Modelling Zinc Batteries with Ionic Liquid Electrolyte

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Rechargeable zinc ion batteries are potential candidates for low-cost and efficient energy storage devices [1]. Zinc is an abundant element which is non-toxic, cheap and environmentally benign. Primary zinc batteries have a long history and are established commercially [2]. However, technical problems associated with zinc ion batteries are yet to be resolved [1]. The key component is the electrolyte because it must be stable over a wide electrochemical window and allow reversible metal deposition.

Ionic liquids are promising candidates for stable battery electrolytes [3]. Their advantages comprise a large electrochemical window (up to 6V), chemical and thermal stability, non-flammability (as safety asset) and low vapor pressure [4]. In particular, ionic liquids minimize dendrite growth during electrodeposition and have high ionic conductivity [4]. Zinc-air batteries with ionic liquids are potentially stable towards moisture as well as carbon dioxide and can support a reversible oxygen electrochemistry.

In this talk, we present a thermodynamically consistent transport theory of zinc batteries based on room temperature ionic liquids. Upon this framework we model a zinc ion secondary battery with a mixture of ionic liquid and water as electrolyte. This setup is described experimentally in Ref. [1]. The battery comprises a zinc anode and a Prussian blue analogue cathode in combination with a choline-acetate-water mixture, [Ch]OAc+30%wt water. [Ch]OAc, is a biodegradable, biocompatible, and inexpensive ionic liquid.

Our focus lies on the systematic derivation of a set of fully coupled transport equations for the ions, charge and heat based on the development of modeling methodologies for lithium-ion batteries [5]. The battery is simulated along one dimension and good agreement with the experimental observations described in Ref. [1] is found.

For the understanding of microscopic structures, we incorporate the hardcore particle nature of the medium into our transport theory. In the vicinity of an electrified interphase, we find a quasi-crystalline structure with crowding and overscreening [6].

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