

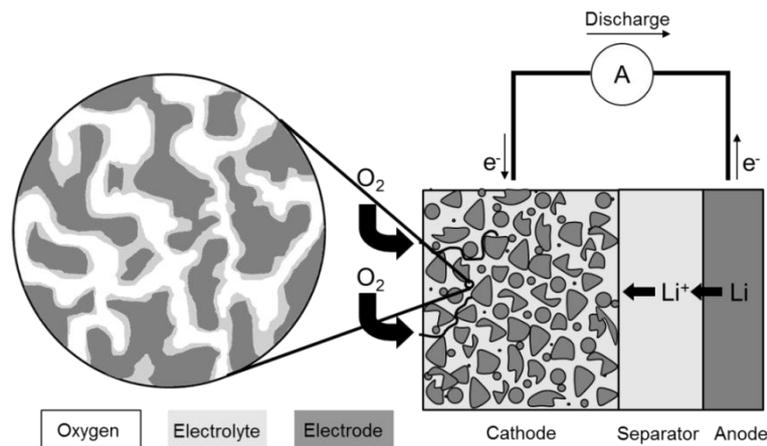
Modeling Crystal Growth and Multi-Phase Flow in Metal-Air Batteries

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We contributed to research on lithium-air batteries with aqueous as well as non-aqueous electrolytes on the pore level and the cell level. Based on the developed modeling methodologies, we study silicon-air and zinc-air batteries.

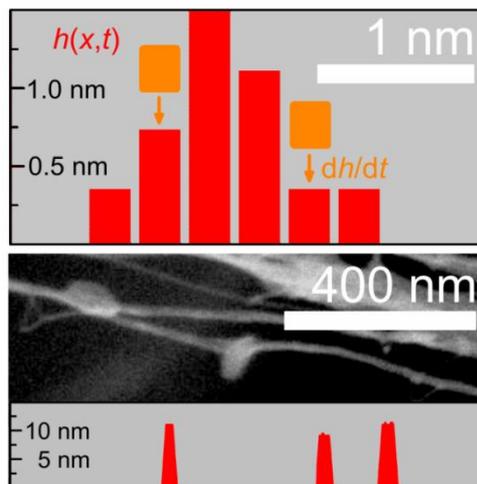
In aqueous alkaline electrolytes, lithium ions react with oxygen to form lithium hydroxide in a gas diffusion electrode (GDE), where liquid and gas coexist in a porous structure. We model the electrochemical dynamics within a GDE including the effects of pressure-driven convection and multi-phase coexistence with continuum models and Lattice-Boltzmann theory [1,2]. The lithium hydroxide concentration in alkaline lithium-air batteries is accumulating during discharge until it precipitates. We rationalize that this precipitation is inhomogeneous due to fundamental transport effects in alkaline electrolytes and discuss adjusted cell designs [1]. On a microscopic level, we study the elementary kinetics of the oxygen reduction reaction on the active surfaces [3].



A second line of our research is devoted to aprotic solvents in lithium-air batteries. On a cell level, we found that slow oxygen transport in flooded electrodes is a limiting factor for power density [4]. On a pore level, we studied the nucleation of lithium peroxide on the active surfaces of the cathode [5]. The discharge product lithium peroxide is found in different morphologies inside lithium air batteries: either it forms films that passivate the active surface, or it forms particles that grow into the electrolyte pore space. We found out and explained that nucleation of lithium peroxide particles happens at discharge currents below the exchange current of the oxygen reduction reaction.

Furthermore, we are performing research on metal-air batteries based upon zinc- or silicon-ions [6]. Our model explains the experimentally observed dependence of cell capacity on water content in the electrolyte of silicon-air batteries. The addition of water to the electrolyte affects the spatial distribution of the precipitation reaction and thus the balance between anode and cathode capacity.

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