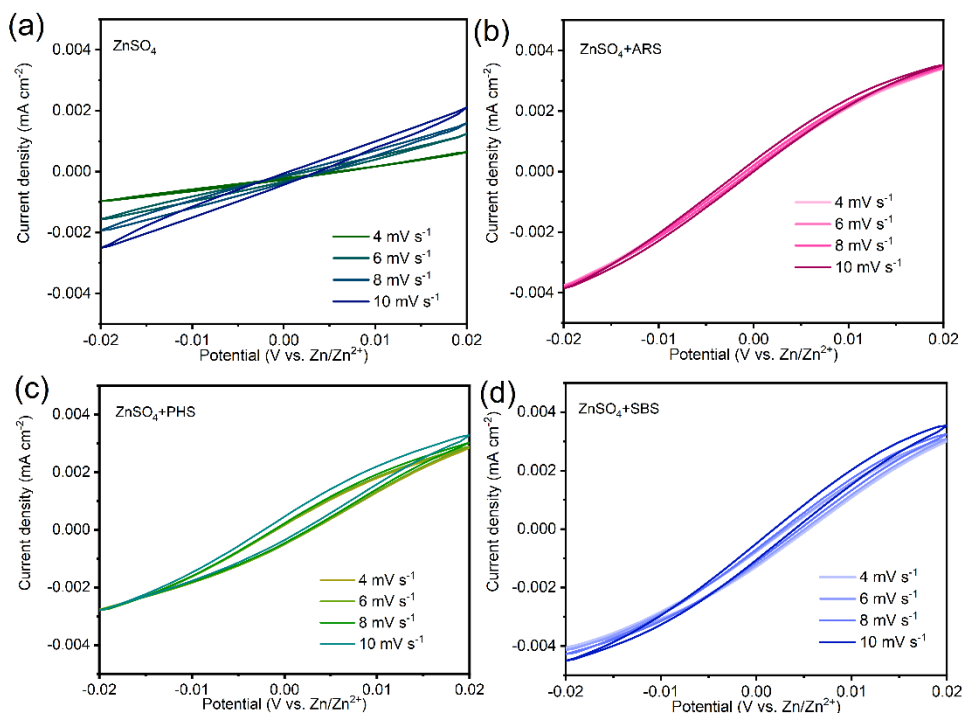


Figure S12. The EDL capacitance of the Zn electrode in the ZnSO₄, ZnSO₄ + ARS, ZnSO₄ + PHS, and ZnSO₄ + SBS electrolytes.

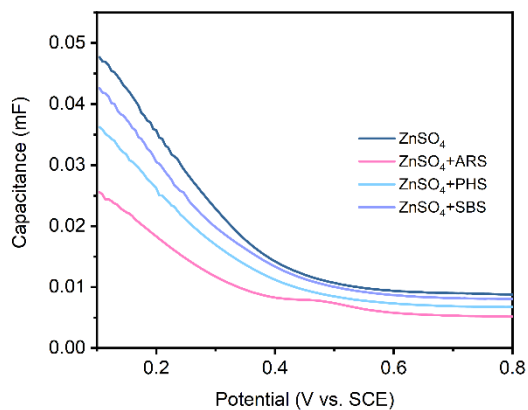


Figure S13. The differential capacitance curves with ZnSO₄, ZnSO₄ + ARS, ZnSO₄ + PHS, and ZnSO₄ + SBS electrolytes measured in the Ti//Zn cells.

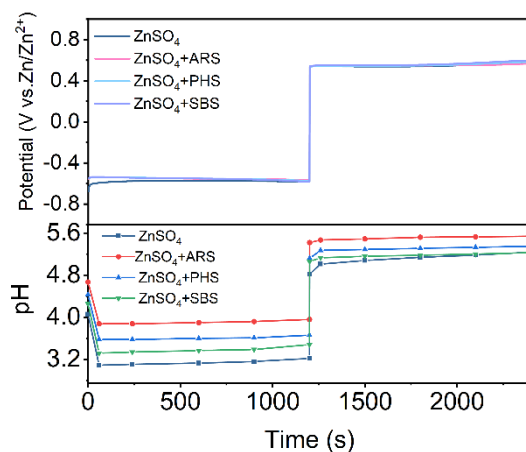


Figure S14. The potential-time curves and real-time pH values near the Zn anode in the ZnSO_4 , $\text{ZnSO}_4 + \text{ARS}$, $\text{ZnSO}_4 + \text{PHS}$, and $\text{ZnSO}_4 + \text{SBS}$ electrolytes during the plating/stripping process.

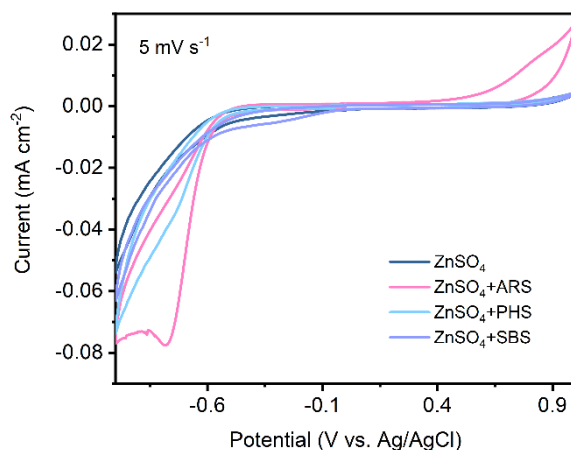


Figure S15. CV curves of the Zn electrode in the ZnSO_4 , $\text{ZnSO}_4 + \text{ARS}$, $\text{ZnSO}_4 + \text{PHS}$, and $\text{ZnSO}_4 + \text{SBS}$ electrolytes.

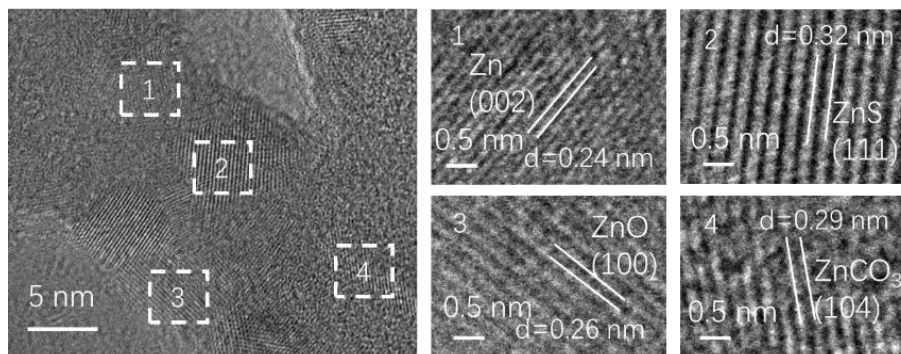


Figure S16. The HRTEM images of the Zn anode cycled in ZnSO_4 electrolytes.

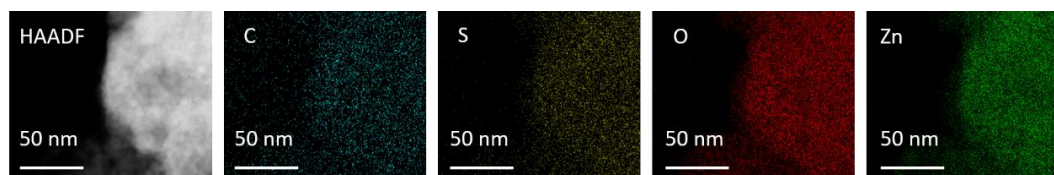


Figure S17. The EDX elemental maps of the Zn anode cycled in ZnSO_4 electrolytes.

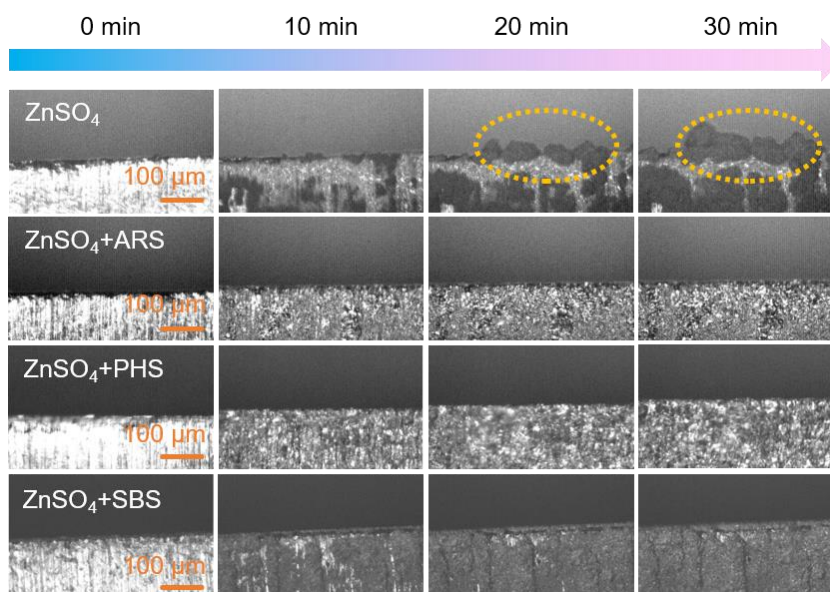


Figure S18. *In situ* optical microscopy images of the Zn plating process in different electrolytes.

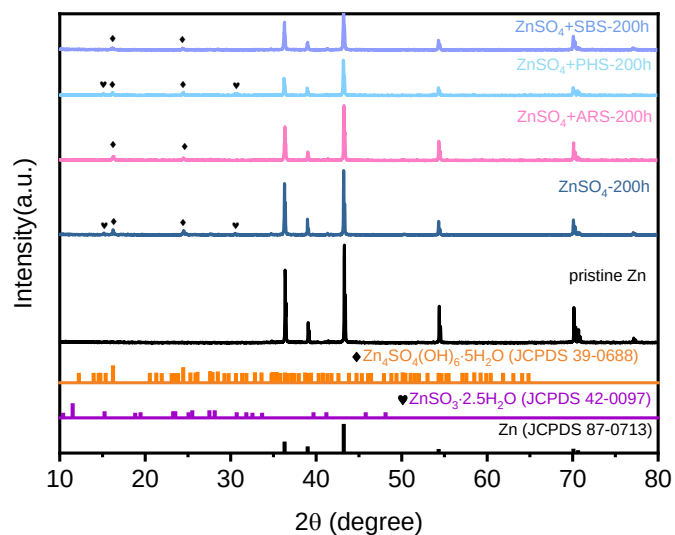


Figure S19. XRD patterns of the Zn electrodes cycled in ZnSO_4 , $\text{ZnSO}_4 + \text{ARS}$, $\text{ZnSO}_4 + \text{PHS}$, and $\text{ZnSO}_4 + \text{SBS}$ electrolytes.

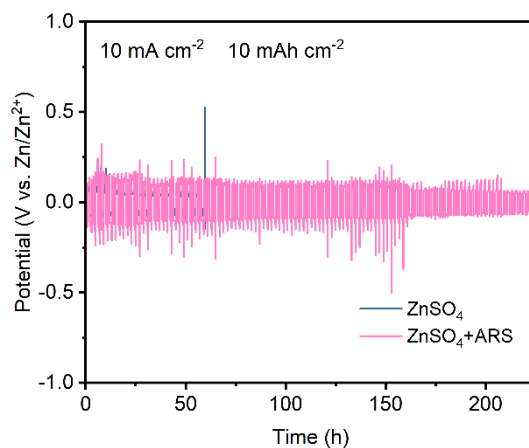


Figure S20. Cycling performance of Zn//Zn cells with ZnSO₄ and ZnSO₄ + ARS electrolytes at 10 mA cm⁻², 10 mAh cm⁻².

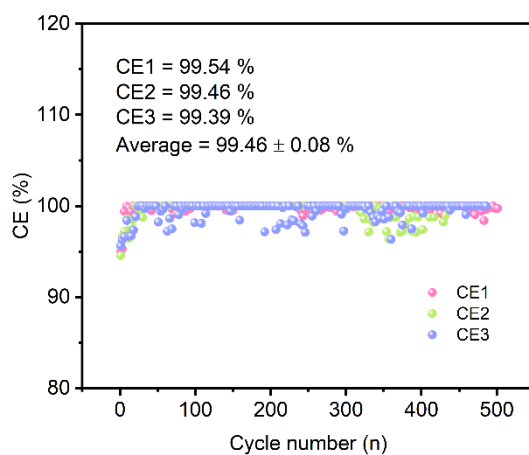


Figure S21. CE results of Ti//Zn cells with the ZnSO₄ + ARS electrolyte under the current density of 1.0 mA cm⁻².

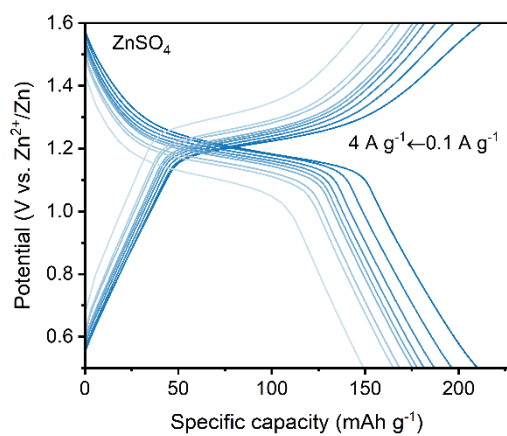


Figure S22. The galvanostatic charge /discharge profiles of the Zn//I₂ batteries using ZnSO₄ electrolytes under the current densities of 0.1 A g⁻¹ - 4.0 A g⁻¹.