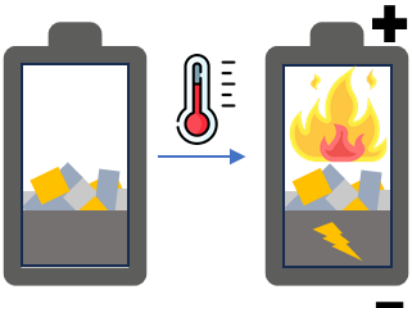
Karlsruher Institut für Technologie

Institute for Applied Materials
Electrochemical Technologies
Adenauerring 20 b
76131 Karlsruhe

Bachelor- / Master thesis / Internship

Study of thermal Degradation and Interfacial Layer Growth in Lithium-Ion Batteries



Field of Science

- ☒ Batteries
- ☐ Fuel Cells and Electrolyser
- ☐ Electrocatalysis

Focus

- ☐ Experimental
- ☐ Thermodynamic analysis
- ☐ Reaction chemistry
- ☒ Structuring Code
- ☒ Simulation
- ☒ Literature research

Studies

- ☒ Chemistry
- ☒ Chemical engineering
- ☒ Electrical engineering
- ☒ Mechanical engineering
- ☒ Computer Science
- ☒ Material science

Starting date

Immediately

Contact person

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Motivation

As electromobility and renewable energy storage technologies continue to advance, the demand for safe and thermally stable lithium-ion batteries is increasing. A major risk is thermal runaway a self-reinforcing process that may lead to cell rupture or explosion. The processes that trigger this behaviour begin long before the event occurs, at the molecular level of the interface between the anode and the electrolyte. This interface is known as the **solid electrolyte interphase** (SEI).

The SEI is made up of electrolyte decomposition products, and its properties are influenced by many factors, including electrolyte composition and cell charging conditions. The SEI is able to both significantly help or hinder battery performance, but it is not well-understood due to its complex and variable nature. Especially at elevated temperatures, the SEI may decompose, which can initiate self-reinforcing heat generation. The detailed mechanisms, particularly the interaction between exothermic and endothermic processes, as well as gas and heat evolution, are not yet fully understood. At IAM-ET, we have developed a novel 3-D Kinetic Monte Carlo modelling method that is able to simulate the complex molecular- scale electrochemical phenomena that influence SEI growth and behaviour. By understanding the fundamental mechanisms that drive SEI behaviour, we can inform the development of systems that generate more favourable SEIs, and thus lower the risk of thermal runaway. Depending on your interests, the thesis can focus on either developing models (100% simulation) or parameterising models supported by experiments (>50% simulation).
Possible tasks include:

- conducting a literature review on electrolyte degradation, thermal runaway, lithium-ion batteries and kinetic Monte Carlo modelling;
- Engage with the current model.

Focus: Model development

- Integration of new physico-chemical processes.
- Simulation of SEI formation and decomposition under various temperature conditions.

Focus: Parameter identification.

- Assembly of experimental 3-electrode battery cells.
- Electrochemical testing of experimental cells.
- Analysis and processing of experimental data for model building.

About us

We offer you excellent support and the opportunity to work in an interdisciplinary team in a pioneering field. You should be able to work independently and be motivated to familiarize yourself with new topics. If you are interested, please send your resume and current transcript of your grades, to Sebastian Frentzen.

Prof. Dr.-Ing. Ulrike Krewer