Modeling Aqueous Zinc-Ion Batteries: The Influence of Electrolyte Speciation on Cell Performance

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Zinc-based batteries are among the longest-used cell systems, yet they show increasing research interest in the last years[1]. The high specific capacity of zinc metal anodes combined with their stability in aqueous electrolytes and abundance highlights their potential in a growing market for energy storage systems. The long-commercialized alkaline cell chemistry, a zinc metal anode and a manganese dioxide cathode, showed increased rechargeability when switching to mildly acidic electrolytes[2]. While the charge transport of Zn^{2+} is widely acknowledged and distinguishes them from alkaline electrolytes, in-detail charge storage mechanisms are under debate[3]. The electrolyte's role in this process and its influence on cell performance and stability is often overlooked.

We employ a thermodynamically consistent dynamic cell model to describe aqueous zinc-ion batteries' behavior in our work. The model includes a thermodynamical equilibrium description of complex formations. Species composition significantly alters the transport properties and stability of both the electrolyte and the cathode. We predict cell behavior and cycling performance for different electrolytes and electrode materials. Putting this into the context of cell parametrization and rate limitations, we describe possible pitfalls and identify goals for the ongoing optimization of zinc-ion batteries.

This work is supported by the Federal Ministry of Education and Research (BMBF) via the project ZIB.

Literature

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