NETWORK OF RESEARCH PILOT LINES
FOR LITHIUM BATTERY CELLS

Modeling and simulation of cells

Date and time:

Part 1: 27 October 2021 – 14:00 - 16:00pm

Part 2: 28 October 2021 – 14:00 - 16:00pm

Computational multi-scale modeling plays key roles in Battery designing and manufacturing which ranges from atomic scale to macroscale. Atomistic scale modeling produces the fundamental physical and chemical characteristics of the materials such as diffusion pathways and coefficient, structural evolution, and phase transition and therefore help to modify and design the materials from the atomic level. However, for optimizing the processing conditions to achieve the desired cell performance the physics-based electrochemical modelling play essential role. In addition, recent ML methodologies provide a platform to accelerate the modelling process and derive models to predict the behaviour of cell on special conditions. In addition, ML-based algorithms are employed to discover new materials consist desired properties predict the properties of materials. The first part of this virtual training starts by introducing various strategies of modelling in Battery designing and manufacturing such as atomistic modelling, electrochemical model and ML. Then, the details of atomistic modelling and its capability in battery designing and it´s integration with ML will explains. Furthermore, it will provide basic concepts of designing physics-based electrochemical model and the insights they provide on the processing-performance mapping using case studies.

After a general introduction to the different model scales, this training will focus on the continuum scale models as well as in ML models. The main aspects and purposes of such models will be discussed. Continuum model equations will be described as well as state of the art in numerical algorithms and optimization algorithms will be briefly mentioned. Model parametrization aspects will be described as well as the required parameters for each of the models will be enumerated. Similarly, the general overview of the current ML models for battery predictions will be described showing the advantages of these models in computation costs. Finally, some examples of the usage cases will be shared for both models. This training is suitable for theoretical and experimental researchers alike as well as managers to have a basic understanding of model development and design principles. Participants are only expected to have a basic understanding of the working of an electrochemical cell.

Learning outcomes

This virtual training empowers you to:

- understand the atomistic modeling and its application in battery designing
- identify ML methodologies and its application in prediction battery behavior
- understand the elements in electrochemical modeling for lithium-ion batteries
- identify the relation of processing conditions to electrode microstructure and cell performance
- learn how to tune the model for more realistic simulations

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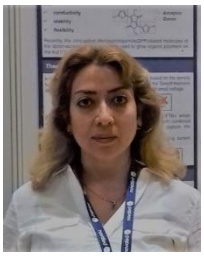
- understand the scope and approach of continuum models
- understand how model-based design can be applied to real usage
- understand how models can accelerate the battery parametrization activities

Who are the experts?

Part 1



Dr. Seddigheh Nikipar is the Team lead for ABEE Battery modelling Platform. She leads the activities related to developing software for multiscale modeling in Lithium ion and Solid-State Batteries (ranging from atomistic to microstructure scale). She has managed several scientific projects in atomistic and large-scale ab initio modeling of molecular structures & nano materials through applying first principles techniques in physics (e.g., DFT, DFTB & NEGF) integrated with programing in Fortran, C++, Python, MATLAB. In addition, she executed projects in computational physics and numerical modeling of semiconductor & mesoscopic devices, optical systems (localized plasmon resonance) and optimization performance of lithium battery cells based on FEM methods within ANSYS, COMSOL. She represents ABEE in H2020 EU projects, such as Safelimove, SUBLIME and Defacto.

Part 2

Ms. Elixabete Ayerbe is a Team Leader in Modeling and Post-mortem in the Materials for Energy Unit of CIDETEC Energy Storage, coordinating the activities related to multiphysics and data-driven models, as well as the parameterization and post-mortem analysis for Li-ion and advanced Li-ion batteries. She is currently coordinating H2020 DEFACTO project and coordinated in the past the FP7 SHEL project. In addition, she represents the multiphysics modeling activity of CIDETEC in several H2020 EU projects, such as SPICY, HIFI ELEMENTS, SPIDER, CoFBAT, BIG-MAP and Battery2030PLUS, and leads the area of Manufacturability in Battery 2030+ initiative.

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