List of topics for research modules and theses

Powerful and safe batteries are of great importance for the realisation of a sustainable energy economy. The Battery Management Methods research group investigates innovative methods for increasing the service life and safety of current and next-generation battery systems.

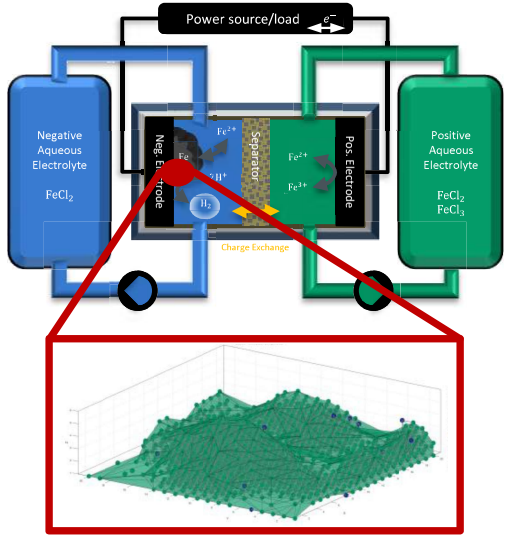
Methoden des Batteriemanagements

Modeling hydrogen evolution reaction (HER) in all-iron redox flow batteries using the kinetic Monte-Carlo method

The growing demand for cost-effective and environmentally friendly energy storage systems is driving the development of **iron-based redox flow batteries** (all-Fe RFBs). These are **hybrid systems**, as **metallic iron is deposited on the anode** during the charging process. Its practical implementation is currently limited by inhomogeneous Fe plating, hydrogen evolution reaction (HER), and pH instability [1].

The **kinetic Monte-Carlo method (kMC)** is suitable for a deeper understanding of the metallic deposition of iron. It can be used to represent molecular processes such as sorption, diffusion, and reactions on the electrode surface in detail [2].

The aim of this work is to **determine the reaction rates for HER** in a kMC simulation, taking into account the three sub-reactions: **Volmer, Heyrovsky, and Tafel steps**. The rates are to be parameterized **as a function of temperature, pH value, and the bonding properties** of graphite and metal surfaces are to be included [3].



3d-kMC model of anode surface with metal deposit (green) and intermediates of HER (blue)

Requirements:

- Basic knowledge of redox flow batteries
- Good programming skills (MATLAB)
- Communicative, reliable, and independent working style

Advantageous knowledge:

- Experience with the kinetic Monte Carlo method

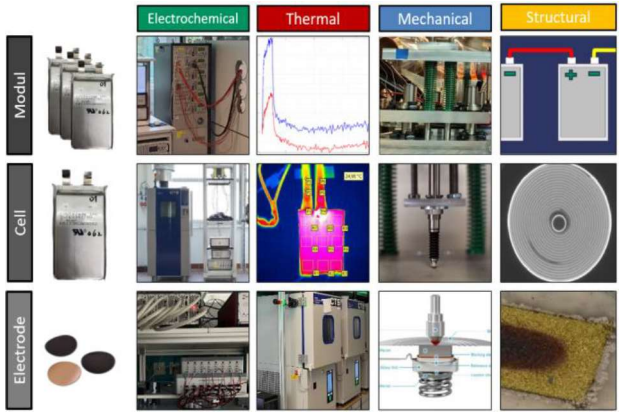
Contact:

Steffen Zappe
✉ steffen.zappe@uni-bayreuth.de

[1] Roth, Noack et al. (Hg.) 2023 – Flow batteries
[2] Andersen, Panosetti et al. 2019 – A Practical Guide to Surface Kinetic Monte Carlo Simulations
[3] Pašti, Leetmaa et al. 2016 – General principles for designing supported catalysts for hydrogen evolution reaction based on conceptual Kinetic Monte Carlo modeling

Methoden des Batteriemanagements

Multi-scale, multi-physics determination of charging limits in Li-ion cells



Fast charging is essential for electric mobility and high-utilization energy storage. However, it is limited by coupled electrochemical, thermal, and mechanical processes that are hard to observe in isolation[1]. Traditional testing across SoC–temperature–C-rate grids is slow and expensive, and it often misses the multi-physics and multi-scale interactions that actually set the limit. ILAB provides the tools to study these interactions directly and to design better charging strategies based on evidence [2], [3].

About the ILAB: The Intelligent Battery Laboratory (ILAB) is a multi-scale, multi-physics facility for research on fast charging and performance of lithium-ion cells.

We study batteries from the electrode level (materials and microstructure) to the full cell and module level. Our instruments capture electrochemical, thermal, mechanical, and structural in a synchronized way. This integrated approach allows us to connect local phenomena at the electrode (for example, lithium plating) to the behavior of the complete cell during fast charging. We provide both experimental and modeling capabilities. You can build and test your own cells, and then use physics-based models to interpret the results.

Required qualifications:

- Good experimental experience and programming skills (MATLAB)
- Knowledge of lithium-ion batteries
- Communicative, reliable & independent work style

Contact:

Hossein Harimi
✉ hossein.harimi@uni-bayreuth.de

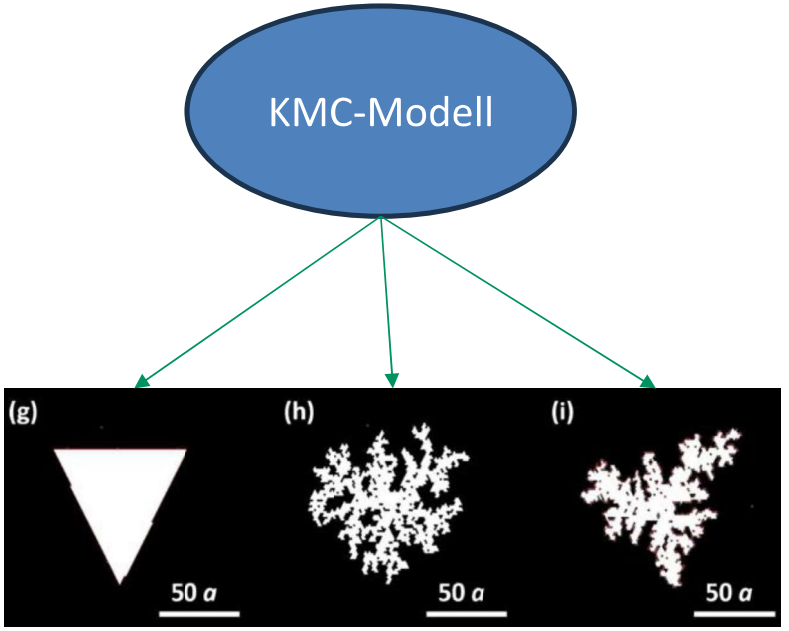
[1] Laue, V., Röder, F, Practical identifability of electrochemical P2D models, DOI: 10.1007/s10800-021-01579-5
[2] Bridging battery degradation and safety: Challenges and opportunities, 10.1016/j.etran.2025.100497
[3] Novel Operating Modes for the Charging of Lithium-ion Batteries, 10.1149/1945-7111/ac9a80

Methoden des Batteriemanagements

Simulation and quantification of 2D crystal growth using WSe2 as an example

This research module investigates the growth of WSe2 monolayers using Kinetic Monte Carlo (KMC) simulation [1]. The aim is to replicate the model developed by Nie et al. (2016) [2] using an existing Python framework. To this end, the energetic parameters, such as binding energies and diffusion barriers, must be extracted from the published DFT data and implemented in the simulation.

Another focus is on the development of a quantitative metric for lattice states. This should enable the stochastic simulation results to be classified objectively and ensure that morphologically equivalent structures are reliably identified under the same initial conditions.



Required qualifications:

- Programming skills (Python)
- Communicative, reliable and independent working style

Advantageous knowledge:

- Basic knowledge of kinetic Monte Carlo simulations

Contact:
Luis Henkelmann
✉ luis.henkelmann@uni-bayreuth.de

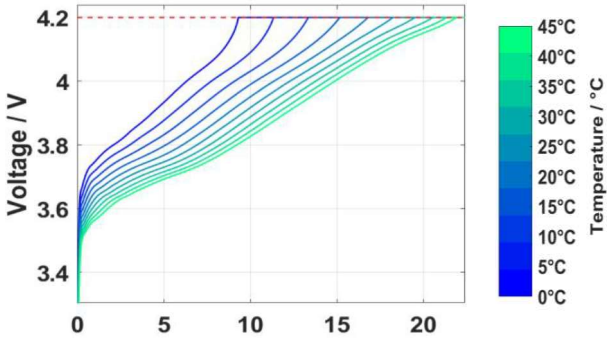
[1] Andersen et al. 2019 – A Practical Guide to Surface Kinetic Monte Carlo Simulations
[2] Nie et al 2016 - First principles kinetic Monte Carlo study on the growth patterns of WSe2 monolayer

Methoden des Batteriemanagements

Multi-scale, multi-physics determination of charging limits in Li-ion cells

You can select one of the following projects or combine elements to fit your interests and background. Each project has a clear experimental core, a modeling component, and a data analysis deliverable.

Si/C vs. graphite anodes under fast charging: build half-cells and full cells; measure OCV, EIS, and rate capability; quantify plating risk and thickness change; compare charging limits at different temperatures.



Fast Charging map: construct an SoC–temperature–C-rate map with safe and unsafe regions

NMC vs. LMFP cathodes: Comparative Entropy analysis of LMFP and NMC cathode materials

Optical cell studies: observe changes to the surface of the electrode during high-rate charging and correlate visual features (e.g. particle movement) in different electrode technologies.

Protocol optimization: use P2D model to charging profiles (e.g., multi-step CC) and validation with experimental cell.

Electrode microstructure and rate: analyze particle size distribution, and coating thickness from imaging; relate microstructure to diffusion length and rate capability.

Required qualifications:

- Good experimental experience and programming skills (MATLAB)
- Knowledge of lithium-ion batteries
- Communicative, reliable & independent work style

Contact:

Hossein Harimi
✉ hossein.harimi@uni-bayreuth.de

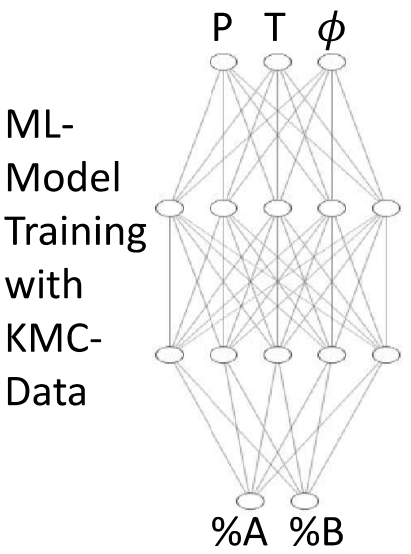
[1] Laue, V., Röder, F, Practical identifability of electrochemical P2D models, DOI: 10.1007/s10800-021-01579-5
[2] Bridging battery degradation and safety: Challenges and opportunities, 10.1016/j.etran.2025.100497
[3] Novel Operating Modes for the Charging of Lithium-ion Batteries, 10.1149/1945-7111/ac9a80

Methoden des Batteriemanagements

Data-driven prediction and optimisation of electrochemical selectivity

Determining the selectivity of electrochemical processes is a central topic in research on electrochemical reactions. Kinetic Monte Carlo (KMC) simulations [1] provide precise insights into reaction pathways and product distributions [2]. However, due to the high computational effort involved, targeted optimization of the input parameters using classical KMC methods is only possible to a limited extent.

In this work, the prediction of selectivity is to be replaced by machine learning (ML). The ML model is trained based on training data from KMC simulations to predict selectivity directly from the input parameters. The model is then used to identify conditions that favor the formation of the desired product. Optionally, the predictions are verified by KMC simulations and compared with the results of conventional KMC-based optimization to evaluate the performance of the ML approach.



Required qualifications:

- Basic Knowledge Machine Learning
- Programming skills (Python)
- Communicative, reliable and independent working style

Advantageous knowledge:

- Experience in developing and training AI models

Contact:

Luis Henkelmann
✉ luis.henkelmann@uni-bayreuth.de

[1] Andersen et al. 2019 – A Practical Guide to Surface Kinetic Monte Carlo Simulations
[2] Wei et al 2025 - Voltage-Dependent Electrochemical Carbon Dioxide Reduction Mechanism Unveiled by Kinetic Monte Carlo Simulation

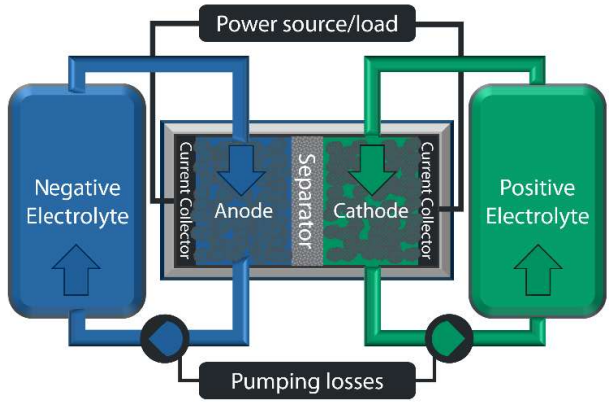
Methoden des Batteriemanagements

Further development of a continuum model and BMS for analyzing Fe plating and inhomogeneities in all-Fe redox flow batteries

The growing demand for sustainable and cost-efficient energy storage systems is driving the development of **iron-based redox flow batteries**. The all-Fe RFB is a **hybrid system** in which **metallic iron is deposited on the anode** during the charging process. Its technical implementation is limited by inhomogeneous Fe plating, hydrogen evolution reaction (HER), and pH instabilities [1].

For safe and efficient operation, a **battery management system (BMS)** is required that visualizes both the **state of charge (SoC)** and **state of health (SoH)** and uses this information to **control operating parameters** such as pH value, electrolyte flow, current intensity, and recombination cells [2].

The aim of this work is to **further develop an existing 0d continuums model** to describe the processes in the cell and a tank model for concentration balancing. Attention is paid to **inhomogeneities** in current density, pH value, and concentration distribution, and to the **use of recombination cells** [3,4].



[3]

Requirements:

- Basic knowledge of redox flow batteries
- Good programming skills (MATLAB)
- Communicative, reliable, and independent working style

Advantageous knowledge:

- Basic knowledge of continuum modeling

Contact:

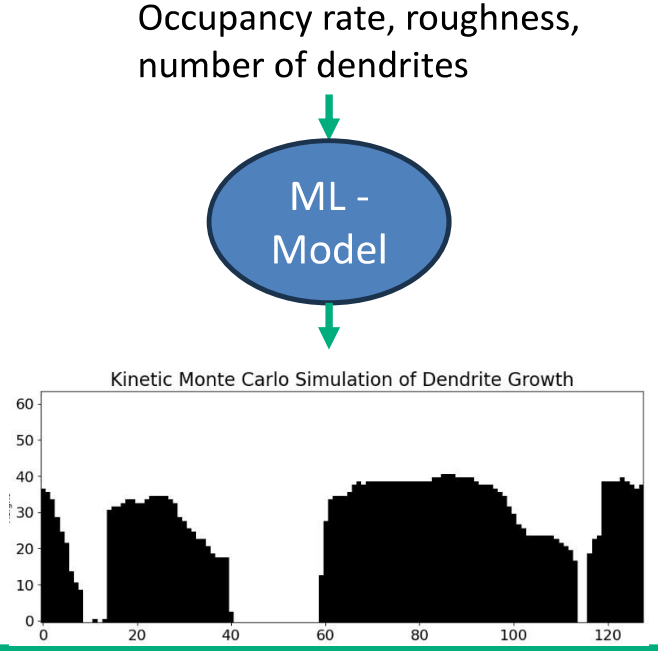
Steffen Zappe
✉ steffen.zappe@uni-bayreuth.de

[1] Roth, Noack et al. (Hg.) 2023 – Flow batteries
[2] Noack, Wernado et al. 2020 – Studies on Fe/Fe Redox Flow Batteries with Recombination Cell
[3] D'Adamo, Badenhorst et al. 2025 – Modeling an All-Copper Redox Flow Battery for Microgrid Applications: Impact of Current and Flow Rate on Capacity Fading and Deposition
[4] Chakrabarti, Kalamaras et al. 2020 – Modelling of redox flow battery electrode processes at a range of length scales: a review

Methoden des Batteriemanagements

Generative AI for reconstructing lattice structures from lattice statistics in KMC models

In classical kinetic Monte Carlo (KMC) models, lattice statistics such as occupancy rate, number of dendrites or the roughness of a profile can be read relatively easily. The aim of this work is to investigate whether generative AI methods can reconstruct or regenerate plausible dendrite structures on the lattice from such statistical data. In addition, we will examine whether the approach is also suitable for the efficient storage of simulation or measurement data and for the reconstruction of lattice structures from experimentally obtained statistics. This would allow a generative model to serve as a bridge between simulation and experiment.



Required qualifications:

- Basic Knowledge Machine Learning
- Programming skills (Python)
- Communicative, reliable and independent working style

Advantageous knowledge:

- Experience in developing and training AI models

Contact:

Luis Henkelmann
✉ luis.henkelmann@uni-bayreuth.de

[1] Mirzaee and Kamrava 2025 - Inverse design of microstructures using conditional continuous normalizing flows