Einladung zum Vortrag

Modeling and simulation of Lithium intercalation and conversion batteries

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The majority of modern Li Ion batteries use porous materials as electrodes as well as separators. The electrodes of most of the conventional Li ion batteries are produced from powders which are kept together by mixing them with binder materials and black carbon to enhance their conductivity. Even if all chemical requirements for constructing a working battery as e.g. mutual chemical compatibility of electrolytes and materials, used for the electrodes, separator and the binder are fulfilled, it is not guaranteed, that the final battery can reach its theoretical capacity or the required power density under operation condition. These properties are strongly influenced by the interplay of the morphological properties of the porous electrodes and the transport and reaction mechanisms of the chemical active ions. Even the extent and the type of degradation mechanisms are likely to be influenced by the morphology of the electrodes. For being able to better understand, evaluate and optimize these dependencies, proper electrochemical and physical reaction and transport models as well as efficient numerical algorithms are needed to study the resulting coupled nonlinear partial differential equations in the complex microstructure of Li ion batteries.
After giving a short introduction in the functionality and general properties of Li ion batteries the differences between Li based intercalation and conversion batteries are explained. For intercalation batteries a validated fully thermodynamically consistent model for transport and chemical reactions in the microstructure of the battery is presented. The importance of a self consistent formulation of interface conditions between electrolyte and active particles and transport theory is discussed. Simulation examples with the software BEST, which was developed at the Fraunhofer ITWM in the group of the presenting author, are used to demonstrate the importance of the microstructure on the distribution of ions, and currents in the microstructure of Li ion intercalation batteries.
In the second part the challenges of modeling the next generation Li based conversion batteries like Li air and Li–Sulfur batteries are outlined. Results of an elementary kinetic modeling approach developed at the DLR and the HIU in a simple 1D effective porous media setting are shown. At the end an outlook on future research at the HIU on modeling properties of Li intercalation and conversion batteries is given.

Freitag, 18. Oktober 2013 **11:00 Uhr**
TUM Exzellenzzentrum **Seminarraum EG**
Boltzmannstr. 17, Garching

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