Battery Modelling and Simulation on the Particle Scale

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Lithium-ion batteries (LIBs) play a key role in the current transformation of our global energy system. A typical LIB cell consists of two electrodes (an anode and a cathode) with a porous separator in between them and an electrolyte which conducts Lithium ions. Most state-of-the-art electrodes consist of active material (AM) particles, conductive additives and binding agents which form a complex microstructure which is soaked with the liquid electrolyte. Together with other effects like degradation phenomena, this leads to a complex interplay over multiple length scales. In order to further advance the technology, a good understanding of individual transport processes as well as their interplay is necessary.

Modelling LIBs on the various length-scales helps in understanding fundamental mechanisms inside batteries as well as in improving battery performance in general. To obtain simulation results based on experimentally measurable quantities which also allow a connection of the different length-scales, it is important to use physics-based approaches. Using a previously developed transport model (A. Latz and J. Zausch, "Thermodynamic consistent transport theory of Li-ion batteries" in J. Pow. Sour., vol. 196 (6), pp. 3296-3302, 2011), simulations can be conducted on LIB-electrodes that resolve their microstructure. As this continuum modelling approach is based on fundamental thermodynamic principles and general conservation laws, it allows the connection to DFT-calculated parameters and only requires experimentally accessible quantities as input. One of its current simplifications is, that the AM particles internal microstructure is not resolved.

As advanced imaging techniques reveal, that these particles inherit a complex inner structure, which has significant influence on the electrode and consequently battery performance, understanding the transport processes on this so-called particle scale has become increasingly interesting. To allow simulative investigations, an extension of the previously mentioned model is required.

We will show results of our work on an extension of the already well-established model, that allows simulations resolving the microstructure of AM particles. Furthermore, a new enhanced-electrochemistry model, that utilizes additional information about redox-reactions of the active material allows to capture rate-dependencies more accurately in the simulation among other advantages.