The Fraunhofer Battery Alliance, consisting of 19 Fraunhofer institutes, carries out research in the field of electrochemical energy storage devices (batteries and supercapacitors) in order to develop technical and conceptual solutions for commercial applications. Particular consideration is given to the social, economic and ecological implications of the technology.

Beside materials, cell production, systems and testing, a further competence of the Alliance is in the field of simulation.

**Simulation activities range from quantum chemical methods for material characterization and physical continuum models for cell design through to real-time-capable battery models for integration into battery management systems, test stands or battery simulations in hardware-in-the-loop (HIL) systems.**

**Materials and atomistic processes**
Quantum chemical methods provide insights into the functioning of materials that cannot be obtained experimentally. This information deepens understanding of the properties of new materials and processes, for example those arising during the charging / discharging of a battery system. Macroscopic parameters, which determine the efficiency of the material, can be calculated using modern multi-scale processes. In addition, numerical simulation on the nanoscale offers the possibility of improving qualitative understanding of the basic processes involved.

**Electrode and cell design**
Beside the material properties, geometric factors also play an important role in the battery behavior at cell level. Based on the physical processes of ion, charge and heat transportation, models have been developed to enable one- and three-dimensional predictive simulations of battery cells.
The influence of the electrode microstructure (for example particle size and topology), and the influence of the macroscopic cell layout can also be investigated using a computer. Detailed local information about the conditions inside the virtual cell furthermore improves understanding of the specific cell properties.

**Cell structure and safety**
Numerical simulations can make an important contribution to predicting the failure of cells, for example where short-circuiting occurs under crash loads. Beside compression and bending tests on cells, extreme scenarios such as perforation can be analyzed, and the cell structure or protective casing can be optimized. For these simulations it is particularly important to use material models suitable for describing the behavior of the materials under high dynamic loads. Specialized material characterization provides the fundamental data necessary, which must then be connected with experiments to determine suitable failure or hazard criteria.

**System design**
Tailored and efficient simulation models are essential for the design of the entire system. Starting with the measurement analysis of storage cells or detailed models, simulation models are available that describe the electrical and thermal operational behavior or the aging of a battery cell so accurately and quickly that they can form a basis for the design and testing of battery systems. This enables better analysis and an application-oriented dimensioning of the energy storage, cooling and battery management systems. Real-time simulations even enable the use of virtual batteries in HIL systems.

In order to configure the models for electrical and thermal behavior, a highly flexible testing infrastructure is available with modular power electronics, highly accurate measurement systems and a wide temperature range on both the cell and the system level.

**Our offer**
- Physical model development from the quantum mechanical level to the whole battery.
- Measurement of model parameters for all the model approaches used
- Virtual cell design
- Generation of detailed and analogous models for strength analysis or crash simulation with failure modeling
- Optimization of cell structures with regard to operational and crash safety
- Analysis of the influence of nano-structures on material parameters
- Quantum chemical material modeling
- Analysis and application-oriented dimensioning of energy storage systems, including optimal energy management
- Measurement of optimal circuit variations of individual cells, and the design and operation strategy of balancing circuits
- Development of a battery management system for monitoring state of charge (SOC), aging (SOH) and interior cell temperature, and for diagnosing storage modules
- Testing and evaluation of on-board systems, battery management systems or holistic systems such as electric vehicles with virtual batteries (HIL battery emulators)

**Products**
- BEST (Battery and Electrochemistry Simulation Tool) is used for cell design and performance analysis on the microscopic (material) and on the macroscopic (cell) scale, and is based on a continuum description of battery transportation processes.
  www.itwm.fraunhofer.de/best
- BaSiS – Battery Simulation Studio dynamically simulates all relevant electrochemical processes in Li-ions and lead-acid cells and batteries under various operating conditions (U, I, T, SOC, SOH) and their aging. Through an interface with Simulink®, the software has been successfully deployed in the automotive industry. A real-time variant for “hardware in the loop” test systems is available.
  www.iee.fraunhofer.de/basis

3 Graphic user interface for ISET-LIB. Photo: Fraunhofer IEE.
4 Simulation of an air-cooled pouch cell. Photo: Fraunhofer ICT.