

Birger Horstmann

Frühjahrsakademie Universität Ulm

Warum braucht man „Batterie-Modelle?“

Verständnis für Batterie überprüfen und entwickeln

- Entwicklung neuer Batterie-Materialien bzw. Batterie-Designs
- Optimierung der vorhandenen Batterietypen
- Vorhersage der Batteriealterung
- Optimierung der Betriebsstrategien

Multi-Skalen Simulation von Batterien

Quantum Chemistry on
Quantum Computers



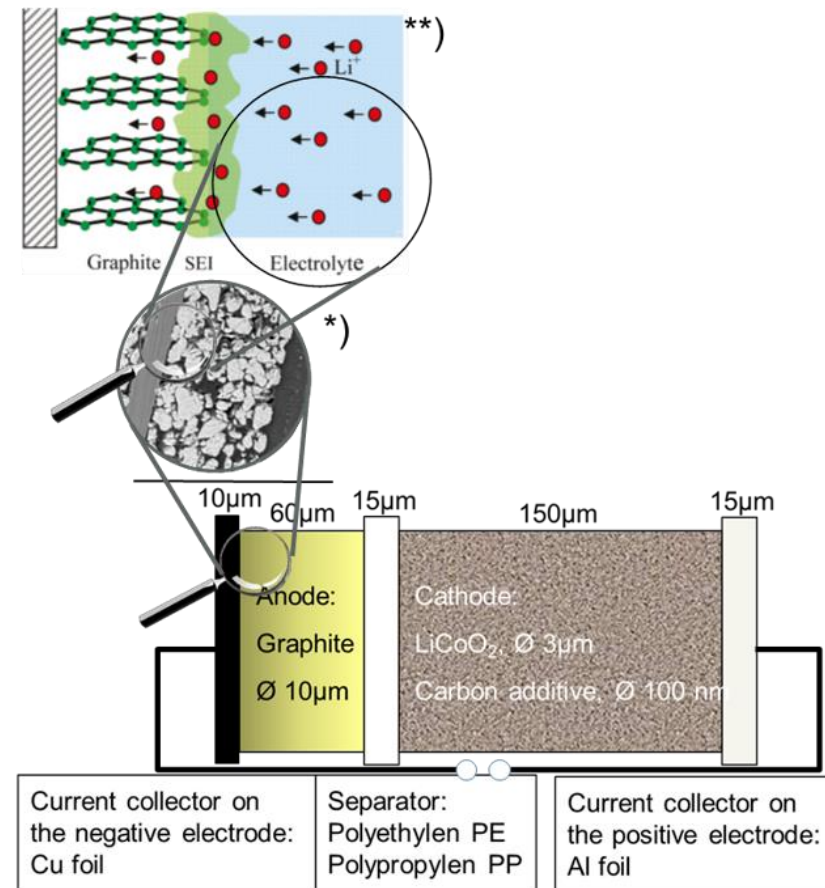
Interfaces &
Interphases



Continuum Cell
Modelling

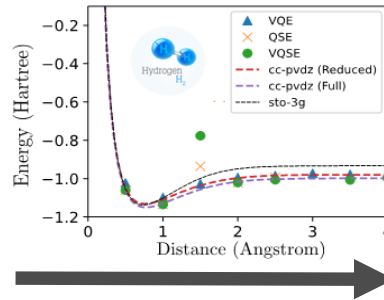


Data-Driven Modelling



Overview

Energy of molecules

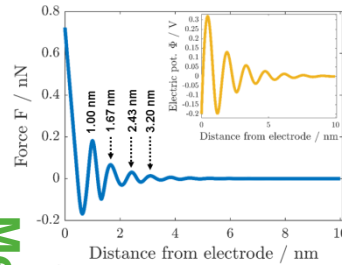


Quantum chemistry of materials

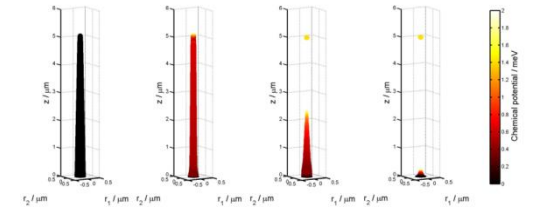
Nano

Meso

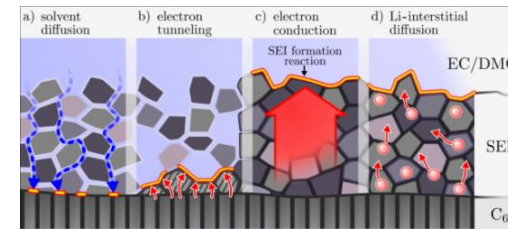
Theory-based modelling



Charged layers in novel electrolytes



Lithium dendrites



SEI – interlayers

Meso

Macro

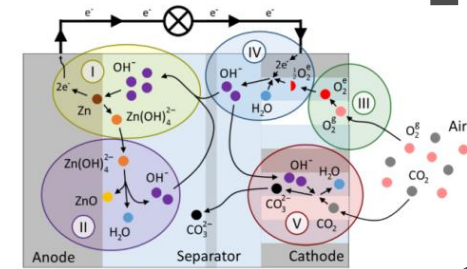
Maschinelles Lernen

System

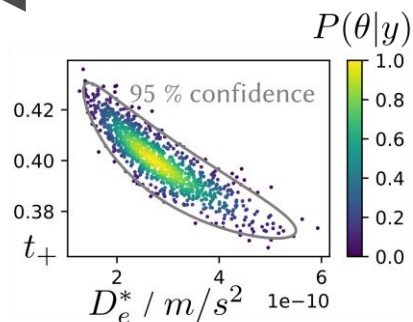
Macro

Simulation of ion fluxes

1D Electrolyte- & cell design

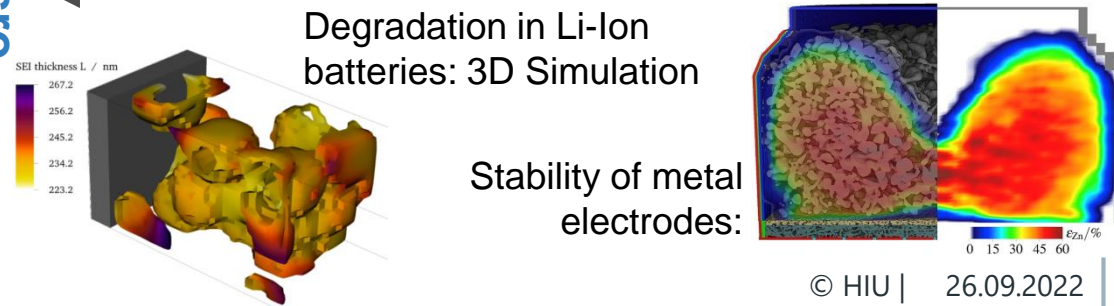


Parameter identification

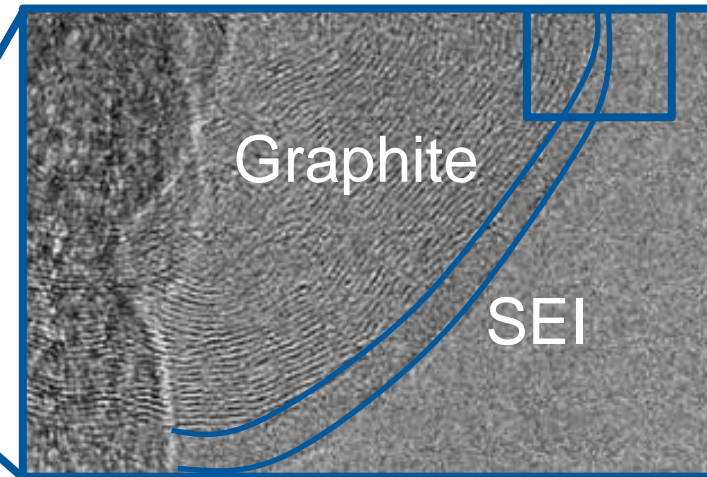
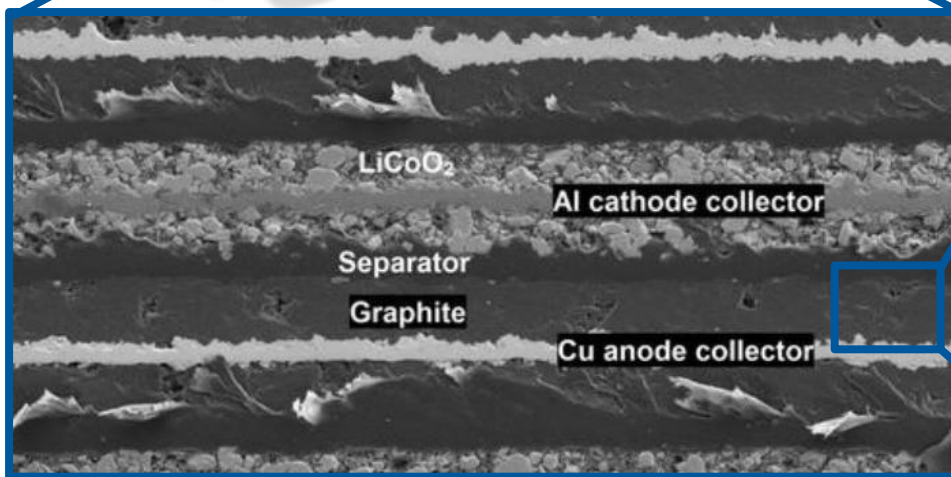
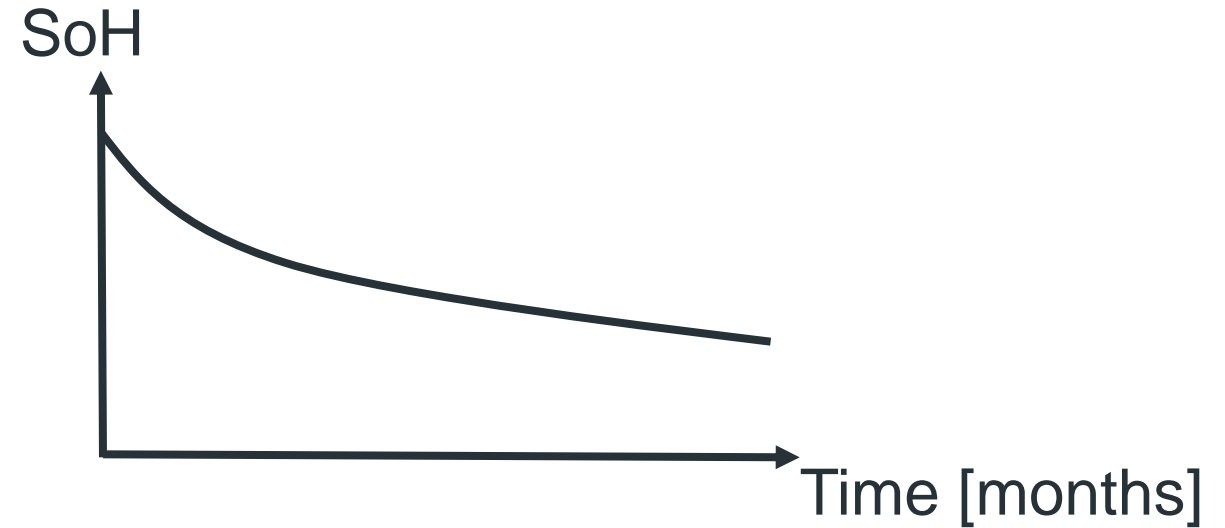
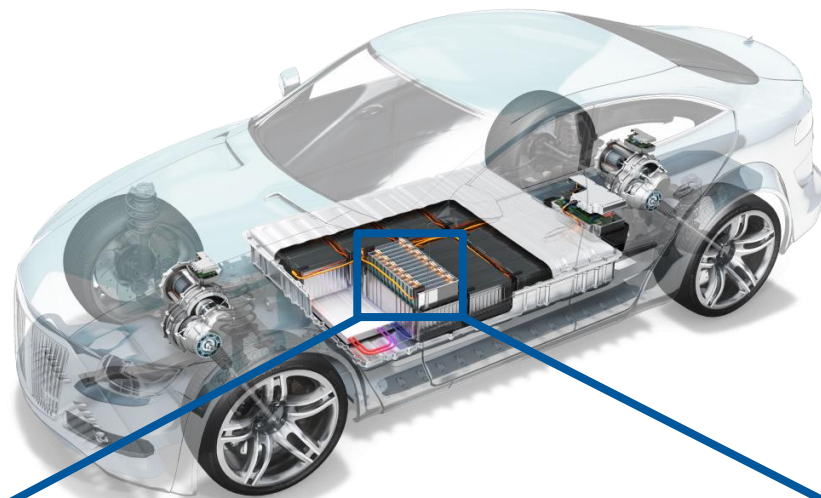


Degradation in Li-Ion batteries: 3D Simulation

Stability of metal electrodes:



Capacity Fade in Li-Ion Batteries

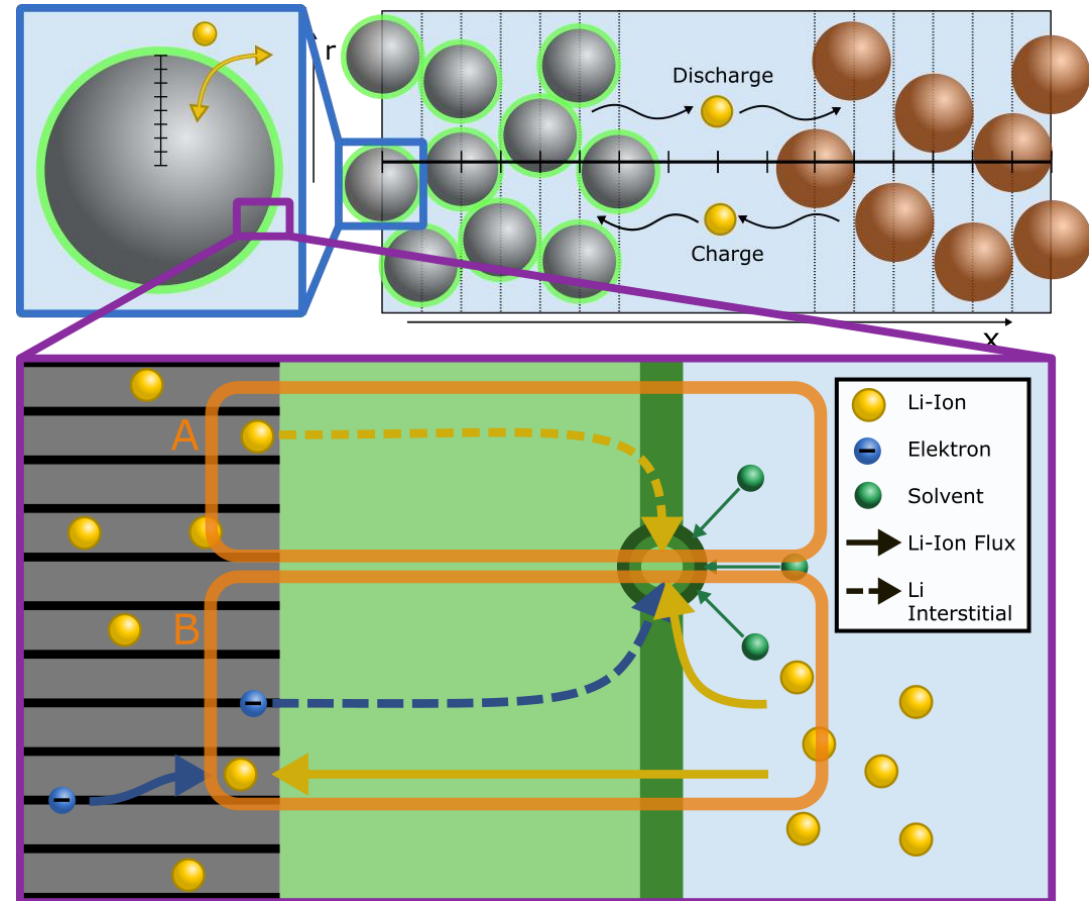


Huang, William, et al. *Nano letters* (2019).
<https://qnovo.com/category/safety/page/4/>
http://henkeladhesivesna.com/blog/wp-content/uploads/2019/03/04_Car-Integration-1024x768.png

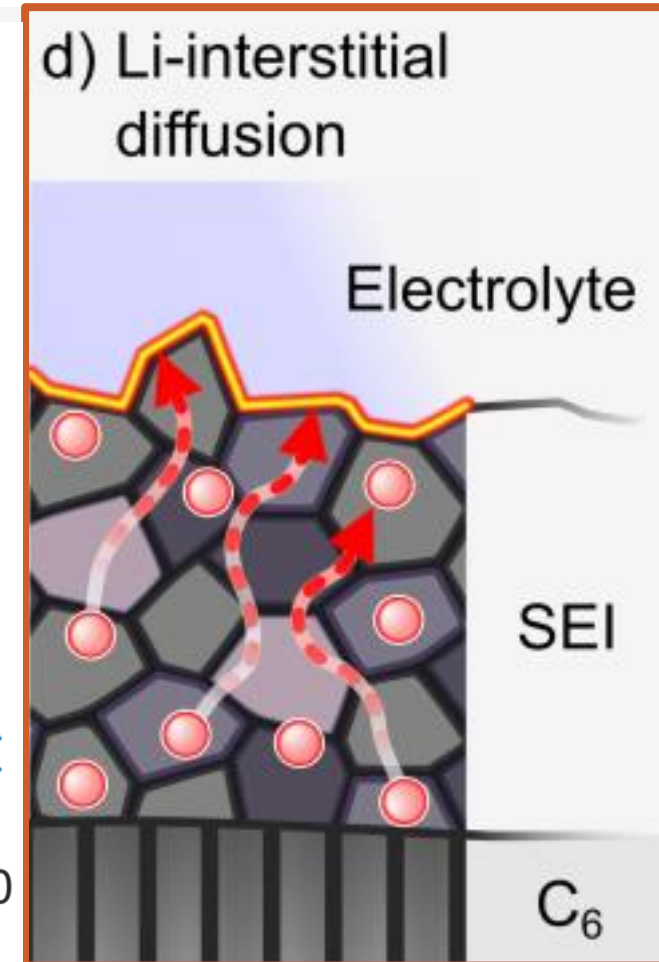
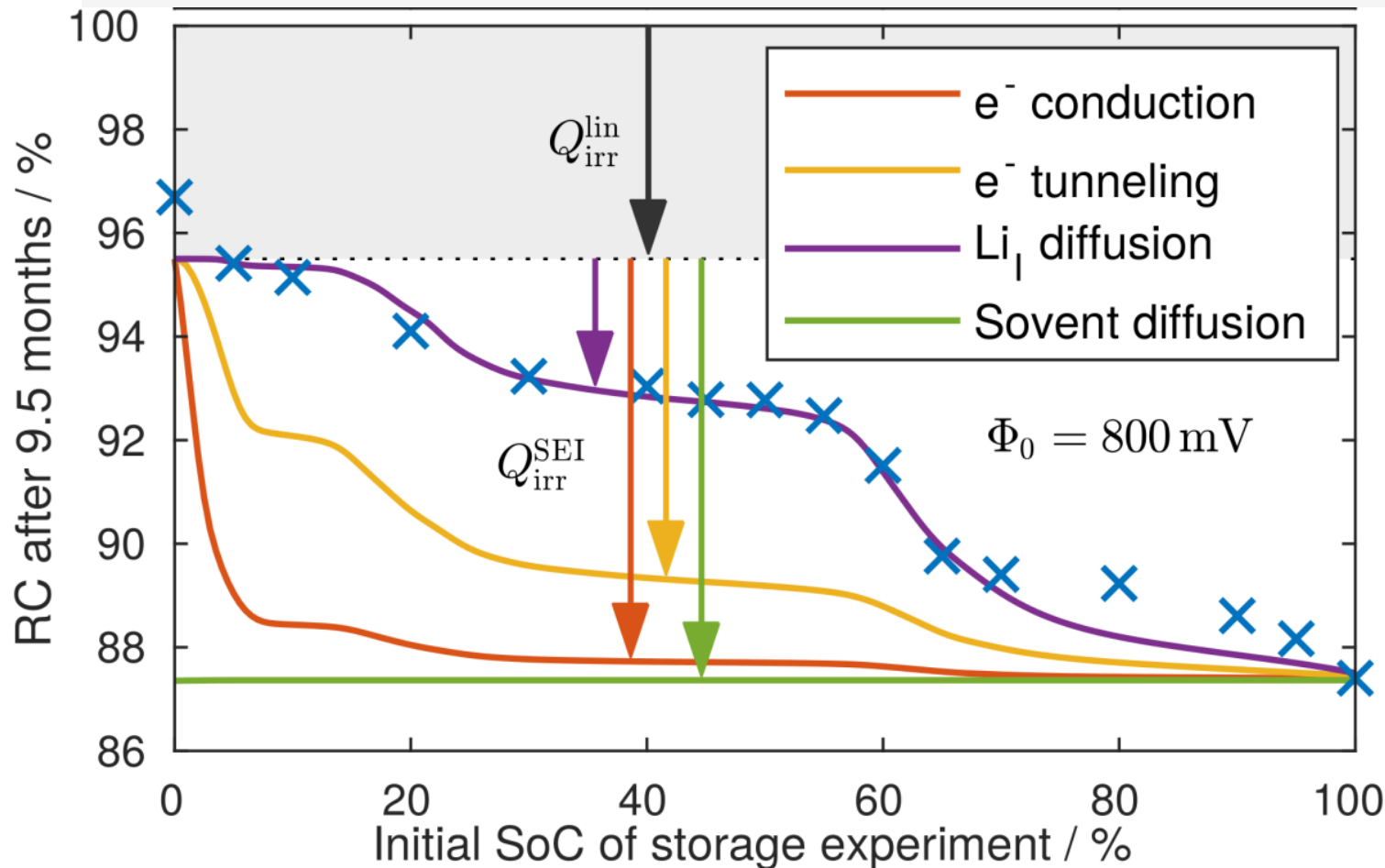
Physics-based Model for Battery Cycling and Aging

Multi-scale problem

- **Cell scale:** ions flow between electrodes
- **Particle scale:** lithium diffusion in electrode particles
- **Interface scale:** reactions and degradation



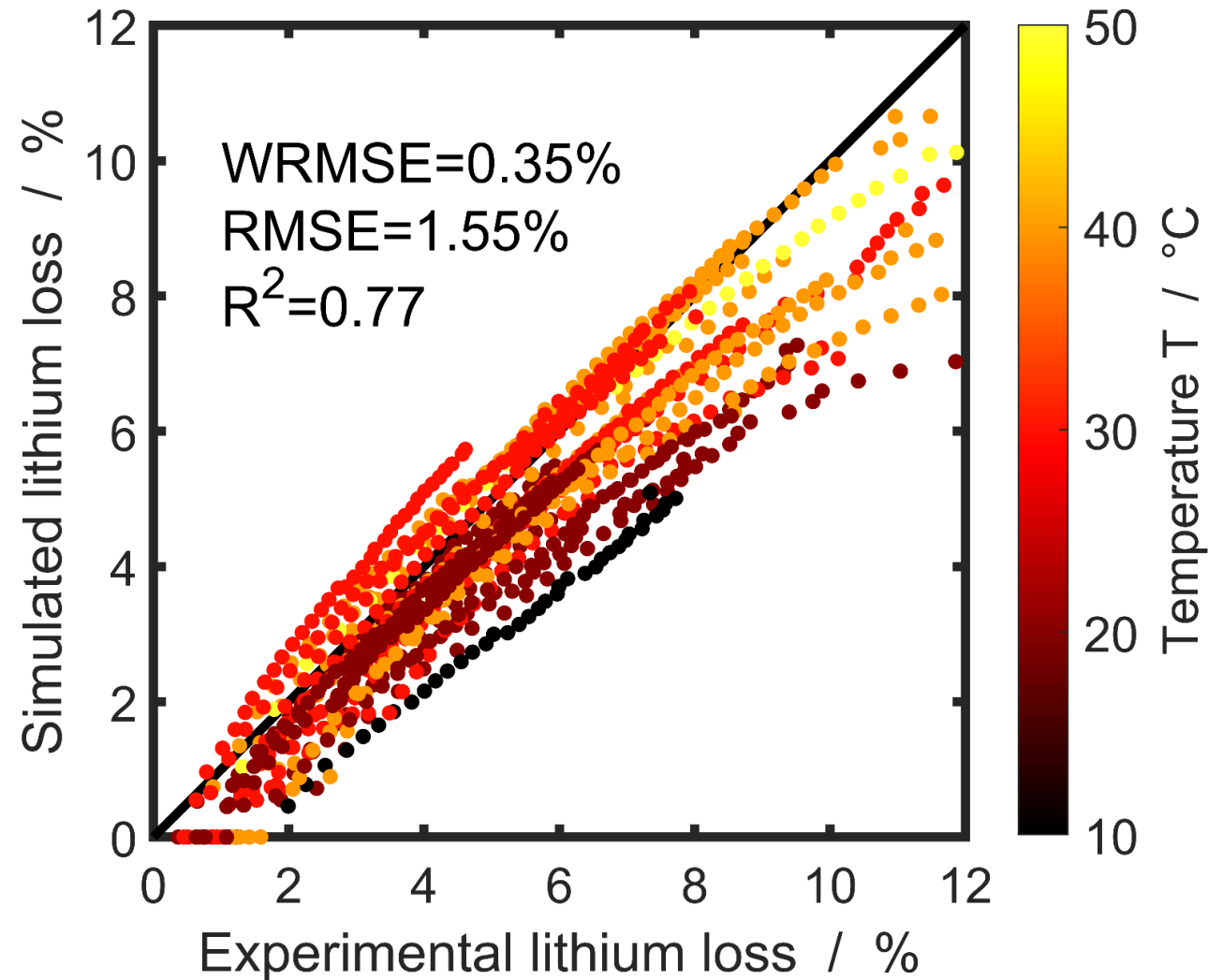
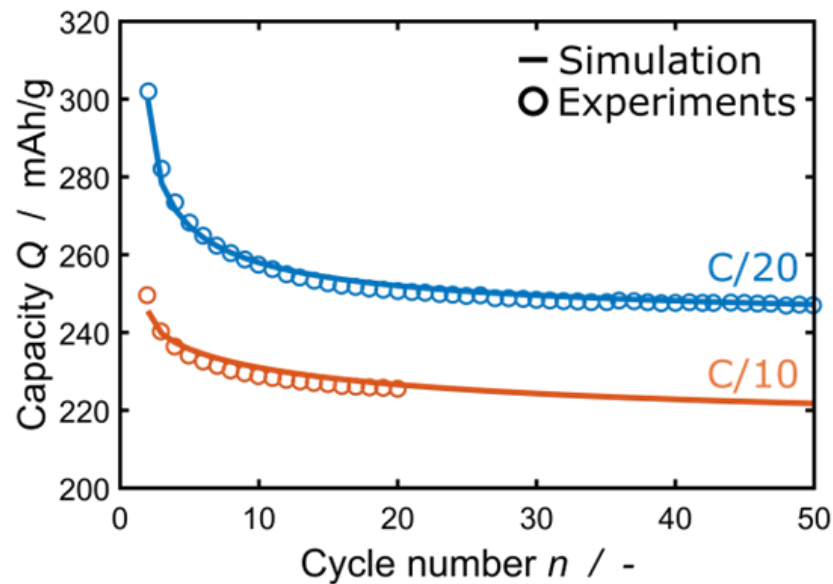
Identifying the Long-Term Growth Mechanism for Battery Storage



Validation for Battery Operation

Model performs well overall

- 62 large format pouch cells
- Driving cycle from automotive industry



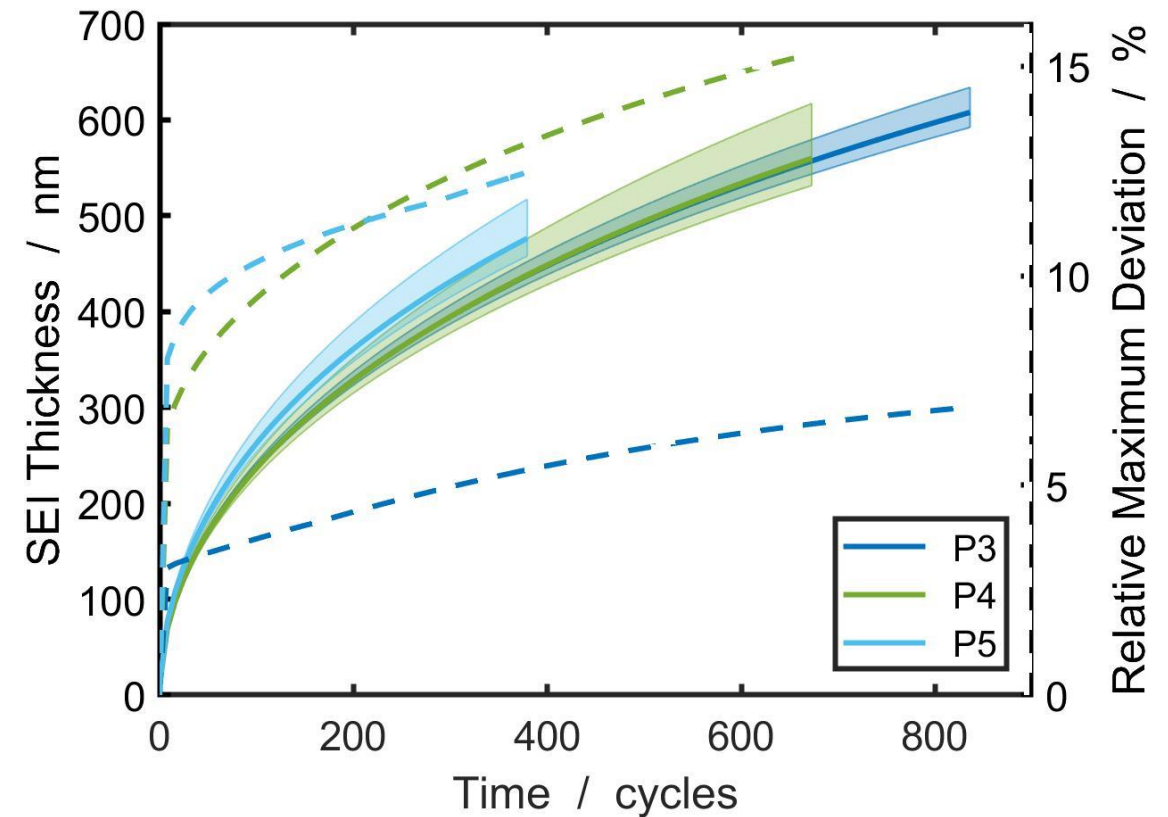
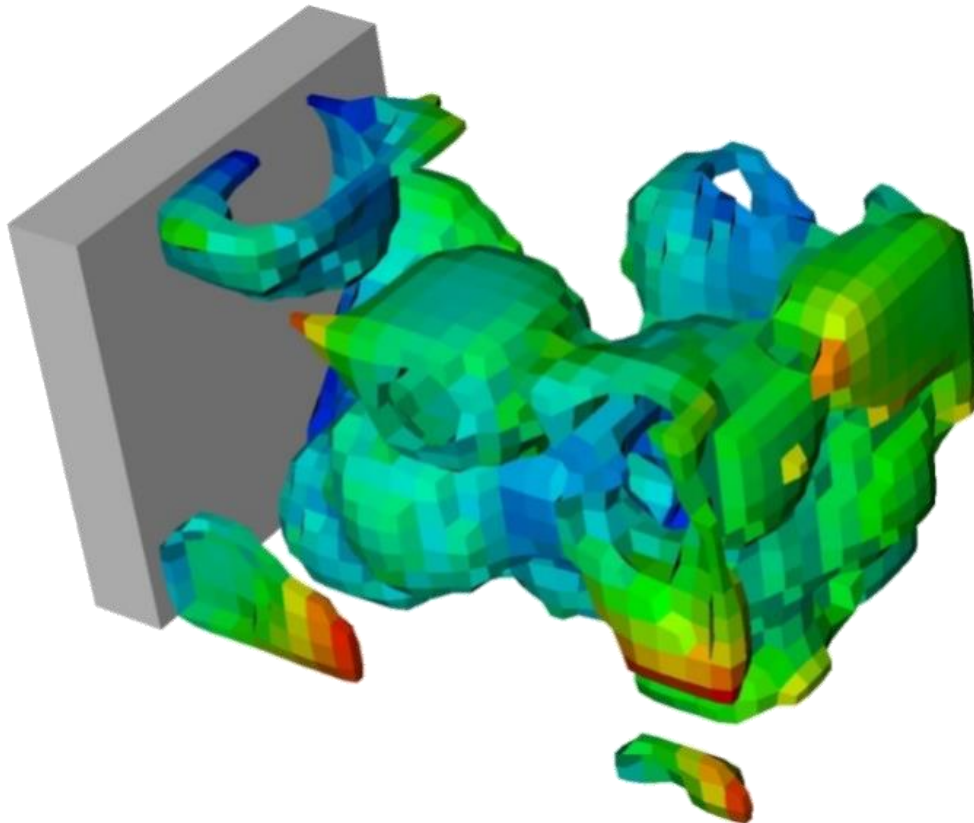
von Kolzenberg, Lars, Arnulf Latz, and Birger Horstmann.

ChemSusChem 13, 3901-3910 (2022).

von Kolzenberg, Lars, et al. *Journal of Power Sources* 539, 231560 (2022).

3D Micro-Structure Resolved Simulations

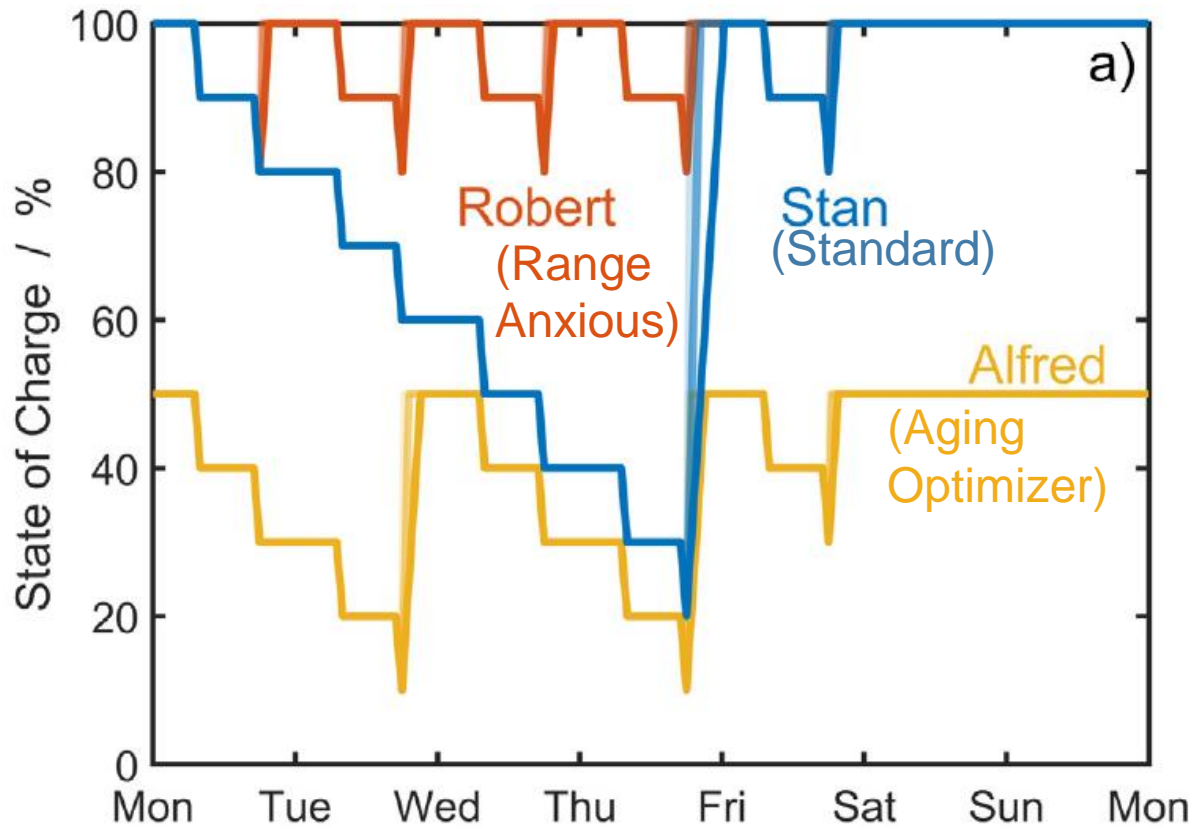
- Inhomogeneous Degradation



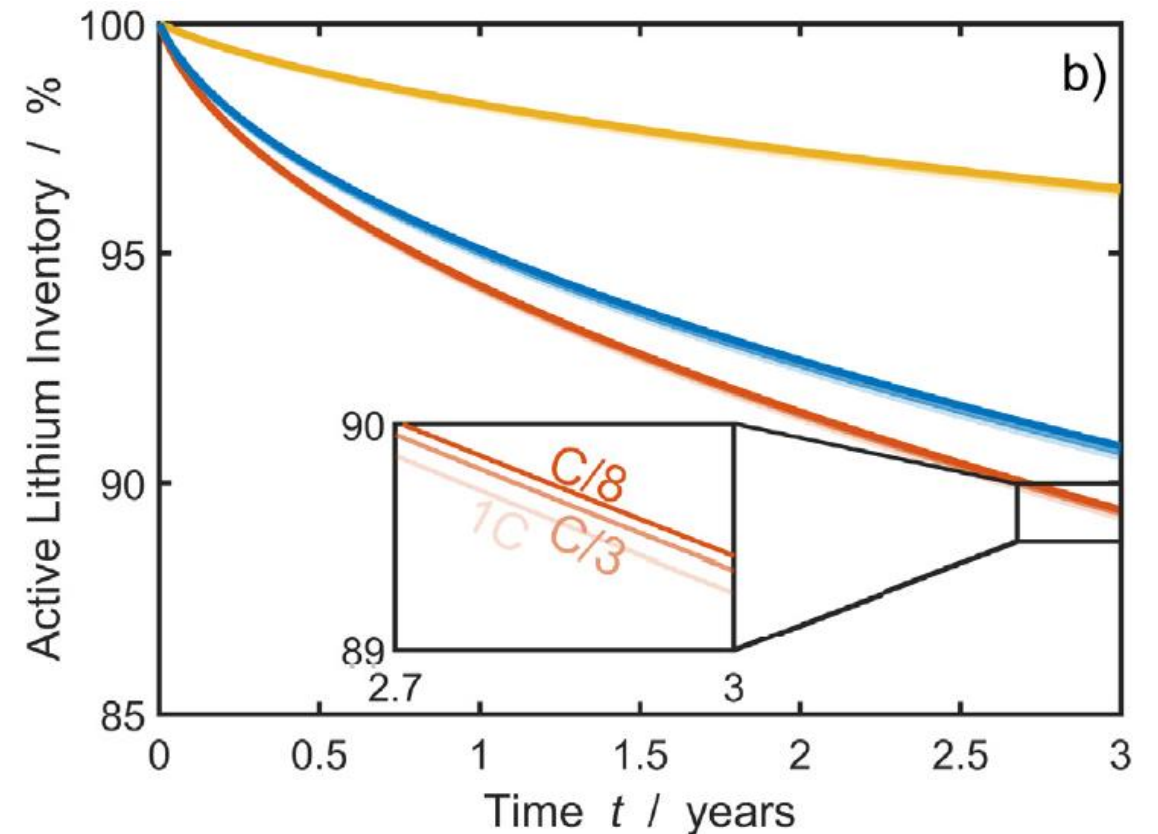
Bolay, Linda J., et al. *Journal of Power Sources Advances* 14, 100083 (2022).

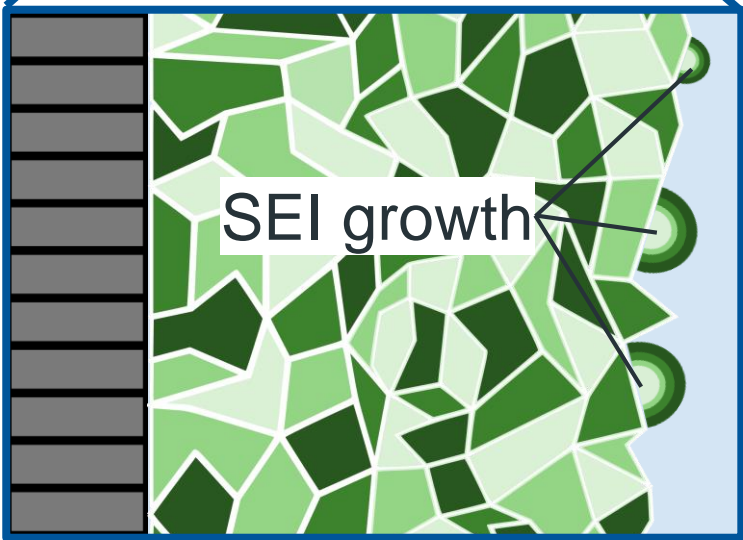
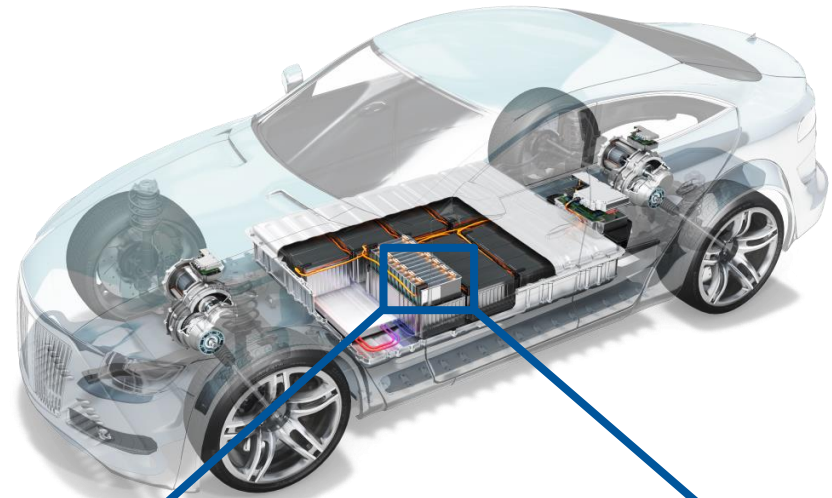
Extrapolation

Three real-life motivated use cases:

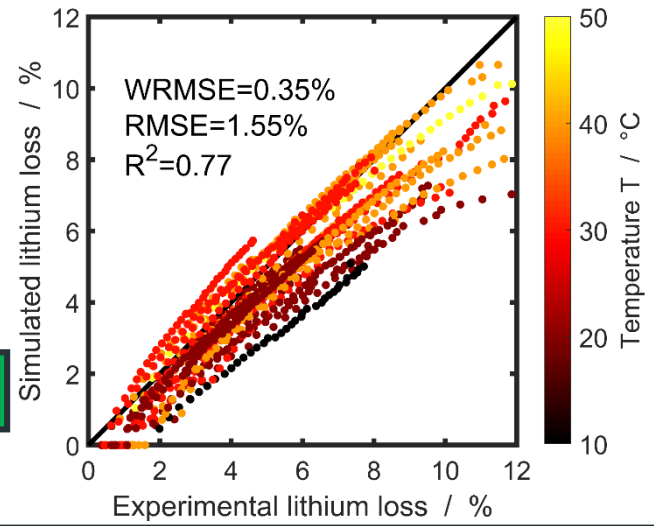


Mean SoC is main aging driver!
Charging Current of minor importance

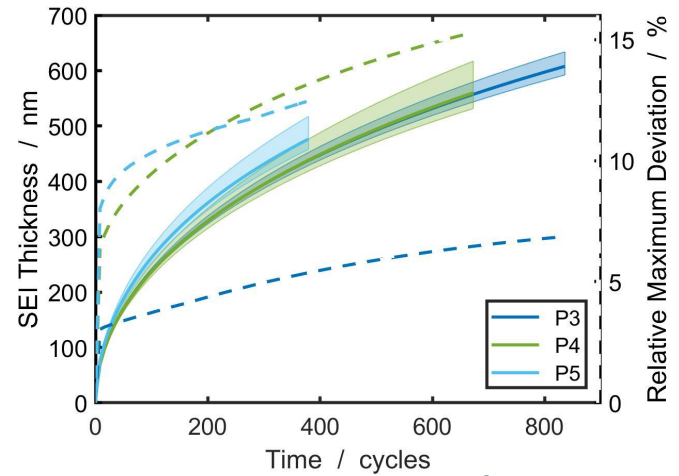
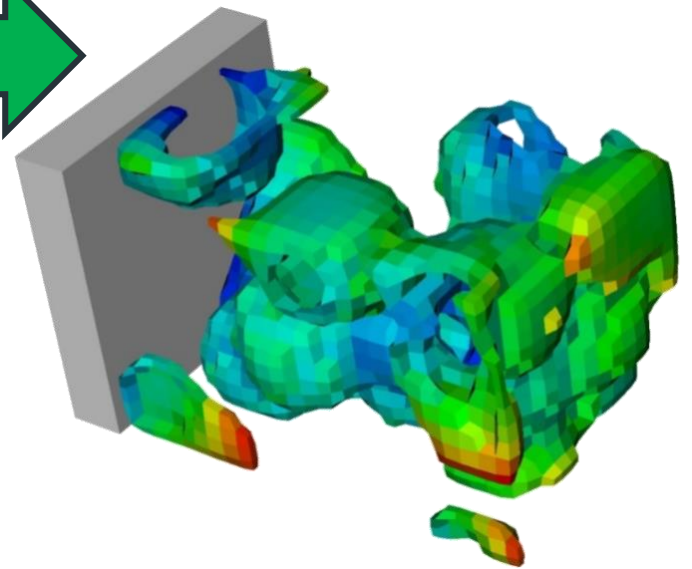




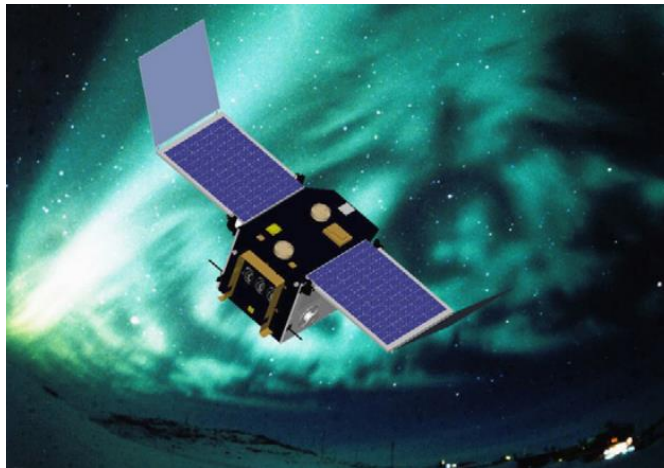
Battery Operation



Micro-structure

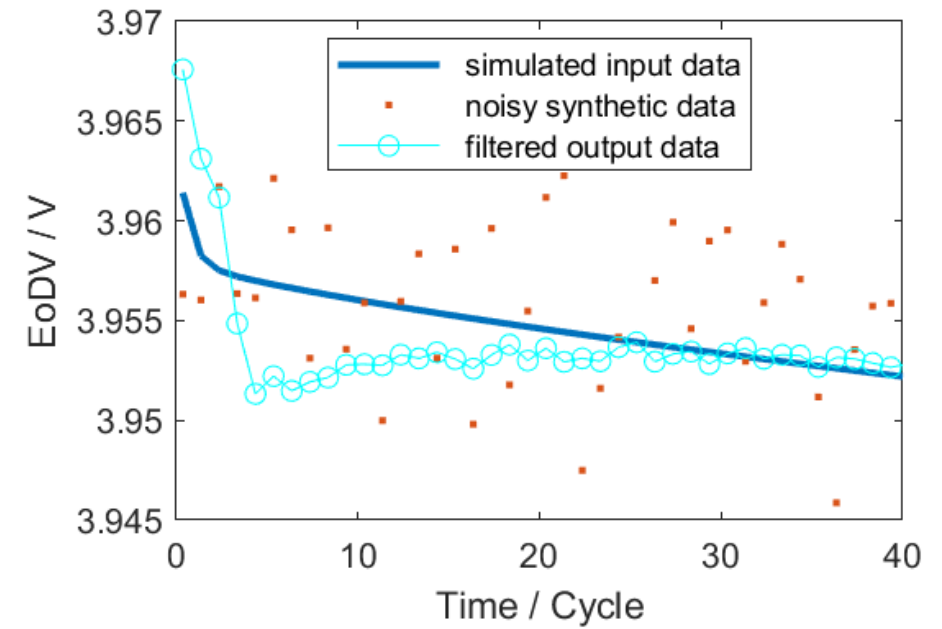
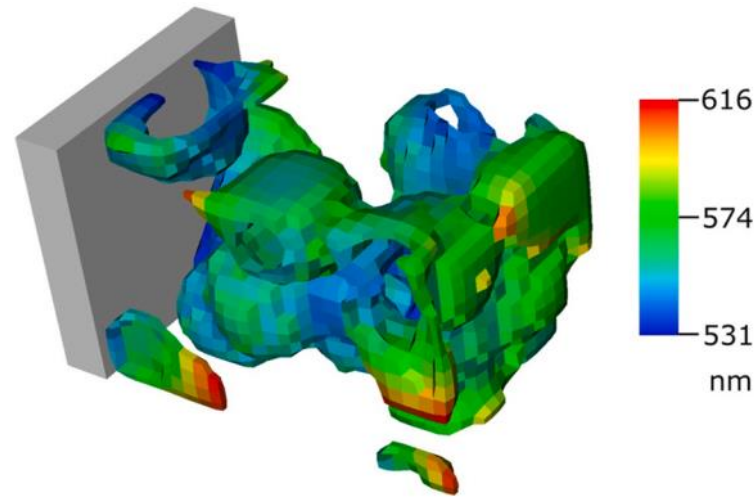


Remote monitoring of batteries



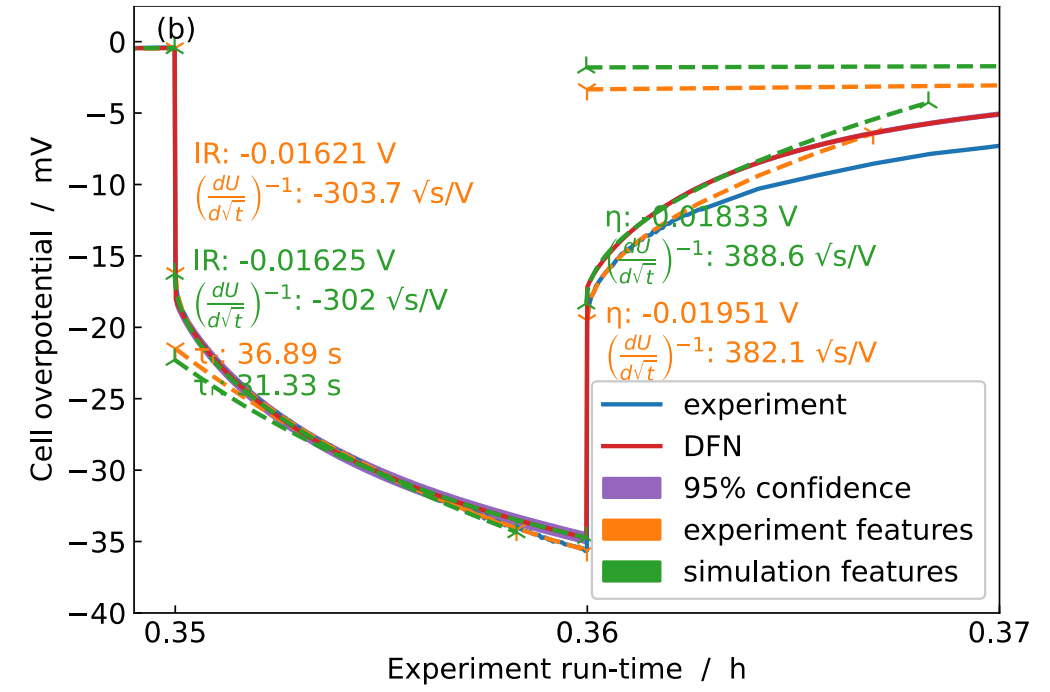
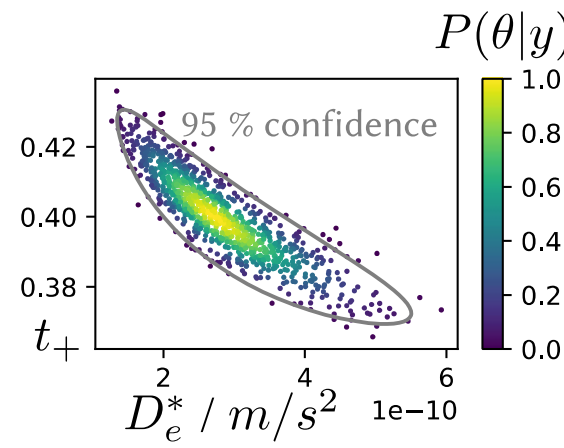
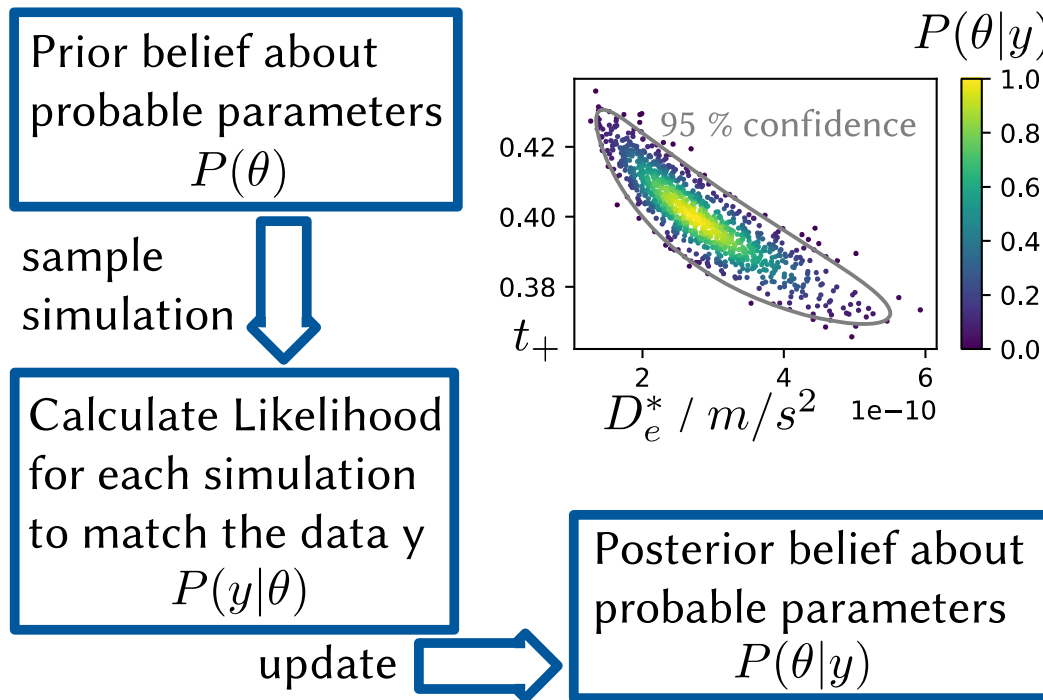
JAXA satellite REIMEI

DLR software BEST



Prediction of Battery health

Automatische Parametrisierung von Modellen



Thank you for your attention!



Bundesministerium
für Bildung
und Forschung

DFG


CELEST


DLR