

Modeling of Species and Charge Transport in Li-Ion Batteries

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In order to improve the design of Li ion batteries the complex interplay of various physical phenomena in the active particles of the electrodes and the electrolyte has to be balanced. The separate transport phenomena in the electrolyte and in the active particle as well as their coupling due to the electrochemical reactions at the interfaces between the electrode particles and the electrolyte will influence the performance and the lifetime of a battery. Any modelling of the complex phenomena during the usage of a battery has therefore to be based on sound physical and chemical principles in order to allow reliable predictions for the response of the battery to changing load conditions. We will present a modelling approach for the transport processes in the electrolyte and the electrode based on non-equilibrium thermodynamics and transport theory. Numerical solution of the resulting highly nonlinear coupled equations for ion concentrations, ion flux and electrical currents, is a challenging task. Here we briefly present some simulation results obtained with our research code BEST (Battery and Electrochemistry Simulation Tool), which is developed at the Fraunhofer ITWM in cooperation with Institute for Parallel Processing, Sofia. More detailed discussions on numerical approaches for this system will be presented in two other talks in this special session.