

## Molecular dynamics study of single-ion conducting covalent organic framework for aqueous Zn-ion batteries

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Aqueous Zn-ion battery has emerged as a promising alternative to Li-ion battery, owing to its low cost, reduced toxicity, high ionic conductivity, and high volumetric density. However, some challenges arise from the lack of suitable electrolytes which can ensure interfacial stability with electrodes. Here, we theoretically investigated the role of zinc sulfonated covalent organic framework (TpPa-SO<sub>3</sub>Zn<sub>0.5</sub>) as a solid electrolyte (SE) in aqueous Zn-ion battery system. We utilized molecular dynamics (MD) simulations to investigate the Zn-ion migration behavior in the SE system in comparison with the conventional liquid electrolyte (LE) (i.e., 2 M ZnSO<sub>4</sub> in H<sub>2</sub>O). We found that the immobile covalently tethered anion in the TpPa-SO<sub>3</sub><sup>-</sup> framework allowed more uniform Zn-ion flow across the system as opposed to non-uniform flow in LE system. The non-uniform flow of ions in LE system can be attributed to the strong electrostatic interaction between Zn<sup>2+</sup> ion with SO<sub>4</sub><sup>2-</sup>, leading to the formation of aggregates under electric field. Benefiting from this unusual single-ion conduction behavior in SE system, high redox reversibility and long-term cyclability of battery system was achieved.