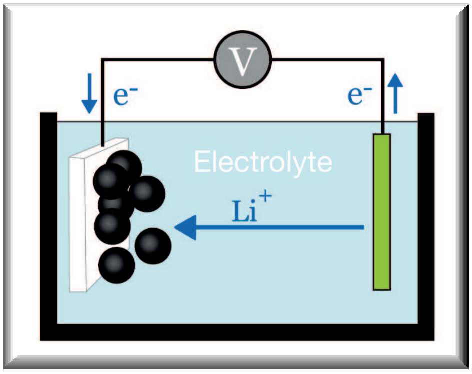
Lithium-Ion Batteries

Mathematical Modeling and Simulation

Background

Energy storage is widely considered as being the crucial bottleneck in renewable energy supply chains, and lithium-ion batteries are therefore of significant importance. They differ from other batteries by the necessity to improve the classical battery models. For example, originally lithium atoms were considered to be simultaneously stored in the individual storage particles. The Fokker-Planck equation embodies the new idea that the particles are loaded one after the other. The voltage-charge plot shows hysteresis and a phase transition during the storage process. Our model predicts this behavior for the first time.



Our Services

We develop new mathematical models for all components of lithium-ion batteries. These include many-particle-electrodes, graphite electrodes, electrolytes, and electrolyte-electrode interfaces. The models describe electrochemical processes and transport phenomena by means of partial differential equations in the bulk and by transition conditions at the interfaces and are able to predict the voltage-charge properties of the corresponding component.

Key Features

- The slow charging and discharging process is described by a Fokker-Planck equation for a many-particle cathode.
- The fast charging regime is modeled by a coupled system of viscous Cahn-Hilliard and Lame equations that takes the coupling of diffusion and mechanical stresses within the electrode into account.
- The anodes are usually represented by carbon electrodes with a layered structure. Here the model describes the reversible storage of lithium within the layers. The storage process is also described by a Fokker-Planck equation.
- The electrolyte is described by a completely new model that overcomes the deficiencies of the popular Nernst-Planck models which usually form the basis for the existing commercial numerical codes.
- The contact surface between the electrolyte and the electrode is modeled by new jump conditions that take chemical reactions at the electrode surface into account. The equations of the model generalize and correct the Butler-Volmer formulas.

Fields of Application

- Automotive Industry
- Industrial and consumer products sector (smartphones, notebooks, tablet computers, etc.)

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