

Supplementary Materials

Cosolvent-involved hybrid solvation models for aqueous Zn-ion electrolytes: a case study of ethylene glycol-H₂O-ZnSO₄ system

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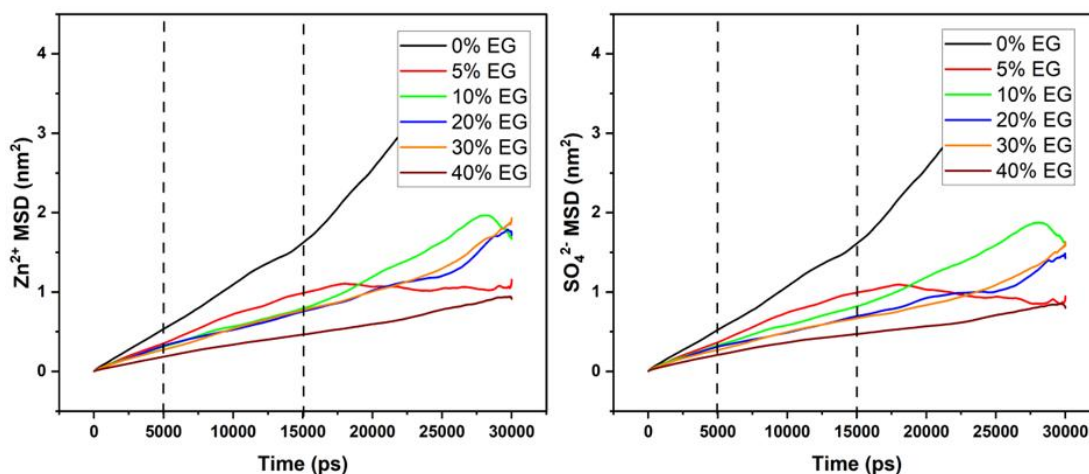
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Supplementary Table 1. EG and ZnSO₄ concentrations in MD simulation

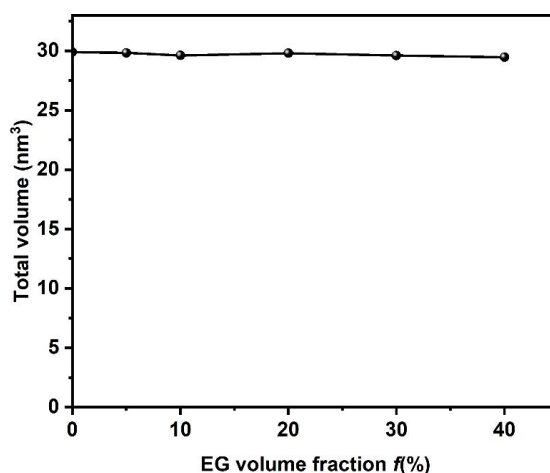
EG volume fraction $f(\%)$	The number of water molecules $N_w = 1000(1 - f)$	The number of EG molecules $N_{EG} = 323.22f$	Number of ZnSO ₄	
			Zn ²⁺	SO ₄ ²⁻
0	1000	0	36	36
5	950	16	36	36
10	900	32	36	36
20	800	65	36	36
30	700	97	36	36
40	600	129	36	36

Supplementary Table 2. Diffusion coefficients calculated from MSDs in Supplementary Table Figure 1

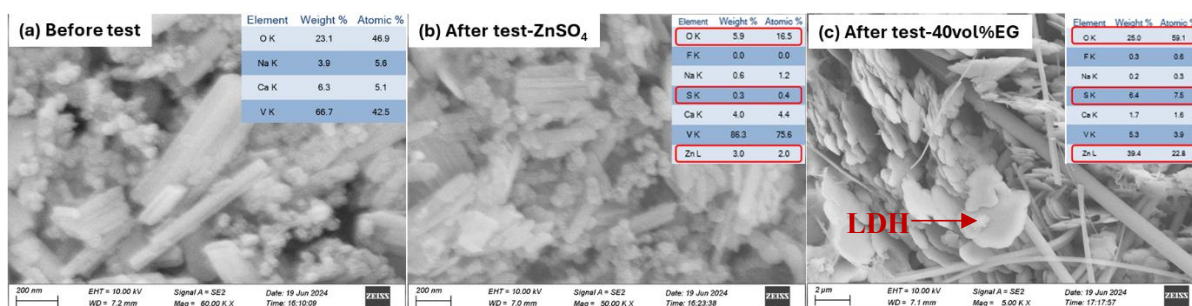
EG volume fraction $f(\%)$	D(Zn ²⁺) (1e-5 cm ² /s)	D(SO ₄ ²⁻) (1e-5 cm ² /s)
0	0.0182 (+/- 0.0026)	0.0184 (+/- 0.0013)
5	0.0106 (+/- 0.0032)	0.0105 (+/- 0.0039)
10	0.00778 (+/- 0.001421)	0.00806 (+/- 0.0008821)
20	0.00692 (+/- 0.0011)	0.006358 (+/- 0.00109)
30	0.008526 (+/- 0.001325)	0.006784 (+/- 0.002103)
40	0.004555 (+/- 0.0009483)	0.004356 (+/- 0.001883)



Supplementary Figure 1. Mean squared displacements (MSDs) of Zn^{2+} and SO_4^{2-} ions in electrolytes of different EG volume fractions.



Supplementary Figure 2. The equilibrium volumes for systems with different EG volume fractions.



Supplementary Figure 3. SEM-EDX results of a $\text{NaCa}_{0.6}\text{V}_6\text{O}_{16}$ cathode (a) before, and after test at 0.5A/g for 500 cycles using 2M ZnSO_4 electrolyte with (b) pure H_2O , and (c) $40\text{vol}\%\text{EG-H}_2\text{O}$ as solvent. The flakes shown in Figure (c) is LDH ($\text{Zn}_x\text{SO}_4\text{y}(\text{OH})_z \cdot n\text{H}_2\text{O}$) with high oxygen content.