Description of Additional Supplementary Files

Supplementary Data 1. Adsorption energy: The adsorption models of various electrolyte solvent molecules and ions with S_8 and ZnS.

Supplementary Data 2. Electrostatic potential: The optimized computational models of DMF molecules adsorbed on the surface of ZnS.

Supplementary Data 3. HOMO energy level: The models for energy calculation of various electrode and electrolyte components.

Supplementary Data 4. Charge density difference: Interfacial adsorption model of Zn^{2+} solvation structures on sulfur electrode.

Supplementary Data 5. Bader charge: The models for charge calculation of Zn atom.

Supplementary Data 6. MD simulations: The initial and final configurations of solvation structures in $ZnSO_4$−ZnI_2−H_2O and $ZnSO_4$−ZnI_2−H_2O−DMF electrolytes.