Materials Research on Li-ion batteries and beyond

Minisymposium

Fr., May 06, 2022 from 14:00 – 17:30 h

Faculty of Chemistry, Seminar room 1, 2nd floor, Währingerstraße 38, 1090 Wien

Lectures

Fast charging, thermoregulation and aging of lithium-ion batteries: multi-scale and multi-domain modeling

Dr. Johann C. Wurzenberger, AVL List GmbH, Graz, Austria

Solid electrolytes for lithium-ion batteries

Dr. Alexander Beutl, AIT, Vienna, Austria

Electrochemical energy storage - insights from in operando measurements

Univ.Prof.Dr. Helmut Ehrenberg, KIT, Karlsruhe, Germany

Organizer: H. Flandorfer, F. Kleitz, Department of Inorganic Chemistry – functional Materials. In the framework of the "Seminar for Materials Chemistry", SS2022

Fast charging, thermoregulation and aging of lithium-ion batteries:

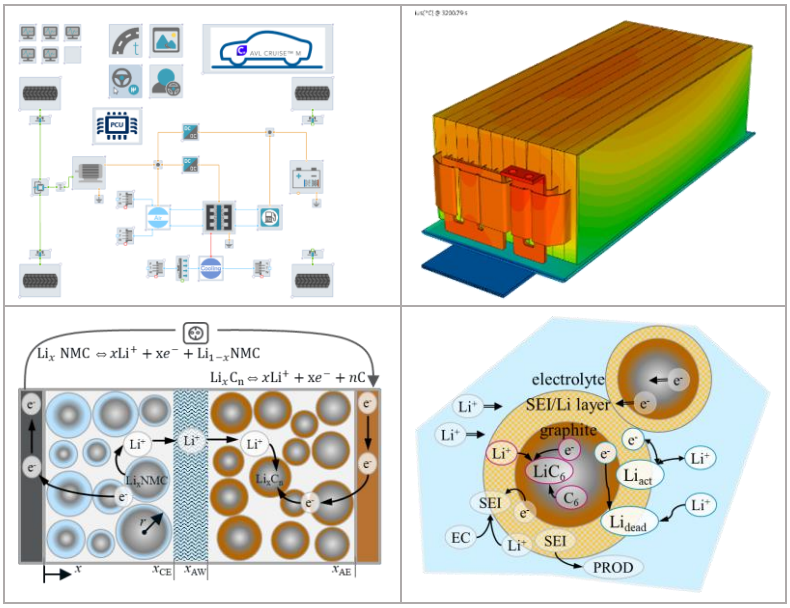
multi-scale and multi-domain modeling

Dr. Johann C. Wurzenberger, AVL List GmbH, Graz, Austria

Battery electric vehicles together with renewable energy sources are an attractive alternative to make future mobility more sustainable. Lithium-ion batteries have been established in recent years as a suitable energy storage technology in mobile applications in full-electric, plug-in electric, hybrid electric and fuel cell powered vehicles. Common requirements of these applications are high performance, capacity, long life and safety of the battery in operation. However, there is also application-specific demands derived from different vehicle classes, individual load profiles and driving ranges. Hence, one single battery design is not sufficient to meet all requirements. There is the need of customized battery systems to aim on approaching engineering limits. This is today's challenge for development engineers.

The use of virtual prototypes and model-based development methods is essential to meet the multitude of requirements in battery development in a timely manner. In addition, the performance of battery systems results from the interaction of phenomena on different spatial and temporal scales, which are difficult or even impossible to observe experimentally. Energy density and aging phenomena are strongly influenced by material properties and, at the same time, depend on the cell design, on the design of the battery pack, the thermoregulation system and the load requirements from the particular driving situation.

This paper deals with electrochemical and thermal modeling and simulation of lithium-ion batteries. The model considers different scales for vehicle, pack, modules, electrode and electrode-electrolyte interface. The different sub-models are discussed and validation comparisons to experimental data are shown. Several examples are presented for the application of the model. These include simulation of fast charging, thermoregulation, and cell aging.



Solid electrolytes for lithium-ion batteries

Dr. Alexander Beutl, AIT, Vienna, Austria

Electric vehicles are seen as one of the key ingredients in achieving the energy transition objectives that are set by more and more countries globally. Market volume predictions estimate 320 million units sold by 2040, which will make up a 40-50% share of the total sales market.

One of the main reasons for these optimistic prospects is the expected technological advancement and concomitantly performance increase of conventional lithium ion batteries, which seem to reach their limits regarding their specific energy (~200-250 Wh/kg).

In this regard, all-solid-state batteries have been the focus of research, promising higher energy density, faster charging rates, higher safety and lower cost. In such battery cells, the conventional electrolyte, which is based on volatile organic liquids, is exchanged with a solid ion conductor. The latter is selected from a variety of different materials, ranging from organic polymers to oxide ceramics. Although this exchange comes with some benefits (which are highlighted in news reports and press-releases of emerging battery start-ups) it also causes significant challenges and drawbacks.

In this talk a summary of solid-electrolyte development for lithium ion batteries will be given to enable a realistic evaluation of battery performance and future developments in the electric vehicle sector. Thus, a concise review of different electrolyte materials (polymers, sulfides, oxides) being used as solid-electrolytes for lithium ion batteries will be presented and their individual challenges and prospects will be discussed.

Electrochemical Energy Storage - Insights from in operando Measurements

Univ.Prof.Dr. Helmut Ehrenberg, KIT, Karlsruhe, Germany

Intermediate energy storage is one of the most important challenges for a successful transition into a sustainable energy technology based on fluctuating primary sources. Electrochemical energy storage is of high relevance for this purpose, because the high values for the energy efficiencies of the one-step transformations between electrical and chemical energy forms cause only low losses. The key performance indicators of electrochemical energy storage devices depend mainly on the properties of the battery materials used and their specific behavior in a battery cell. Therefore, a systematic optimization of batteries requires a solid knowledge of the working and degradation mechanisms of the involved materials during regular operation conditions. The highly reactive environments inside a cell and the pronounced interactions between the individual components require investigations by dedicated comprehensive and complementary in operando methods, supported by post mortem studies. This contribution presents and discusses in operando techniques using X-ray, synchrotron and neutron radiation with a focus on diffraction and their role in the development of battery materials. Selected examples are shown for Li-ion batteries but also for electrochemical energy storage “beyond lithium”, like Na- and Mg-batteries. During charge and discharge ions are alternatingly inserted and extracted from host structures accompanied with oxidation and reduction reactions. The underlying crystal structure is essential for the ionic transport properties, and the structural response during cycling reflects the working mechanism and changes during ageing and fatigue. Most reliable data are obtained from high-quality commercial cells, but sometimes specially designed test cells are used, especially at low technology readiness levels. Therefore, different types of in operando cells are also compared. Capabilities and challenges of in operando measurements are compiled and discussed.