**Motivation**

- Lithium-Ion batteries are receiving increased attention and importance for portable and mobile applications.
- Fundamental processes on cell and electrode level are still not sufficiently understood.
- Goal: Scientific understanding and model-based optimization of electrochemical and transport processes in lithium-ion batteries for supporting technological development.
- Modeling framework [1] based on microscopic description of thermodynamics, kinetics, transport and structure to predict:
  - Macroscopic electrochemical observables (discharge / charge behavior, capacity, SOC)
  - Ageing processes (SOH) and durability
  - Heat transport and hot spot formation

**Modelling and simulation approach**

Multi-scale approach to understand *macroscopic* electrochemical behavior (capacity, power, SOC) and lifetime (SOH) from *microscopic* physicochemistry

- Charge neutrality condition: \( \sum c_i z_i = 0 \)
- Nernst-Planck equation of ion transport: \( \frac{\nabla c_i}{RT} = \nabla(D_i \nabla c_i) - \frac{2F}{RT} \nabla(D_i \nabla \phi) \)
- Arrhenius behavior of diffusion coefficients: \( D_i = D_0 \exp\left(-\frac{E_{\text{act}}}{RT}\right) \)
- Butler-Volmer equation: \( \eta = n F \frac{E_{\text{cell}}}{RT} \exp\left(-\frac{0.5 F \eta^m}{RT}\right) \)
- Stoichiometry of anode (x) and cathode (y): \( x = \frac{\rho_{\text{M}_x}}{\rho_{\text{M}_L}} \), \( y = \frac{\rho_{\text{M}_y}}{\rho_{\text{M}_{\text{CoO}_2}}} \)
- Half-cell potential of anode and cathode from empirical polynomials [2,3]
- Parameters [2,3,4]: \( D_0 = 1.07 \times 10^{-11} \text{ m}^2/\text{s}, T = 298 \text{ K}, \rho (\text{Anode}) = 3.6 \times 10^2 \text{ A/m}^2, \rho (\text{Cathode}) = 3.6 \times 10^3 \text{ A/m}^2, \rho_{\text{CoO}_2} = 1050 \text{ kg/m}^3, \rho_{\text{Li}_2} = 3225 \text{ kg/m}^3 \)

**Conclusions**

- Demonstrated multi-scale modeling and electrochemical simulation for physically-based prediction of cell behavior.
- 1D simulations show typical discharge behavior. Distribution of loss processes can be quantified.
- Quantification of spatially resolved Li concentration in intercalation electrode and electrolyte.

**Research group**

- Multi-scale approach
- Electrochemical simulation
- Solid oxide fuel cells
- PEFC hybrid vehicle

**Results and discussion**

- 1D model: Simulated discharge characteristics
- Simulation shows typical voltage behavior at low discharge rates
- Amount of intercalation of Li in electrodes depends on location of each particle and differs inside one electrode [3]
- Concentration of Li$^+$ in electrolyte shows good agreement with other studies [4]

**Outlook**

- Half-cell potentials based on physical thermodynamic data in order to reduce empiricism.
- Elementary kinetic models of side reactions such as SEI formation leading to ageing of cells.
- Heat production and heat transport as well as its feedback on electrochemical behavior (e.g., hot spot formation).