TIME TABLE

TIME	Monday	Tuesday	Wednesday	Thursday	Friday
	September 25	**September 26**	**September 27**	**September 28**	**September 29**
09.00 - 09.45	Registration	Qi	Janek	Howey	Howey
09.45 - 10.30	Wall	Qi	Janek	Howey	Howey
11.00 - 11.45	Latz	Janek	Latz	Howey	Qi
11.45 - 12.30	Latz	Janek	Latz	Latz	Wall
14.00 - 14.45	Janek	Wall	Borodin	Borodin	
14.45 - 15.30	Janek	Wall	Borodin	Borodin	
16.00 - 16.45	Wall	Knobbe	Chen	Qi	
16.45 - 17.30	Poster/slide flash	Knobbe	Chen	Qi	
18.00	Welcome aperitif				

ADMISSION AND ACCOMMODATION

The course is offered in a hybrid format giving the possibility to attend the course also by remote (on Microsoft Teams platform). On-site places are limited and assigned on first come first served basis.
The registration fees are:

- **On-site participation, 600.00 Euro + VAT***
This fee includes a complimentary bag, five fixed menu buffet lunches, hot beverages, downloadable lecture notes.
Deadline for on-site application is August 25, 2023.

- **Online participation, 250.00 Euro + VAT***
This fee includes downloadable lecture notes.
Deadline for online application is September 13, 2023.

Application forms should be sent on-line through the following web site: http://www.cism.it
A message of confirmation will be sent to accepted participants.

Upon request a limited number of on-site participants can be accommodated at CISM Guest House at the price of 35 Euro per person/night (mail to: foresteria@cism.it).

** where applicable (bank charges are not included)*
Italian VAT is 22%.

CANCELLATION POLICY

Applicants may cancel their registration and receive a full refund by notifying CISM Secretariat in writing (by email) no later than:
- August 25, 2023 for on-site participants (no refund after the deadline);
- September 13, 2023 for online participants (no refund after the deadline).
Cancellation requests received before these deadlines will be charged a 50.00 Euro handling fee. Incorrect payments are subject to Euro 50,00 handling fee.

GRANTS

A limited number of participants from universities and research centres who are not supported by their own institutions can request the waiver of the registration fee and/or free lodging.
Requests should be sent to CISM Secretariat by **July 25**, **2023** along with the applicant's curriculum and a letter of recommendation by the head of the department or a supervisor confirming that the institute cannot provide funding. Preference will be given to applicants from countries that sponsor CISM.

For further information please contact:
CISM
Palazzo del Torso - Piazza Garibaldi 18 - 33100 Udine (Italy)
tel. +39 0432 248511 (6 lines)
e-mail: cism@cism.it | www.cism.it

Centre International des Sciences Mécaniques
International Centre for Mechanical Sciences
ACADEMIC YEAR 2023
The Morton Gurtin Session

BATTERIES - BASIC PRINCIPLES, EXPERIMENTAL INVESTIGATIONS AND MODELING ACROSS SCALES

Advanced School
coordinated by

Arnulf Latz
German Aerospace Center at the Helmholtz Institute
Ulm for Electrochemical Energy Storage
Germany

Wolfgang Wall
Technical University of Munich
Germany

Udine ***September 25 - 29*** **2023**

BATTERIES - BASIC PRINCIPLES, EXPERIMENTAL INVESTIGATIONS AND MODELING ACROSS SCALES

Batteries are considered to be a key technology in a future energy and mobility system based on renewable and fluctuating energy sources. Depending on the application, the specifications for energy density, power density, safety, and lifetime of batteries can vary considerably. Therefore, the need for optimization tools to balance application-specific conflicting constraints on batteries is obvious. In addition, the demand for rapid developments of new energy storage materials and battery designs requires the transition to a rational, knowledge-based battery development strategy based on validated models and sophisticated simulation tools. The challenge is to describe mathematically all electrochemical, physical, and mechanical processes necessary for an efficient and safe operation of batteries, which, for such highly complex electrochemical storage devices, means modeling and coupling processes on a large range of scales.

The course will cover theoretical methods as well as experimental insights on these different scales. Predictive modeling starting from Density Functional Theory calculations allow investigating thermodynamic, mechanical, and electrochemical stability of materials and combination of materials. They provide fundamental electrode material parameters to be used in the continuum modeling and give insights into the kinetics of electrochemical reactions. A crucial factor for the stability and power density of batteries is the choice of electrolyte. Finding the right compromise between electrochemical stability, excellent transport properties, and forming interfaces that support the reaction kinetics at positive and negative electrodes is a challenging task. The method of choice to investigate the behavior of electrolytes is molecular dynamics simulation (MD), either ab initio MD or classical MD, with fine-tuned force fields for the electrolyte under investigation. For optimizing the structural design of the electrodes and the cell design from nanometer to cm scale continuum theories are necessary to describe the complex interplay of transport, reactions, and mechanical processes during battery operation. To allow for a systematic coupling of continuum theories and underlying atomistic theories, it is important to derive continuum models within rigorous theoretical concepts. The course will give an introduction to state-of-the-art continuum modeling and simulation techniques for electrochemical as well as mechanical processes on electrode and device scales. This part will be complemented by an overview of experimental techniques for investigating battery behavior and validating continuum theories of batteries. On the largest scale, the system scale, simulation tools are required which maintain the essential features of the underlying detailed models but are systematically simplified to allow for real-time control of the battery operation in order to guarantee safety and preserve the lifetime of the battery. The description of the art of model reduction and real-time simulations of battery responses on system requests rounds up this CISM course.

The course aims at doctoral students as well as (junior) researchers, from different backgrounds, both from academia and industry. In the afternoon of the first day, a poster/slide flash will be held to give participants the opportunity to briefly present their interests or working area. This will enable fostering a collegial discussion during the course.

PRELIMINARY SUGGESTED READINGS

Overview:

A. Van der Ven, Z. Deng, S. Banerjee and S. Ping Ong, Rechargeable Alkali-Ion Battery Materials: Theory and Computation, Chemical Reviews 2020, 120, 14, 6977-7019 (Review).

DFT and MD Simulation:

M.P. Allen and Tildesley, "Computer Simulation of Liquids", Clarendon Press, Oxford, UK; Oxford University Press, New York; 1987.

D. Sholl and J. Steckel, “Density Functional Theory, a Practical Introduction”, Wiley; 2009.

F. Jensen, " Introduction to Computational Chemistry", Wiley. John Wiley and Sons, New York (1999).

Continuum Scale:

A. Kovetz, (2006). Electromagnetic Theory. Oxford: Oxford University Press.

J. Newman, J., & K. E. Thomas-Alyea. (2004). Electrochemical Systems. Wiley.

System Scale:

G. Plett, Battery management systems, Volumes 1 and 2, Artech House 2015.

For Battery Introduction and History:

M. Winter, B. Barnett, K. Xu, "Before Li-Ion Batteries" Chem. Rev. 2018, 118, 23, 11433-11456.

Lithium Batteries and Cathode Materials:

M. Stanley Whittingham, Chemical Reviews 2004, 104, 10, 4271-4302 (Review).

Electrolytes and Interphases in Li-Ion Batteries and Beyond:

K. Xu, Chemical Reviews 2014, 114, 23, 11503-11618 (Review).

LECTURES

All lectures will be given in English. Lecture notes can be downloaded from the CISM web site. Instructions will be sent to accepted participants.

INVITED LECTURERS

Oleg Borodin - Adelphi, Maryland, USA
4 lectures on: Molecular modeling of electrolytes with a focus on electrolyte electrochemical stability, oxidation/reduction of electrolytes vs HOMO/LUMO, electrical double layer structure and its importance to stability, SEI, the Li cation transport mechanism, transference number and its relations to electrolyte structure.

David Howey - University of Oxford, UK
5 lectures on: Overview of energy storage devices, Ragone plots. Electrical equivalent circuit models of batteries. Introduction to electrochemical models and deep dive on the single particle model. Pack modelling. Thermal models. Degradation models. Battery management systems.

Jürgen Janek - Justus-Liebig-Universität Gießen, Germany
6 lectures on: Overview on experimental approaches assessing cell behavior on different levels (atomistic, component, cell level). Electrochemical techniques, diffraction, spectroscopy, microscopy (in situ/operando). Transport of ions/electrons in active materials and electrolytes, interface kinetics, thermal and mechanical properties. Evaluation of energy, power density, capacity fading, aging, etc.

Arnulf Latz - German Aerospace Center at the Helmholtz Institute Ulm for Electrochemical Energy Storage, Germany
5 lectures on: Non equilibrium thermodynamics and statistical physics for ionic materials in electric fields. Free energy based derivation of transport theories and complex double layer formation in highly concentrated electrolytes. Models for electrochemical reactions. Microstructure resolved models of batteries. Upscaling from microstructure to extended porous electrode theory.

Yue Qi - Brown University, Providence, RI, USA
5 lectures on: Multiscale modeling strategy starts from Density Functional Theory (DFT) calculations and atomistic simulations. Predictive modeling of thermodynamic, mechanical, transport, and kinetic properties of the solid-state materials in batteries, including electrodes, solid electrolytes, solid electrolyte interphases (SEI), and interfaces.

Wolfgang A. Wall - Technical University of Munich, Germany
5 lectures on: Brief introduction to nonlinear continuum mechanics and coupled (monolithic & partitioned) multiphysics simulations. Coupled models for batteries with liquid electrolytes. Introduction to coupled thermo-electro-chemo-mechanical models for solid-state batteries. Modeling of electrode-electrolyte contact and thin layer in all-solid-state batteries.

GUEST LECTURERS

Long-Qing Chen - Pennsylvania State University, USA
Phase field modeling of batteries.

Edwin Knobbe - Battery Cell Competence Center, BMW AG, Germany
Challenges to simulate interaction of mechanics and electro-chemistry in battery cells – perspective of a cell developer.