Master 2 internship at CNRS in LRCS Lab (Amiens, France)

AI-Enhanced Phase Field Modeling for Lithiation Dynamics in Li-ion Battery Cathodes: A Data-Driven and Physics-Informed Approach

Laboratory: LRCS lab (CNRS)
Address: 15 Rue Baudelocque, 80000 Amiens, France
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Required skills: Physics, Machine/Deep Learning, Python coding
Contract dates: from March to July 2025
Salary: 578€/month (net)
Keywords: Phase field, Lithiation Dynamics, Deep learning, Physics-informed model, battery

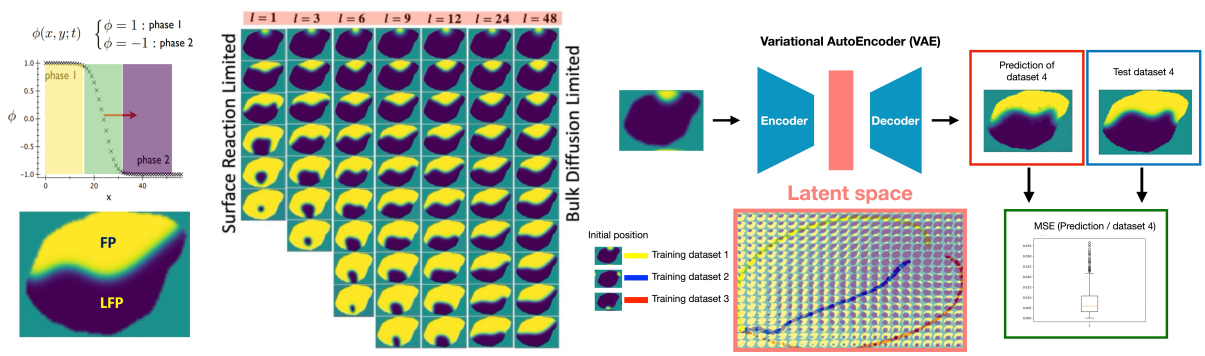

Figure-left. Preliminary results of our Allen-Cahn phase field model on the lithiation dynamics based on a real particle morphology in which surface reaction limited and bulk diffusion limited modes have been identified as a function of the kinetic parameter ***l***. **Figure-right.** Schematics of the VAE data-driven approach. Three Ph-F simulations are performed, and their time evolution is used as training data for VAE. A fourth simulation is performed (Test dataset) and compared with the prediction from the DL algorithm. The deviation (boxplot) is measured via MSE (Mean Square Error).

Context and Objectives

The performance, durability, and safety of lithium-ion batteries are intrinsically linked to the dynamics of lithiation and phase transformations in their cathode materials. The internship project aims to develop a novel methodology to study these dynamics at the microscopic scale, integrating Phase Field (PhF) modeling and machine learning approaches, such as Variational Autoencoders (VAE) and Physics-Informed Neural Networks (PINNs).

The intern will contribute to an **advanced numerical framework** that combines:

- **Phase Field Modeling** based on the Allen-Cahn approach to simulate lithiation dynamics in realistic cathode particle morphologies.

- **Machine Learning Approaches** (VAE and PINNs) to optimize simulation efficiency, reduce computational costs, and improve predictive capabilities.

Key Tasks
The selected candidate will be involved in:

1. **Phase Field Simulations**
   - Implement and optimize PhF models to describe lithiation/delithiation dynamics.
   - Incorporate realistic boundary conditions for electrode/electrolyte interfaces.
   - Analyze microstructural evolution during battery cycling.
2. **Machine Learning for Accelerated Simulations**
   - Train **Variational Autoencoders (VAE)** to interpolate and predict phase transformations.
   - Implement **Physics-Informed Neural Networks (PINNs)** to enforce physical consistency in simulations.
   - Explore data-driven surrogate models to reduce simulation time.

Required Skills :

- **Computational Physics / Materials Science**: Familiarity with **phase field models**, diffusion-reaction processes, or battery materials is an advantage.
- **Programming & Simulation**: Experience with **Python, AI libraries and numerical solvers** is a plus.
- **Machine Learning**: Basic understanding of **deep learning (PyTorch/TensorFlow)**; prior experience with **autoencoders, physics-informed AI, or generative models** is a plus.
- **Motivation for Interdisciplinary Research**: Enthusiasm for bridging physics-based modeling, and complexed AI development.

Expected Outcomes :

- Development of a **computational framework** for studying lithiation dynamics.
- Implementation of **VAE and PINN models** for accelerating and improving predictions.
- Comparison of numerical results, leading to potential publication.

Application Process:

Interested candidates should send:

- A **CV**
- A **motivation letter** outlining relevant experience and interest in the project

This internship offers a unique opportunity to work at the interface of **computational materials science, battery research, and AI-driven modeling**, contributing to the next generation of energy storage technologies.