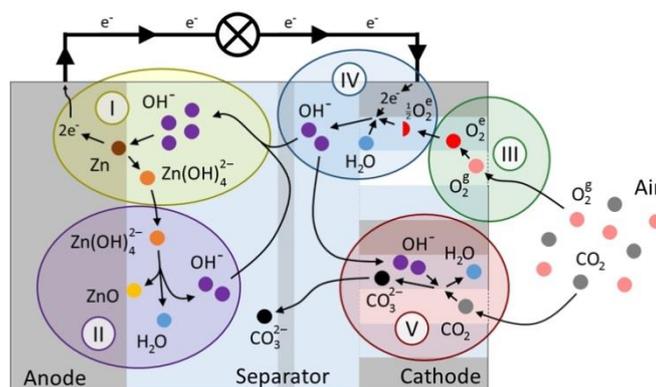


# Theory of Electrolytes for Zinc-Air Batteries

Birger Horstmann<sup>1,2</sup>, Simon Clark<sup>1,2</sup>, Johannes Stamm<sup>1,2,4</sup>, Max Schammer<sup>1,2,3</sup>, Timo Danner<sup>1,2</sup>, Arnulf Latz<sup>1,2,3</sup>

- 1) Helmholtz Institute Ulm, Helmholtzsstraße 11, 89081 Ulm
- 2) German Aerospace Center, Institute of Engineering Thermodynamics, Pfaffenwaldring 38, 70569 Stuttgart
- 3) University of Ulm, Albert-Einstein-Allee 47, 89081 Ulm
- 4) University of Münster, Einsteinstraße 62, 48149 Münster



Abundant resources and large energy density make Zinc-air batteries (Zn-O) attractive for distributed stationary energy storage. Furthermore, Zn-O batteries are commercialized as primary button cells for hearing aids for decades. The standard alkaline electrolytes limit the lifetime due to reaction with atmospheric carbon dioxide<sup>1</sup> and zinc shape change. Therefore, we study its substitution by novel electrolytes, i.e., aqueous neutral electrolytes<sup>2,3</sup> and ionic liquids<sup>4</sup>.

Experimental progress is speed up with mathematical models which describe consistently transport, chemistry, and electrochemical reactions on the pore and the cell scale<sup>5,6</sup>. These models allow studying the expected performance of the cell as well as local electrochemical conditions and degradation mechanisms depending on operation condition and cell design.

First, we model a commercial Zn-O button cell with alkaline electrolytes and validate our understanding of nucleation and growth processes in these batteries. Our model demonstrates that contamination due to carbon dioxide limits their lifetime to a few months.

Therefore, we study the impact of exchanging the electrolyte and present the first model of Zn-O batteries with aqueous neutral electrolytes<sup>2,3</sup>. We model the dynamics of electrolyte composition and discuss its impact on solid discharge products. We validate our model against experiments in the literature<sup>2</sup> and propose design changes. As an alternative, ionic liquids are proposed as electrolytes for Zn-O batteries. We formulate a theory-based model and study the interfacial structure in the electrolyte.

To sum up, we evaluate the prospects of novel electrolytes for Zn-O batteries. Our models elucidate the complexity of these electrolytes and guide the experimental progress towards their application. We validate the theory against experiments and improve it with this feedback.

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