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, testing and systems, a further competence of the Alliance is in the field of simulation.

**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, 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 electrical and thermal design of the whole system. Starting with the measurement analysis of storage cells or detailed models, faster computable cell models are deduced to describe the electrical and thermal operational behavior with a sufficient degree of accuracy. These form the basis for the analysis and application-oriented dimensioning of energy storage systems, including cooling and battery management 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.

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**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 nanostructures 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 Controlling of wiring systems, electric vehicles and battery management systems with virtual batteries (battery emulators)

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**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
- The software ISET-LIB simulates all relevant physical and electrochemical processes in Lithium Ion cells & batteries under different operating conditions (U, I, T, SOC, SOH). The software has been successfully deployed in the automotive industry. A real-time variant for “Hardware in the Loop” test system is available.  
  http://battery-simulation.de/
- ISET-LAB simulates the dynamic behavior of Lead Acid batteries. All common real-time operating systems are being supported.  
  http://battery-simulation.de/

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1 Graphic user interface for ISET-LIB. Photograph: Fraunhofer IWES.
2 Simulation of an air-cooled pouch cell. Photograph: Fraunhofer ICT.