A Multi-Process Cathode Model for MnO_2-based Aqueous Zinc-Ion Batteries

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Rapidly rising electricity prices on the European energy market flared up an accompanying discussion about the revival of nuclear power and gas-fired power plants as bridging technologies. This situation emphasises the urgency of powerful and affordable electrochemical energy storage systems for a rapid energy transition. Next-generation storage technologies are in a tight race competing in energy density, environmental safety and cost per capacity. Zinc-based anodes are commercial highly successful for several decades, yet there is no commercialised zinc-insertion cathode yet [1]. Manganese dioxide cathodes, which are widely used in alkaline cells, were shown to have a reversible zinc storage capacity in mild electrolytes. This increased the research interest in zinc-ion batteries in the last decade, and many successful systems were proposed [2].

Aqueous metal batteries face a series of challenges. The dynamic electrolyte composition and pH profile heavily influence performance, and many side reactions occur. This contribution presents a thermodynamically consistent dynamic cell model, which considers the electrolyte's complex formation and related transport properties. Additionally, it implements a multi-process model for the MnO_2 cathode, reflecting the most reported side reactions in literature, manganese dissolution, and proton co-insertion. We use this to identify well-known experimental characteristics, describe possible pitfalls, and identify goals for further optimising zinc-ion batteries.

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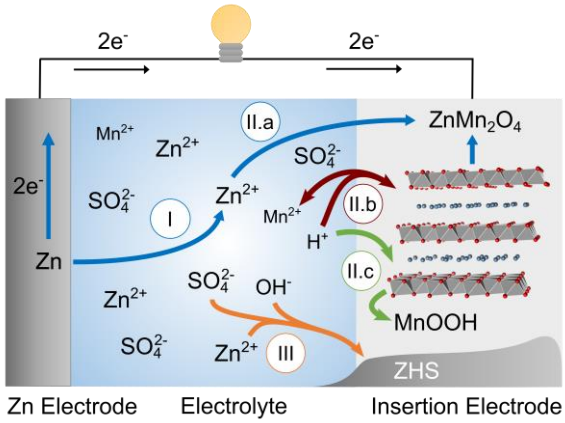

Figure 1: Cell schematic depicting the relevant processes in the developed model for Zn-MnO_2 batteries; adapted from [2].

***Keywords**:* Zinc-Ion Batteries, Aqueous Electrolyte, Electrolyte Complexation, Full-Cell Models

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