TIME TABLE

TIME	Monday	Tuesday	Wednesday	Thursday	Friday
	September 21	September 22	September 23	September 24	September 25
9.00 - 9.45	Registration	xxxx	xxxx	xxxxx	xxxxx
9.45 - 10.30	Wall	xxxx	xxxx	xxxxx	xxxxx
11.00 - 11.45	Latz	xxxx	xxxx	xxxxx	xxxxx
11.45 - 12.30	Howey	xxxx	xxxx	xxxxx	xxxxx
14.00 - 14.45	Janek	xxxx	xxxx	xxxxx	
14.45 - 15.30	Borodin	xxxx	xxxx	xxxxx	
16.00 - 16.45	Qi	xxxx	xxxx	xxxxx	
16.45 - 17.30	xxxx	xxxx	xxxx	xxxxx	
18.00	Welcome Aperitif				

ADMISSION AND ACCOMMODATION

The registration fee is 600.00 Euro + VAT*, where applicable (bank charges are not included). The registration fee includes a complimentary bag, four fixed menu buffet lunches (on Friday upon request), hot beverages, downloadable lecture notes and wi-fi internet access.

Applicants must apply at least one month before the beginning of the course. 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. Applicants requiring assistance with the registration should contact the secretariat at the following email address: cism@cism.it.

Applicants may cancel their course registration and receive a full refund by notifying CISM Secretariat in writing (by email to cism@cism.it) no later than two weeks prior to the start of the course.

Cancellation requests received during the two weeks prior to the start of the course will be charged a 50.00 Euro handling fee. Incorrect payments are also subject to a 50.00 Euro handling fee.

A limited number of participants from universities and research centres who are not supported by their own institutions can be offered lodging and/or board, if available, in a reasonably priced hotel or student guest house.

Requests should be sent to CISM Secretariat by **July 21, 2020** 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.

Information about travel and accommodation is available on the web site www.cism.it, or can be mailed upon request.

* Italian VAT is 22%.

For further information please contact:
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ACADEMIC YEAR 2020
The Shinozuka Session
Centre International des Sciences Mécaniques
International Centre for Mechanical Sciences

BATTERIES - BASIC PRINCIPLES, EXPERIMENTAL INVESTIGATIONS AND MODELLING ACROSS SCALES

Advanced School
coordinated by

Arnulf Latz
German Aerospace Center
Ulm, Germany

Wolfgang A. Wall
Technical University of Munich
Germany

Udine ***September 21 - 25*** **2020**

BATTERIES - BASIC PRINCIPLES, EXPERIMENTAL INVESTIGATIONS AND MODELING ACROSS SCALES

This CISM course is aims at theoretical and experimental foundations of batteries and will cover the whole spectrum from atomistic over microstructure to cell and system scale. 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. The probability to identify a universal battery which could maximize all parameters simultaneously is very small. 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. This means for batteries as highly complex electrochemical storage devices to model and couple processes on all scales from Angstrom to Meter scale. The course will cover theoretical methods as well as experimental insights on all these scales. Atomistic theories allow investigating thermodynamic and electrochemical stability of materials and combination of materials. They provide fundamental electrode material parameters as e.g. diffusion coefficients or elastic constants and they give insights in the reaction kinetics for intercalation and conversion, the two main electrochemical reaction mechanisms in batteries, but also in the occurrence of unwanted side reactions. A very crucial factor for stability and power density of batteries is the choice of the electrolyte. Finding the right compromise between electrochemical stability, excellent transport properties and forming interfaces which 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. To find the best materials is by far not sufficient to guarantee optimal performance and life time of batteries. Both optimization variables are strongly influenced by the structural design of the electrodes and their constituents (particles of active materials, binder and electronic conduction enhancing additives) as well as on the cell design on micrometer to cm scale. To model these scales continuum theories are necessary to describe the complex interplay of transport, reactions and mechanical processes during operation of the battery. Contrary to ab initio density functional and molecular dynamic simulations which are based on rigorous theorems of quantum and classical mechanics, the continuum modeling approaches for processes beyond the molecular scale are often used heuristically. Fortunately, also continuum methods can be derived within rigorous theoretical concepts. This is especially important for allowing coupling to underlying atomistic theories and simulations on the scale of the electrode microstructure of electrochemical devices, where local in situ experimental methods to verify the simulation results are still rare. The course will give an introduction in state of the art continuum modeling and simulation techniques for electrochemical as well as mechanical processes on electrode and device scale. This part will be complemented by an overview over experimental techniques for investigating battery behavior and validating continuum theories of batteries. To optimize 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 a real time control of the battery operation in order to guarantee safety and preserve 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.

PRELIMINARY SUGGESTED READINGS

INVITED LECTURERS

Oleg Borodin - Electrochemistry Branch, Sensor and Electron Devices Directorate, Army Research Laboratory, Adelphi, MD, USA
X lectures on:
Molecular Dynamic simulations of electrolytes.

David A. Howey - University of Oxford, UK
X lectures on:
System modeling and diagnostics of batteries.

Jürgen Janek - Justus-Liebig-Universität Gießen, Gießen, Germany
X lectures on:
Experimental approaches for investigating battery behavior.

Arnulf Latz - *Deutsches Zentrum für Luft- und Raumfahrt e.V. (DLR) German Aerospace Center, Institute of Engineering Thermodynamics | Computational Electrochemistry and Helmholtz Institute Ulm for Electrochemical Energy Storage, Ulm*, Germany
X lectures on:
Theory based continuum modeling and microstructure simulation of batteries.

Yue Qi - Michigan State University, East Lansing, MI, USA
X lectures on:
Atomistic simulations of transport and kinetics in batteries.

Wolfgang A. Wall - Technical University of Munich, Germany
X lectures on:
Computational modeling of coupled thermo-electrochemo-mechanical phenomena on the continuum scale.

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.