Modelling the cycling of zinc-ion batteries

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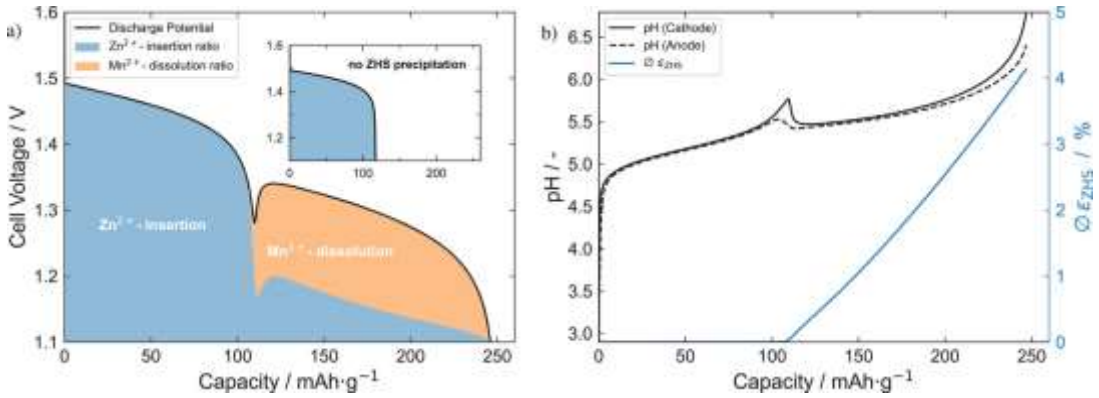
Manganese-oxide (MnO_2) cathodes are a well-studied candidate for zinc-ion batteries (ZIB) are [1]. ZIBs with aqueous neutral electrolytes exhibit two distinct phases during charge and discharge. Experiments have revealed that the second discharge phase goes hand-in-hand with the precipitation of zinc-hydroxide sulfate (ZHS) at the cathode [2]. Besides the most desired zinc insertion, the proposed working mechanisms of the MnO_2 cathodes are the (co-)-insertion of protons into the cathode and the reversible dissolution of the MnO_2 itself, both having similar effects on the local pH evolution eventually leading to ZHS precipitation. Our work uses a continuum full-cell model supported by DFT calculation to investigate the implications and details of the experimentally observed properties and deduced claims [3]. We find that the precipitation of ZHS stabilizes electrolyte pH accelerating MnO_2 dissolution in the second discharge phase. Thus, we can propose operating strategies for mitigating the shape-changing MnO_2 dissolution [3]. Finally, we compare the discharge behavior of various electrolytes [4].



***Keywords**:* Zinc-air, air electrode, zinc-nickel, zinc-manganese, aqueous battery.

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