Karlsruher Institut für Technologie

Institute for Applied Materials
Electrochemical Technologies
Adenauerring 20 b
76131 Karlsruhe

Student thesis

Model-based Study of Electrolyte Decomposition and Interfacial Layer Growth in Sodium Ion Batteries

Field of Science

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

Focus

- ☐ Experimental
- ☒ Thermodynamic analysis
- ☒ Reaction chemistry
- ☐ Development of setups
- ☒ Simulation
- ☒ Literature research

Studies

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

Starting date

Immediately

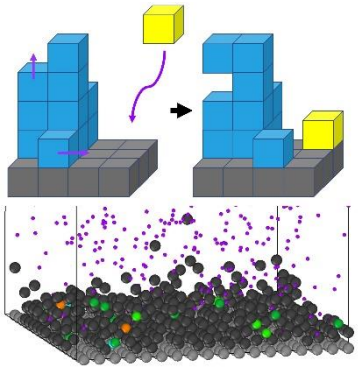
Contact person

Kie Hankins
Building 70.03
Room: 004
E-Mail: Kie.Hankins@kit.edu

https://www.iam.kit.edu/et/english/index.php

Motivation

Sodium ion batteries are promising candidates for sustainable next-generation enegy storage, but face challenges with long-term stability. One of the most significant driving forces of this instability is the degredation of the **solid electrolyte interphase** (SEI), a thin layer that forms on the anode surface. The SEI is made up of electrolyte decomposition products, and its properties are influenced by many factors, including electrolyte chemistry 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. At IAM-ET, we have developed a novel 3-D **Kinetic Monte Carlo** modeling method that is able to simulate the complex molecular-scale electrochemical behavior that influence SEI growth and behavior. By understanding the fundamental mechanisms that drive SEI behavior, we can inform the development of systems that generate more favorable SEIs, and thus more stable and effective batteries.



Tasks:

- Literature research on electrolyte degradation, SEI formation, sodium ion batteries, kinetic Monte Carlo modeling.
- Initial familiarization with the existing model.
- Possible implementation of new features to the model.
- Study of SEI formation and behavior

About IAM-ET:

We offer excellent supervision and the opportunity to work in an interdisciplinary team on a cutting-edge topic. The IAM-ET offers a constantly growing team with expertise in battery, fuel cell and electrocatalysis research focused on simulation (Campus East KIT) and experimental (Campus South KIT). Independent work and the motivation to work on current research topics are required. For further information, please contact Kie Hankins. If you are interested, please send your curriculum vitae and a current overview of your grades to kie.hankins@kit.edu.

Prof. Dr. -Ing. Ulrike Krewer