BayBatt
Bayerisches Zentrum für Batterietechnik

UNIVERSITÄT BAYREUTH

Bavarian Center for Battery Technology (BayBatt)

Researching the battery of the future.

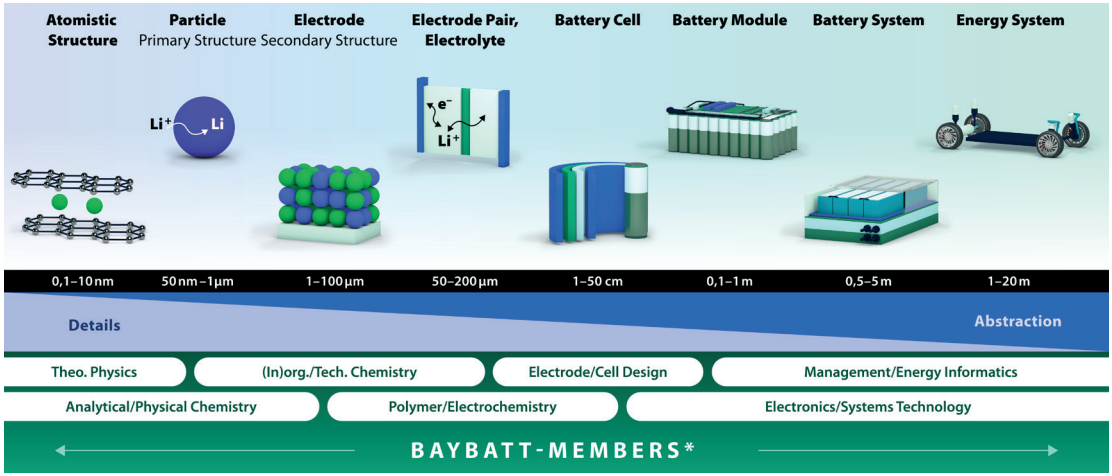
Bavarian Center for Battery Technology (BayBatt)

Smart – Safe - Sustainable: Developing energy storage systems of the future

The research work at the Bavarian Center for Battery Technology (BayBatt) covers the entire spectrum of innovative battery technology: it ranges from molecular fundamentals to the structuring of electrodes and cell production to the use of batteries in networked energy storage systems. The range of disciplines, which is unique in Germany, is also reflected in the subject profiles of the participating chairs and their main research areas. Questions about improved recycling potentials are addressed just as much as the development of solid-state batteries based on sodium for safety or aspects of modern battery management systems. BayBatt deals with all the central challenges of the energy transition and electromobility on an interdisciplinary basis.

The research work of the center is extensive and far-reaching, dealing with modern battery storage technologies at different scales. Core topics are the safety and sustainability of batteries and their components, the intelligence of the storage medium itself as well as its economic viability.

In line with the interdisciplinary orientation, the BayBatt members come from four different faculties and cover all size scales of battery research and all stages of the battery value chain, respectively.



Battery research at BayBatt. Graphic: Daniela Leitner, Design meets science.

Bavarian Center for Battery Technology (BayBatt)

A center for the next generations of batteries

Supraregional competence center in Bayreuth

E-mobility, energy storage of the future, smart batteries and power grids – current issues that represent a major challenge for industry, research and society. This is where the BayBatt comes in and is dedicated to researching and developing new battery technologies for sustainable energy supply solutions. At BayBatt, battery storage systems for mobile and stationary applications in electric vehicles, buildings and grids are researched and further developed to become smart, reliable, safe, long-lasting, powerful and sustainable energy storage systems. To this end, the center builds bridges between basic research in electrochemistry, materials science and engineering and the industrial use of the developed processes and models.

BayBatt brings together battery-specific expertise in physics and chemistry, material and engineering sciences as well as computer science and economics as a supraregional center of excellence located in northern Bavaria.

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BayBatt is advised on its technical and strategic orientation by renowned representatives from industry and science.

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- Dr. Qingsong Wang
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Battery materials and computer-aided material design

The Chair of Theoretical Physics VII focuses on computer- and data-based investigations of charge carrier transport in various materials, such as battery components and photoelectrocatalysts and (metal-) organic semiconductors. Basic processes are simulated using ab initio methods and the data generated are analysed using statistical and machine-learning methods to derive general structure/function relationships.

Battery materials

In view of the increasingly urgent need to switch to a CO_2-neutral economic system, one of the greatest challenges, in addition to the problems of sustainable energy production, is the efficient storage of the energy thus produced. One option, electrochemical battery systems, which have been known in principle for over 200 years, show only inadequate energy densities and long-term stabilities such as those exhibited by fossil fuels. To overcome these limitations, research is being carried out all over the world.

A large part of this research relates to the identification of new materials and the characterization of the microscopic mechanisms involved in order to be able to use them for maximum efficiency. Due to the nature of an electric battery, these mechanisms are based on the transport of charge carriers such as electrons or ions. Over the years, the group has implemented a number of methods that are perfectly suited to investigate the fundamental processes that occur in battery materials.

These microscopic insights can then be used to further optimize already known materials, e.g. by creating defects in specific patterns. In this way, materials can be created that have not only higher conductivities but also better stabilities.

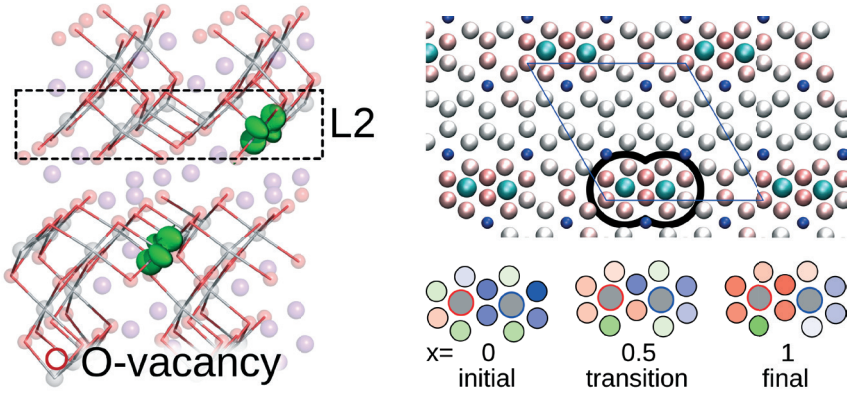
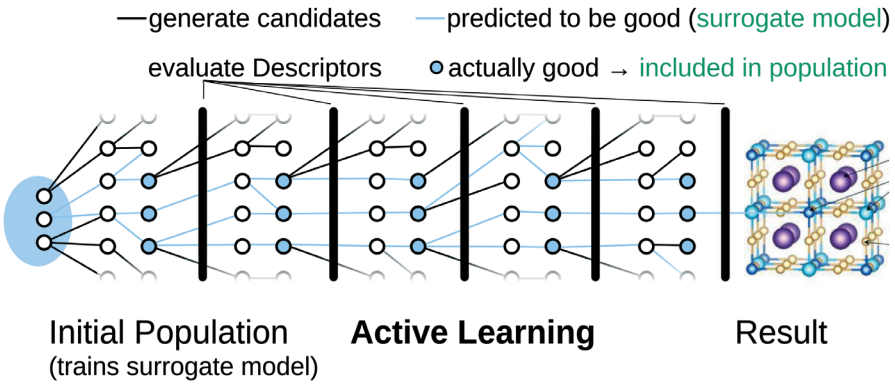


Illustration of a lithium titanate (LTO) cell with an oxygen defect. The resulting electronic polaron states are shown in green.
Top right: Section through the LTO cell in layer L2 at the transition state of a polaron migration. The initial and final states are highlighted in cyan, while shades of red indicate the magnitude of the displacement of the surrounding atoms.

Computer-aided material design

A large part of the group's research is the design of new materials for various applications. However, for organic electronics applications, for example, the signature space of possible molecular crystals is huge, with many billions of possible molecules. For the application, this creates unsurpassed flexibility in terms of possible material or electronic properties, which can be tailored as required. At the same time, this great variability hinders the identification of new materials due to the enormous spaces that would theoretically have to be searched. For this reason, the group is working on the determination of good descriptors, computationally less demanding properties of the systems that correlate with the desired observables, such as charge carrier mobility, as well as methods to calculate them with sufficient accuracy. With these one can then not only identify promising materials in either classical in-silico screening or machine-learned models, but also generate enormous amounts of data for further analysis of the design space. Indeed, in the group's work researchers try to derive general design criteria from a combination of advanced visualization techniques and mathematically sound statistical tests. Visualizations allow for the identification of relationships between chemically similar materials and thus to find areas of the design space that have not yet been sufficiently systematically improved, such as through the synthesis of modified molecules and crystals. The group's rigorously tested design rules, such as specific combinations of molecular building blocks, can provide a way to fully explore design space in this regard.



Schematic representation of polaron migration.

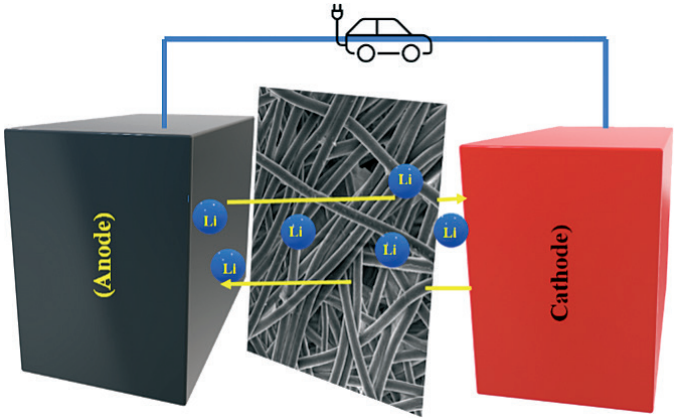
High temperature stable polymer electrospun separators and solid electrolytes

Prof. Seema Agarwal's research group (Macromolecular Chemistry II) has expertise in polymer synthesis, the production and structuring of polymer composites and polymer processing methods. Within BayBatt, battery separators and polymer solid electrolytes based on electrospun high-temperature functional polymers and polymer-ceramic composites are being developed for safe, lightweight and efficient batteries.

Battery materials

Urgently needed technological developments in energy storage are lightweight design, safety and efficiency. We use rationally designed polymers and nanostructures combined with appropriate processing methods to explore the separators and solid electrolytes for the next generation of LIBs and lithium-metal batteries.

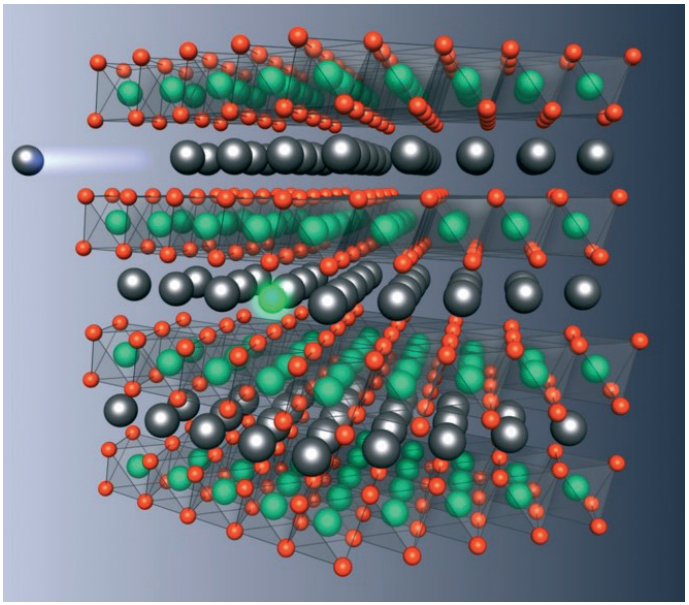
One of our goals is to produce ultra-light, thin, strong and safe separators and/or polymer solid electrolytes with excellent wettability, lithium-ion conductivity at room temperature and without Li-dendrite formation. The separators are based on highly temperature-stable, specially developed polymers with or without inorganic additives. Polymer-ceramic fibre composites are researched for room-temperature conductive solid electrolytes. Electrospinning is used as a processing method to produce defect-free, large-area and extremely thin separators (< 10 µm) and ceramic fibres. The use of scalable synthetic processes and processing methods makes technology transfer on an industrial scale very promising.



Schematic representation showing electrospun separators / solid electrolytes as one of the important parts of a battery cell.

Na-ion battery development and 4SBATT

The focus of the Chair of Inorganic Active Materials for Electrochemical Energy Storage is on improving the current generation of Li-ion batteries and developing next-generation technologies such as Na-ion or solid-state batteries through design, synthesis and characterization of novel electrode materials. Electrode materials are the "heart" of energy storage devices and determine their performance. Improved cathode and anode materials are the key to more powerful and longer-lasting batteries.



Layered structure of a typical electrode material for Li-ion or Na-ion batteries

Na-ion batteries development

Na-ion batteries are potential alternatives to Li-ion batteries (LIBs). They are based on abundant elements (Na, Fe, Mn, ...) and can be cheaper than their Li-ion counterparts. Although their energy density cannot rival NCM-based Li-ion systems, they can achieve similar performances to $LiFePO_4$ (LFP)-based ones. This makes them interesting alternatives to LIBs for lower cost applications. At present, improvements are needed both on the positive and negative electrode. At the positive side, the Bianchini group looks at finding new cathode materials with improved energy density; candidate materials belong to both the layered and polyanionic class of compounds. At the anode, amorphous carbons are used because graphite cannot intercalate Na. Carbons with high capacity and high efficiency are sought, as well as composites with alloying elements.

4SBATT project (ERC Starting Grant)

The Li-ion battery, developed in the last 30 years, is a very successful technology. However, it now faces the challenge of powering the e-mobility revolution, requiring a large increase of raw resources availability. At this point in history, given the roadmap of the European Green Deal and the need to reduce CO_2 emissions, such a scale up should be seen as a unique opportunity to eliminate

unsustainable elements from the batteries. Yet the Li-ion battery relies on a series of elements that are critical, most importantly Li, Co and natural graphite. Moreover, the safety of Li-ion batteries is often in question, and their energy content still needs to increase to satisfy the demand for extended driving ranges. In this context, 4SBATT aims to develop a solid-state battery based on Na, rather than Li, representing the best solution in terms of four key parameters: sustainability, energy density (specific and volumetric), readiness of adoption (i.e. compatibility with existing Li-ion production lines) and safety. To achieve such a challenging goal, 4SBATT will operate at the cross-section between inorganic chemistry, materials science, and engineering. The Bianchini group is developing a combined computational and experimental approach based on density functional theory and in situ x-ray diffraction during synthesis that will allow it to explore large amounts of temperature-dependent multicomponent phase diagrams for various classes of materials.

Thereby the group designs and prepares novel Na-based inorganic compounds for positive electrodes, solid electrolytes and negative electrodes. Then the physical properties of materials and composite electrodes are characterized to understand, improve and engineer their performances. Finally solid-state batteries will be assemble, based on Na and sustainable elements such as Fe, Mn and Si, intrinsically safe due to the non-flammable solid electrolyte, and targeting record energy densities of 300 Wh/kg and 750 Wh/l at the cell level.

Glovebox facilities in the Bianchini group to assemble Li-ion and Na-ion batteries

Developing new active materials

The Chair of Physical Chemistry III combines inorganic synthesis methods with thorough physicochemical characterization. Within the framework of BayBatt, new active materials are developed and structured with regard to optimal wetting behaviour. In addition, co-operation partners carry out detailed electrochemical and spectroscopic investigations on material developments.

The Marschall research group investigates the nanostructuring of known and the synthesis of new active materials for anodes and cathodes in Li-ion and Na-ion batteries. The group has a broad expertise in the synthesis of complex transition metal oxide materials for various catalytic and electrochemical applications. This includes ternary and quaternary solids with layered (e.g. layered perovskites), tunnel-like (e.g. defect pyrochlore) and spinel crystal structures. The portfolio of synthesis methods includes sol-gel synthesis, solid-state synthesis, ammonolysis, hydrothermal synthesis, melt synthesis and microwave-assisted synthesis. The great strengths and broad application possibilities of sol-gel chemistry are used extensively by the Marschall research group, for example for template-assisted syntheses to mesoporous materials in the form of powders and coatings, for controlled nanoparticle syntheses, but also for electrospinning of fibrous oxides. In addition, there are a large number of characterization methods available for material analysis, including physisorption, absorption spectroscopy in diffuse reflection, and DRIFT spectroscopy.

With these competences in the field of material synthesis, structuring and analysis, the Marschall research group is involved in various projects and topics at BayBatt. Mixed oxides of iron, for example, have aroused great interest in recent years for electrodes in lithium-ion and sodium-ion batteries, especially in the field of conversion electrodes. Prof. Marschall's research group is able to produce size-controlled nanoparticles of ternary iron oxides (AFe_2O_4, A= Zn, Mg, Mn, Fe, Co, Ni), for example to obtain a better distribution in the active anode. Their microwave-assisted synthesis is particularly well-suited for this purpose, as the temperature of the sol-gel chemistry can be reached very efficiently and quickly in a laboratory microwave. In some cases, metal oxides produced in this way do not even require a subsequent temperature step, so they can be produced quickly and in a time-saving manner. In addition, a macroporous $CaFe_2O_4$ was recently reported together with the research groups led by Prof. Weber and Prof. Breu. Molybdenum-iron oxides for electro- and photocatalytic applications are currently being investigated by the Marschall research group. These are highly interesting materials for battery applications that can be used as cathode materials for Li, Na and Mg batteries. Up to 2 mol Li+ or Na+ can be incorporated into some iron molybdate structures, while the cell voltage remains almost constant during the intercalation process. Thus, nanostructuring in the form of nanofibres or (porous) nanoparticles can improve the poor reported conductivity and shorten the long Na diffusion paths.

Analytics of heat transport

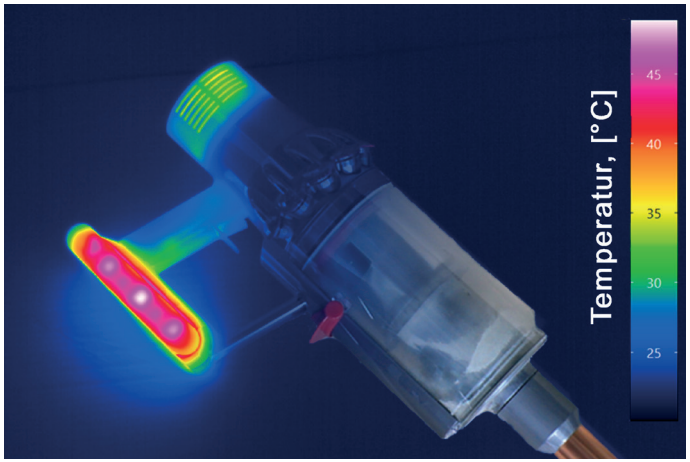
The Chair of Physical Chemistry I specializes in the modelling of heat transport and its analysis, including laser flash analysis, lock-in thermography and photo-acoustic methods. The focus is on heat transport in colloidal materials and thin films. Within BayBatt, operando analyses and real-time methods are being developed based on these activities, which serve to describe the internal current and future cell state and thus allow a sensor-supported, model-based self-assessment of the battery system.

Next generation thermal management

Heat transport in nano- and mesostructured materials plays an important role in many technological applications. Efficient insulation and heat dissipation are the focus of many current research efforts. Within the framework of a Lichtenberg Professorship of the Volkswagen Foundation, the research group has investigated many fundamental heat transport phenomena in colloidal materials. At the same time, the group has established a variety of advanced characterization methods to study thin materials and mesostructured films. Building on this work, they are now investigating aniso-tropic transport phenomena as well as switchable and stimuli-responsive systems.

The vision of controlling the flow of heat, i.e. the transport of phonons, is described in analogy to electronics as "Phononics". One can expect that heat management will tremendously gain relevance for many electronic applications, including batteries.

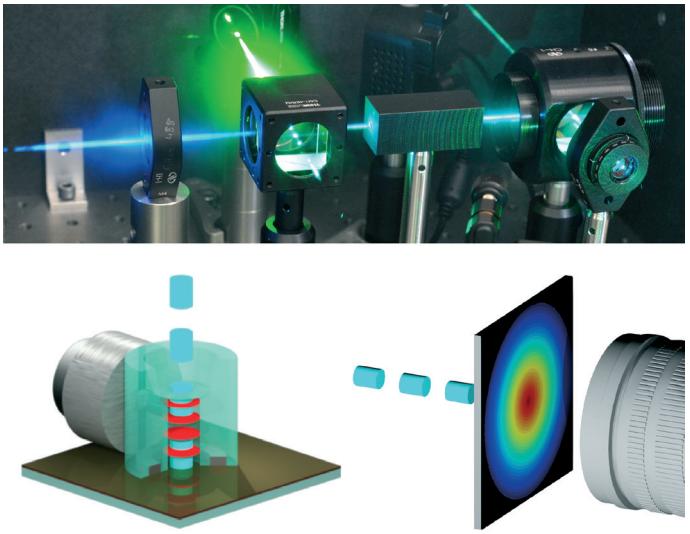
It is the role of interfaces, the microscopic composition of materials and their nanostructuring that is largely responsible for effective heat transport. All of these are abundant in battery cells. The group approaches this task by model systems, e.g. colloidal crystals, because of their well-defined structure together with a large variability of length scales and material composition.



Temperature evolution of a typical battery-driven household appliance during operation.

Prof. Retsch's group investigated colloidal polystyrene crystals, which have a low thermal conductivity of ~ 51 $mWm^{-1}K^{-1}$ at a comparatively high density (740 kgm^{-3}). The open, porous structure (< 200 nm) makes such particle assemblies quite insensitive to the surrounding atmosphere. At the same time, the film formation has an extremely large impact on the effective heat transfer, which increases abruptly when the glass transition temperature is exceeded. The specific structure of colloidal mesostructures is also suitable for realizing specifically programmed steps in the thermal conductance.

With hollow silica nanoparticles, the group investigated another highly porous and highly insulating class of materials. In analogy to aerogels, it is possible to produce extremely efficient thermal insulators. The good structural control in hollow silica nanoparticles also allowed the elaboration of clear structure-property relationships, which underlines the importance of adhesion between neighbouring particles. The group is now extending these studies to a variety of other well-defined colloidal systems, ranging from one-dimensional to three-dimensional systems. On the smallest length scales, the group works with exfoliated layered silicates, single fibres and fibre bundles up to 3D printed bodies. They spend a large part of their work on the development, adaptation and optimization of specific measurement methods. Currently, these are laser flash analysis (LFA), transient heat flux measurement, thermo-reflection in the acoustical frequency range, lock-in thermography (LIT) and photoacoustic characterization (PA). The group is now able to determine thermal transport properties for a very large range of materials and samples. Highlights include anisotropic measurements (also within a sample plane), the variation of temperature and pressure, as well as measurements under external stimulation, e.g. by light. The experimental techniques are supported by the modelling of our hybrid structures, in particular by FEM simulations based on COM- SOL®.



Collection of thermal transport characterization methods including frequency-domain thermoreflectance, photoacoustic characterization, and lock-in thermography.

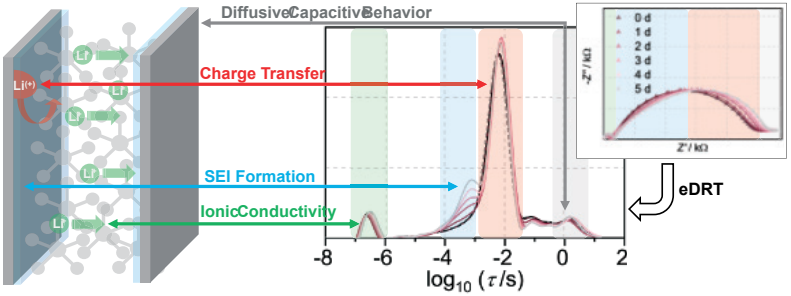
Design and controlled synthesis of novel polymer electrolytes

Prof. Thelakkat's research group focuses on the design and controlled synthesis of novel polymer electrolytes that can replace the current organic liquid-based electrolyte systems on the way to all solid-state lithium metal batteries (ASSLMBs). The challenge is to simultaneously maintain high ionic conductivity, high mechanical stability and well-defined SEI formation in such ASSLMBs. Some of the design concepts and investigated systems are given below.

Next generation thermal management

Both PEO-based and "Beyond PEO" systems were developed and extensively studied for their electrochemical and battery cycle properties. The first objective was to suppress the high crystallinity in PEO systems, which was achieved by the bottlebrush architecture in which different backbones such as polymethacrylate or polynorbornene were decorated with different PEO side chain lengths (ACS Appl. Energy Mater. 2019, 2, 3373–3388). In this architecture, completely amorphous polymers were obtained. Since these novel polymers provide high ionic conductivities only when their T_g is very low, they must be mechanically reinforced by adding fillers such as TiO_2. This led to polymer nanocomposite electrolytes that perform very well, both in terms of low interfacial impedance and long lifetime with considerably high specific capacitance retention at room temperature (Electrochimica Acta 2021, 387, 138455).

In another concept, a series of polyesters with diester side chains were synthesised and tested as "beyond PEO" polyelectrolytes. This new class of polyesters works very well in ASSLMBs in combination with fillers and LFP as cathode (J. Mater. Chem. A 2022, 10, 8932–8947). In a joint work between three research groups within BayBatt, the electrochemical properties of five different SPEs based on three different polymer architectures (linear PEO, methacrylate-based bottlebrushes and poly(glycidylpropargyl ether) (PGPE)-based graft copolymers) and a ceramic electrolyte (LLZO) were compared (Electrochimica Acta 2020, 344, 136060). An in-depth analysis of SEI formation and the influence of different lithium salts was performed. As a reference SPE, PEO+LiTFSI was electrochemically analysed by EIS (see figure below). The measurement data were successfully interpreted and significant differences between the materials were revealed by eDRT.



Investigation of the processes in the battery by means of DRT

Electrical energy conversion with power electronics

The research area covered by the Chair of Mechatronics is electrical energy conversion with power electronics, whereby the investigations range from the semiconductor to the system. This research area thus represents the link between the battery and the consumer or generator.

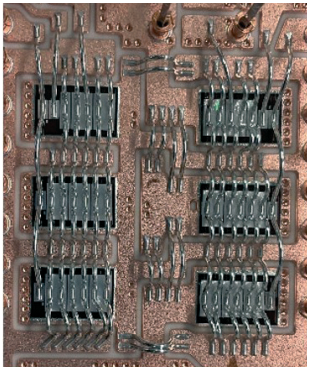
The chair's research focuses on energy and drive technology applications of mechatronics, with power electronics taking on the connecting role. This is where the control meets actuator and sensor technology, which then finds the connection to mechanics in drive technology. The development of new circuit techniques, the use of new types of components and the optimization of systems technology are the focal points of the work:

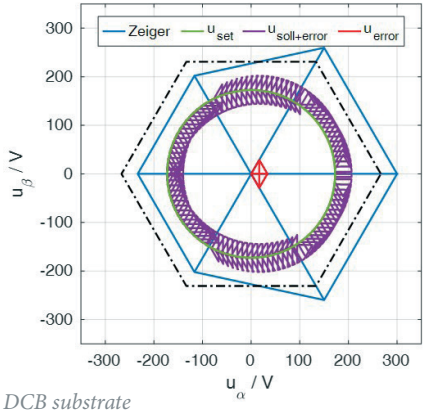
- Electrical energy conversion with increased power density
- Novel components for power electronics
- Integration of energy storage systems
- Energy conversion in the high-power range
- Reliability and service life of electrical energy converters
- Optimization of drive systems especially for traction applications
- Measurement technology on fast power semiconductors

This broad subject area finds its common bracket in power electrics.

The research topics are thus application-oriented, and at the same time, they deal with key technologies on the following topics of the future:

- Electromobility: Electric drives for vehicles from cars to trains to planes
- Integration of renewable energy sources into the grid: HVDC transmission, coupling of DC grids
- Increasing energy efficiency: integration of energy storage systems in drive systems, power electronics with increased efficiency
- Increasing the operational safety and availability of electrical energy conversion circuits





Left: Modern power semiconductors on a DCB substrate
Right: Space vector modulation under asymmetric conditions

Electrode Design

The Chair of Electrode Design for Electrochemical Energy Systems focuses on material development, cell expansion and diagnostics, emphasizing solid-state and quasi-solid-state technologies. Central research areas include the development of innovative materials and devices using first-principle and continuum-level modelling.

Advanced Batteries

For nearly a decade, Prof. Ciucci's team has researched solid and quasi-solid-state batteries, developing new electrolytes using ceramics, ceramic-polymer composites, and polymers. The latter two electrolyte types show the most promise for practical applications. As commercial LIBs struggle with increasing energy density demands and maintaining energy density at sub-zero temperatures, the group designed new quasi-solid-state polymer electrolytes that, when paired with high-capacity, high-voltage electrodes, deliver exceptional performance at room temperature and below freezing. The group also created novel fabrication methods for ultrathin electrolytes and in situ polymerization of polymer electrolytes. Current research includes developing in situ polymerized materials for rapid charging. The team has also explored Na-based battery electrodes, particularly conversion-type sulfide materials like Sb_2S_3 and MoS_2, examining Na insertion mechanisms. By combining these electrodes with carbon materials and sodiophilic compounds, the researchers have enhanced their cycling stability. For emerging, low-cost, Zn-metal rechargeable batteries, they optimized deep eutectic electrolytes.

Reversible Protonic Ceramic Cells for Energy Storage and Power-to-X Applications

Globally, government policies aim to reduce carbon emissions from electricity generation. To minimize reliance on fossil fuels, strategies propose integrating renewable energy sources with grid-scale lithium-ion battery storage. Lithium batteries and fuel cells are both vital in advancing energy storage solutions. Lithium batteries are highly efficient and versatile. Reversible fuel cells complement these benefits for large-scale energy storage, such as seasonal storage. Traditional reversible fuel cells, using oxygen-conducting electrolytes, operate at high temperatures (800–1.000°C), which increases costs and lowers reliability. However, proton-conducting ceramic electrolytes, functioning effectively at lower temperatures (400–600°C), offer improved efficiency, durability, and reduced complexity and costs, making them a promising alternative in the energy landscape.

Although reversible proton ceramic cells hold considerable potential, development faces significant challenges, primarily enhancing cell power density and efficiency. Successful protonic ceramic fuel cell implementation necessitates high-performance, cost-effective cathode catalyst discovery. For instance, rational design guided by theoretical insights led to the development of $Ba_{0.875}Fe_{0.875}Zr_{0.125}O_{3-\delta}$ material, demonstrating exceptional oxygen reduction performance, and surface stability, and achieving record power densities.

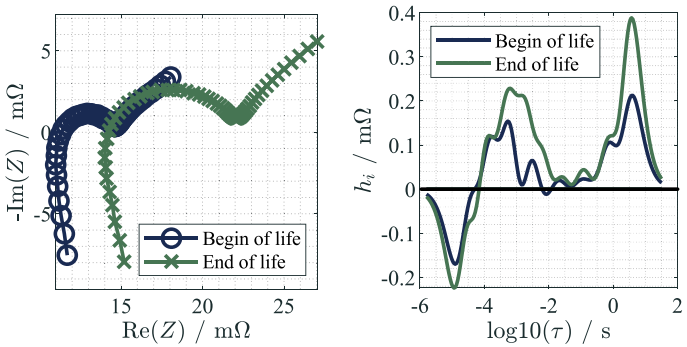
Modelling Impedance Data

Electrochemical spectroscopy has emerged as a valuable tool for investigating energy storage systems. Nevertheless, its usefulness can be limited, especially when multiple experiments are involved. To this end, team has made significant strides in the estimation of relaxation time distributions from electrochemical impedance spectra by harnessing advanced statistical techniques, such as Bayesian statistics, deep learning, Gaussian processes, and neural networks. Leveraging these methods, they have created sophisticated computational tools capable of handling multiple experiments simultaneously, with the capability to provide comprehensive insights into the electrochemical system under investigation. Consequently, their software has gained wide acceptance within the scientific community as a powerful tool for analysing impedance spectra.

Analysis and modelling of lithium-ion batteries

The research area of the Chair of Electrical Energy Systems is the systems engineering analysis of electrical and electrochemical energy storage and converters. Research activities include the analysis and modelling of lithium-ion batteries.

The group's work includes both experimental studies and model-based investigations. Analyses of the performance and aging of electrochemical systems, with a specific focus on electrochemical, electrothermal, and electromechanical effects, are carried out. A wide range of battery scales is covered, spanning from the electrode level to cells, battery packs, and modules.



Non-destructive aging analysis of a battery based on electrochemical impedance spectroscopy (left) and distribution of relaxation times analysis (right).

Therefore, various methods for the in-depth characterization of electrochemical systems are applied but also further developed and improved. The goal is to enable a comprehensive analysis of batteries, with a preference for non-destructive techniques, as they hold significant value for numerous industrial and commercial applications. As depicted below, the electrochemical impedance spectroscopy (EIS) is a powerful tool for this purpose, including the distribution of relaxation times (DRT) analysis. The chair is characterized by extensive expertise in these fields.

When it comes to theoretical considerations, the modelling of short-term (performance) and long-term (aging) behaviour of batteries is another big topic. Beyond that, model-based state estimation and performance, energy, and lifespan prognosis are worked on, as well as model-based algorithms for battery and energy management systems.

A current research topic is the development of new algorithms and approaches that can help to determine the state of a used battery module with respect to its suitability for remanufacturing or refabrication in the context of circular economy decisions. Other research projects range from the investigation and characterization of new battery materials and storage concepts to the optimization of operation strategies of battery energy storage systems (BESS). Current projects are, e.g., dedicated to silicon-based active material, to all-solid-state batteries, and to the operation of a BESS in an industrial context.

Future and sustainable technologies

The Chair of Manufacturing and Remanufacturing Technology works in close cooperation with small and medium-sized enterprises in the research fields of future and sustainability technologies such as additive manufacturing/3D printing, artificial intelligence, digitalization of production, machining and remanufacturing. The Chair's work at BayBatt focuses on the fundamentals of remanufacturing battery storage systems.

Remanufacturing is a key element of the circular economy, closing product loops while maintaining or restoring the product and associated product properties, for reuse. It involves dismantling used products, cleaning, inspection, and sorting of components, then refurbishing and reassembling them into new products. In contrast to repair, remanufacturing is an industrial process, that brings products to at least a quality level of a new product and enables a new product use.

Remanufacturing has environmental, economic and social benefits. Material consumption and environmental impacts are significantly reduced, for example by 88% and 37% respectively in the case of starter motors. Costs are also significantly reduced, as remanufacturing usually costs between 40% and 80% less than manufacturing new products.

For the implementation of remanufacturing in industrial practice, it is necessary to consider the complete life cycle of a product, for which innovative solutions are being researched and developed at the Chair of Manufacturing and Remanufacturing Technology. To this end, the chair's researchers work closely with partners from industry and academia using an interdisciplinary approach.

Keylab Glass Technology | Prof. Dr.-Ing. Thorsten Gerdes

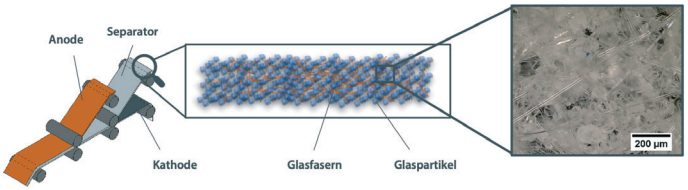
Glass melting and processing technology for functional glasses

The Keylab Glass Technology combines fundamental research with application-oriented development. One focus is on glass melting and processing technology for functional glasses, which enable new applications in batteries. Research activities at BayBatt are glass-based separators that increase the safety of batteries in extreme situations and slow down cell ageing through the chemical composition of the glasses. The separators are tested for various applications in lithium-ion batteries under near-application conditions together with industrial partners.

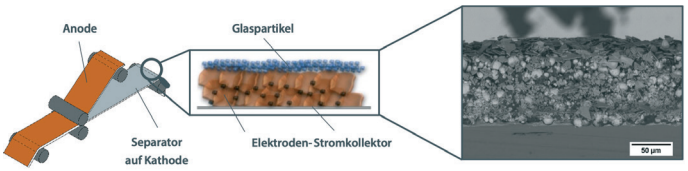
Glass separators

Lithium-ion batteries (LIB) are considered one of the most important energy storage technologies. They are superior to other secondary batteries due to their higher specific energy (density), so that there is a wide range of applications in mobile electrical devices, notebooks and battery-operated hand tools, and even in the automotive sector as energy storage for electric vehicles. In case of overheating due to overcharging or a mechanical defect of the LIB, however, there is a safety risk due to the thermally unstable electrolyte. Contact with atmospheric oxygen or humidity leads to oxidation of the electrolyte and thus to heat generation, which starts a chain reaction known as thermal runaway. The battery separator as a passive, safety-relevant component in LIBs ensures the spatial separation of anode and cathode and thus prevents internal short circuits.

As a temperature-stable alternative to state-of-the-art polymer separators, glass is to be used as separator material. High thermal and chemical resistance as well as good wettability with the battery electrolyte predestine glass for this application. At Keylab Glass Technology, separators based on glass fibres and glass particles are produced and characterized using colloidal processes. In extensive electrochemical testing procedure, the performance and stability of the glass separators could be proven in test cells. However, the higher density of glass reduces the gravimetric energy density of the battery cell, so that the focus of the current research is on reducing the thickness of the separator.



Self-supporting glass separator in the context of battery manufacturing.



Electrode-supported glass separator in the context of battery production

Ecological and techno-economic evaluation of global material

The Chair of Ecological Resource Technology deals with the modelling, simulation and assessment of global material cycles of metals and mineral raw materials. The methodological focus is on material flow analyses, life cycle assessments and raw material criticality evaluations. Particularly relevant for BayBatt are issues relating to the availability of raw materials for cathode and anode materials and the future development of recycling potentials.

Processes from mining through the production and use phase to recycling are considered, taking into account ecological and techno-economic aspects. Relevant research topics include:

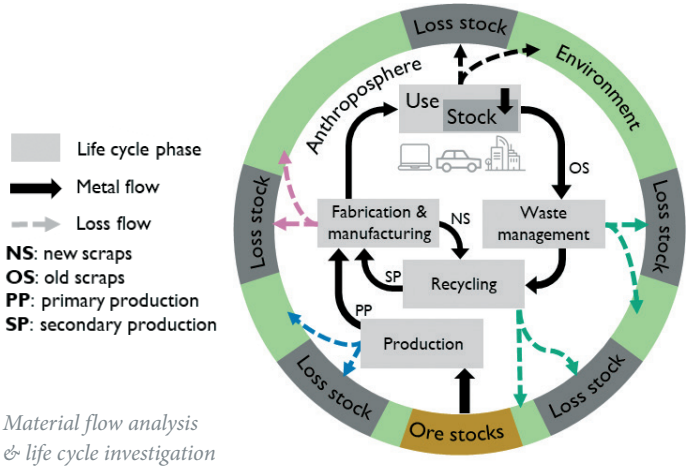
- Supply risks for raw materials,
- the material intensity of infrastructure, energy and mobility systems,
- Phenomena of downcycling in recycling,
- Dissipative material losses
- Environmental impacts of metals and minerals in mining as well as in recycling

The methods used by the Ecological Resource Technology research group are, in particular, material flow analysis, life cycle assessment and raw material criticality assessment. The battery research of the research group comprises the following three focal points:

1. Modelling and simulation of the raw material requirements for battery production and the secondary raw material potential currently and in the next decades in Germany, Europe and worldwide depending on technology development paths.

2. Assessment of the supply risks of battery raw materials and precursors for Europe and European companies on the basis of criticality indicators for material systems

3. Life Cycle Assessment with Life Cycle Costing and Social Life Cycle Assessment for batteries in various fields of application, product composition and manufacturing processes, taking Circular Economy measures into account.



Material flow analysis & life cycle investigation

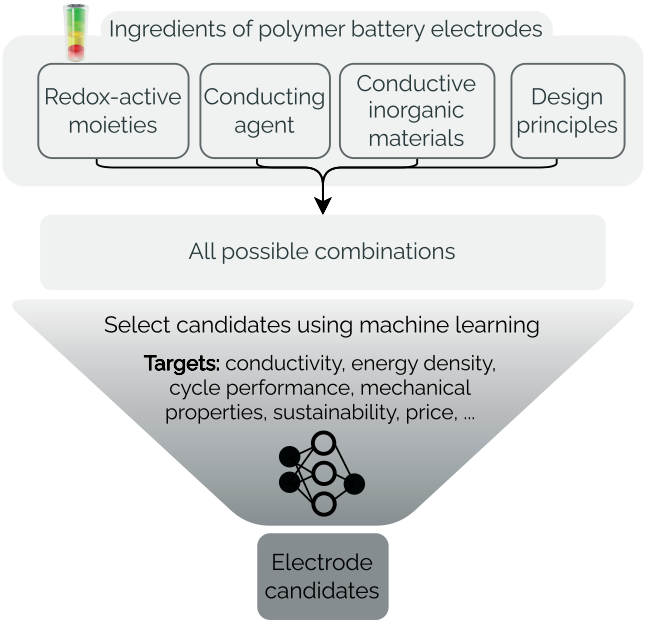
Polymer Battery Informatics

The Kuenneth Group (Junior professorship for Computational Materials Science) is dedicated to democratizing the application of machine learning in materials science to expedite and streamline materials discovery, design, development, and deployment, resulting in increased efficiency, accessibility, and inclusivity. To achieve this objective, they adhere to a materials informatics pipeline centred around machine learning, characterized by four essential pillars: data management, materials representation, machine learning methodologies, and democratization techniques.

Redox-Active Polymer Based Battery Electrodes

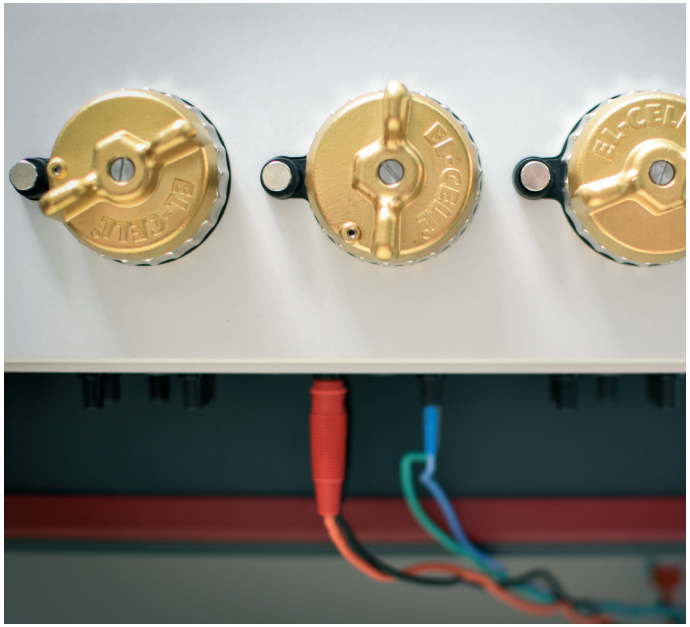
Over the past few decades, significant efforts have been dedicated to the development of batteries using redox-active polymers as the primary electrode material, aiming to achieve properties similar to transition-metal-based batteries. These batteries, which utilize redox-active polymers, offer an alternative to transition-metal-based batteries and are considered environmentally friendly due to their use of earth-abundant elements like hydrogen, oxygen, carbon, and nitrogen. However, a common challenge faced by these batteries is their relatively high susceptibility to dissolution and low electronic conductivity. These issues often require extensive and costly experiments in advanced electrode and material design to find solutions within the expansive chemical landscape of polymer electrodes.

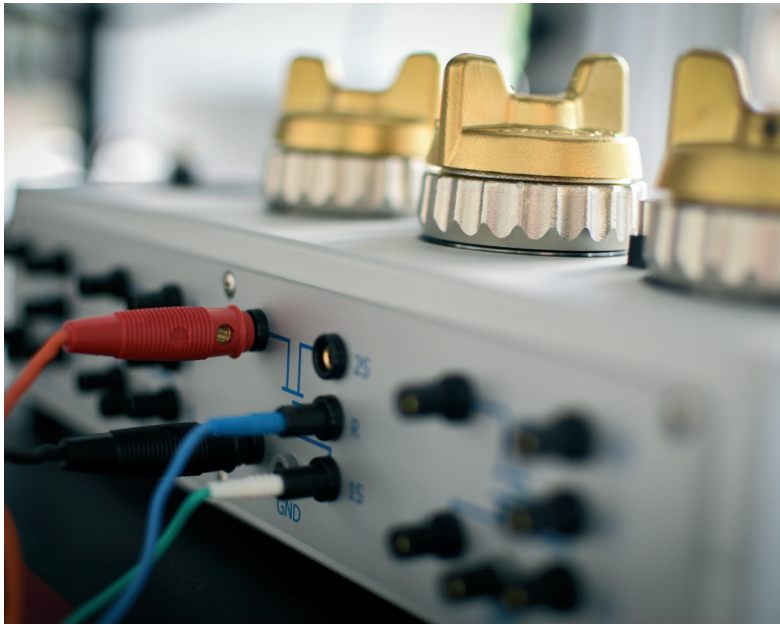
The burgeoning field of polymer battery informatics has emerged as a promising strategy to complement and transcend experimental trial-and-error methods. By harnessing the power of machine learning techniques, this field offers a data-centric exploration path to reconcile electrode design challenges related to dissolution, conductivity, energy density, and mechanical properties, cycle performance, sustainability, and price. Machine learning models are trained using data extracted from experiments,



calculations, literature, and through synergistic combinations of experimental and computational methods to pinpoint potential candidates possessing tailored properties for polymer electrodes.

Machine learning facilitates the exploration of a vast parameter space encompassing various combinations of polymers incorporating redox-active functionalities, conducting agents, and other factors. These models enable the identification of potential electrode candidates that align with specific property criteria. This methodology streamlines and enhances the process of selecting and honing optimal configurations for polymer electrodes, driving forward the development of cutting-edge solutions for energy storage in the next generation.



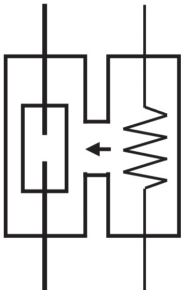


Electronic monitoring and control of electrical energy storage systems

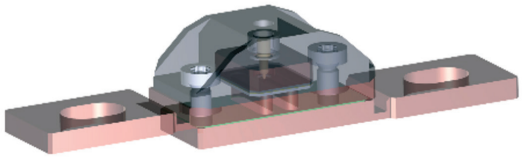
Within BayBatt, the Chair of Electronics for Electrical Energy Storage works together with the Fraunhofer Institute for Integrated Systems and Device Technology (IISB) in Erlangen on solutions for the electronic monitoring and control of electrical energy storage systems such as batteries, supercaps and fuel cells used in mobile and stationary applications. The embedded foxBMS® battery management system platform, which originated from a Fraunhofer IISB initiative in 2015 and is being further developed at BayBatt, enables the research and validation of safer, more robust and reliable battery system architectures for intelligent energy storage systems.

Sensors and actuators for battery systems

Sensor technology plays a central role in battery systems, especially to ensure the safety of the battery system. The chair deals with both the sensor technology and the required actuator technology in order to protect the battery system from dangerous situations. For this purpose, digital and analogue electronics as well as functional system architectures for sensory monitoring are being investigated by the research group in order to guarantee the safe, robust and reliable operation of batteries. Redox-flow batteries and hybrid systems (i.e. combination of battery and fuel cell) are also being considered. Actuator technology makes it possible to eliminate or partially compensate for faults that occur in the battery system. For this purpose, a power antifuse device was developed.



Antifuse:
High-current bidirectional bypass device becoming conductive in an irreversible way after a single thermal event



Ignitor:
Ignition device based on a heating resistor controlled electrically and triggering a one-time exothermal reaction

Power antifuse for bridging defective battery cells

The focus is on resilient electronic systems with a high level of functional safety (i.e. safety: from “fail-safe” to “fail-operational” to “fail-aware”). The reliability and availability of the electrical components has become more important, as the electronics in battery systems are constantly under voltage and are therefore subject to high demands. Components such as electromechanical contactors, electromagnetic fuses and galvanically insulated current sensors are being used and further developed.

Battery management systems
The battery management system (BMS) is the "brain" of the battery system: all important decisions are made there, based on measured physical quantities. The chair develops and validates battery management systems and battery systems by means of hardware and software-in-the-loop concepts, man-machine interfaces, information systems and intelligent communication systems.

For the research work, the chair uses and further develops the foxBMS platform. foxBMS is a free, open and flexible research and development environment for the development of BMS. Most importantly, it is the first universal hardware and software environment to provide a fully open source BMS development platform. It aims to control modern and complex electrical energy storage systems such as lithium-ion batteries. It is also designed to accelerate research, development and testing processes in the field of mobile and stationary electrical energy storage systems through seamless development and integration processes. For this reason, it is ideally suited for research and development, including rapid prototyping and testing.

The foxBMS® performs a number of critical functions such as the electrical management of the battery and the cell balancing (passive and active charge equalization between the cells).

It consists of embedded software (e.g. microcontroller, FPGA, system-on-chip) for distributed systems and controls actuators (e.g. power antifuse as an electrical bypass device in the event of a vehicle crash or a battery fault) via measured physical quantities supplied by sensors (e.g. use of calibration-free current sensors based on quantum technology).

Open source battery management system R&D platform foxBMS

Development of innovative battery concepts

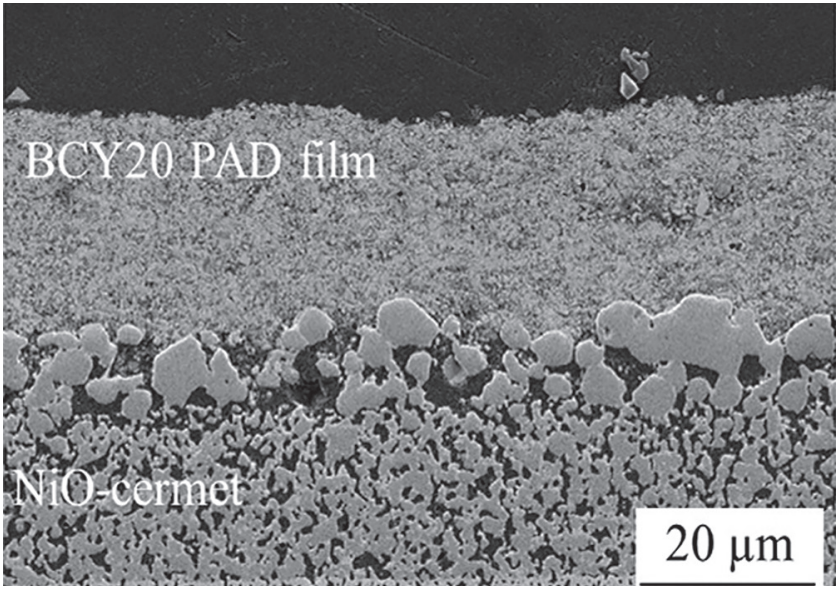
The Chair of Functional Materials works on new materials and technologies for energy conversion. The focus is on novel battery concepts, materials and their processing. This is the basis for the development of innovative battery concepts within BayBatt.

Materials and technologies for energy conversion

The energy transition is a central topic for the future. Replacing fossil fuels with renewable energy from sun, wind and other renewables is inevitable. Electrical energy storage and energy converters play an important role here. New materials are often the driving force of the group's research.

Besides battery materials, thermoelectric materials are components for the conversion of unused waste heat into high-quality electrical energy.

In electrochemical CO_2 electrolysis, the harmful climate gas CO_2 is selectively converted into valuable substances such as ethene using green electricity. The electrode materials and the catalyst coatings on the electrodes play a decisive role here. However, process control is also important. Powerful batteries are important to store electrical energy and for electromobility. The focus here is on new battery concepts, materials and their processing.



Ceramic layer on a porous gas-permeable electrode created using the powder aerosol deposition (PAD) method.
Illustration: Jörg Exner

Model-based methods for battery optimization and operation

The Junior Professorship for Methods for Battery Management addresses the development of modern model-based methods for optimization, monitoring and control of batteries. The aim is to improve lifetime and safety of current battery systems and to develop tailored operation strategies for batteries with novel materials. The research is thus dedicated to central technical challenges for the energy transition and electromobility.

The research focuses on prediction models for batteries, which is the basis for the development of modern battery management systems. Here, especially battery ageing, safety and new materials are addressed.

The electrochemical, chemical, and mechanical processes that take place during the operation of batteries can often not be considered separately from each other and are not limited to a particular length scale. This is especially important for complex degradation and conversion processes that cause significant structural changes within the battery cell. Therefore, multiscale and multiphysical approaches are needed.

The research group develops predictive models on various scales that range from electrochemical interfaces up to large format cells. Further, the dynamic behaviour of batteries is characterized in-depth using modern electrochemical methods. Based on these experiments, model parameters can be identified, and prediction capabilities can be tested.

The research is embedded in an interdisciplinary research environment and acts as an interface between material development and electrical system integration.

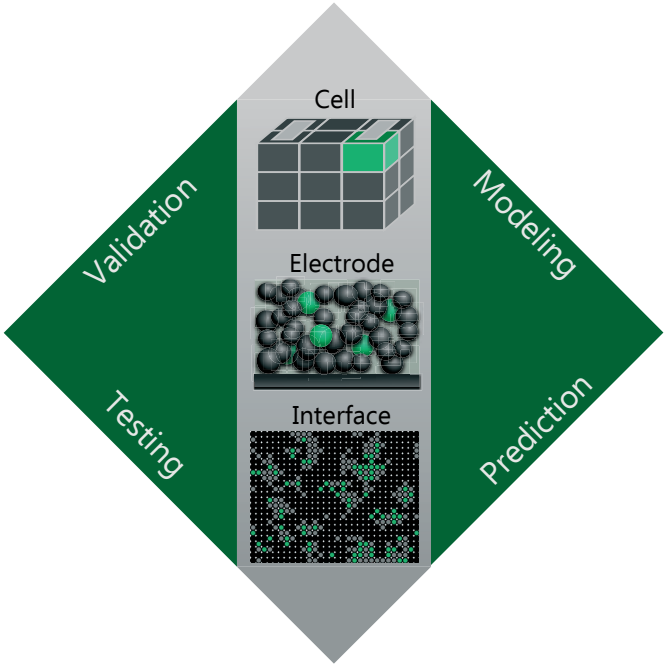


Illustration of the scope of the utilized model-based methods. Their application ranges from the development and integration of new material up to cell integration into energy storage devices.

Materials for electrochemical energy conversion and storage

Research at the Chair of Electrochemical Process Engineering focuses on novel materials and concepts for electrochemical energy conversion and storage. Our activities encompass the development of spectroscopic methods for the in-operando characterization of energy materials as well as the controlled 3D structuring of porous electrodes, e.g. by means of electrospinning and dynamic hydrogen bubble templating. Current battery-related projects are dedicated to the processing and characterization of carbon materials and porous electrodes for lithium-ion and redox-flow batteries.

Lithium-ion batteries

Due to their high volumetric and gravimetric energy density as well as cycle stability, lithium-ion batteries (LiBs) are already commercialised in mobile devices such as laptops and smartphones but are now also increasingly being used in automotive applications.

But while commercial LiBs usually consist of a carbon-based electrode on the anode side and a combination of different transition metals such as nickel or cobalt with lithium on the cathode side, the research group is looking into more environmentally friendly and earth-abundant materials, such as silicon, graphite oxide and sulphur.

Current research focuses on the synthesis of silicon-carbon composites as novel anode materials, the electrochemical characterization of glass-based thin-film separators and the development of in-situ and in-operando analysis strategies to study the complex electrochemical processes at the electrode-electrolyte interface in greater detail.

Redox-flow batteries

Redox-flow batteries store electrical energy chemically in the form of liquid electrolyte solutions. The advantage of redox flow batteries over other storage systems is that the storage capacity can be controlled by the volume of the electrolyte tanks and no phase transitions are required. In some projects, electrospinning and templating are applied to design improved carbonaceous composite electrodes. In others, further insight into the ageing of porous electrodes is obtained using sophisticated electroanalytical methods (RDE, ACCV, DRT-EIS) investigating the relationship between structure and activity.

Electrolyte for redox-flow batteries based on vanadium in different oxidation states

Conception and design of battery storage systems

The Chair of Systems Engineering for Electrical Energy Storage researches optimal design and configuration of battery storage systems from the cell level upwards. Key parameters such as power and energy density as well as system properties such as safety and reliability are only created through the interaction of the subsystems cell, mechanical structure, thermal management, electronics and software. Due to its integrative character, the BayBatt chair represents the bridge from the components to the application of the battery system.

Simulation and design

The development and parameterization of thermal and electrical models is, on the one hand, the basis for potential assessments of component innovations at material and cell level and, on the other hand, an important tool for optimal system design. Both applications are in focus of the chair, whereby the horizon of consideration explicitly includes the necessary periphery of a battery system (current sensor, contactors, etc.), as well as procedures for parameter identification on existing systems.

Diagnosis and impedance spectroscopy

The application of diagnostic algorithms in commercial systems and everyday conditions requires an adaptation of laboratory methods established at cell level. Hence, the chair aims at transferring these methods to the system level, validating them and demonstrating the system benefits or, conversely, deriving the requirements for sensors and data acquisition to achieve the system benefits.

Another central research question is how to derive the quality of a diagnosis. Impedance spectroscopy is a method that seems particularly promising for use in applications. The focus here is on the system level and the consideration of the boundary conditions for operation in the application.

Model-based systems engineering

Using models enables chains of effects and sensitivities to be made visible. The traceability of requirements in the system specification is also ensured and the effects of an adaptation of the architecture can be directly indicated. Model-based systems engineering is therefore helpful in deriving component requirements and, conversely, in quantifying system improvements through component innovations, thus making a significant contribution to collaboration in the context of BayBatt.

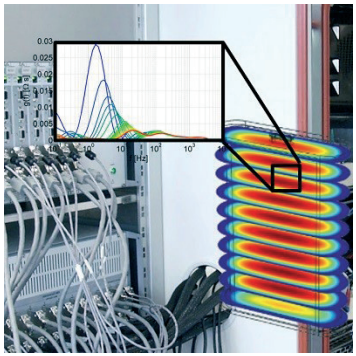


Illustration of the coupling of thermal and electrical properties and the necessary measurement technology: distribution function of the relaxation times over a simulation of the temperature distribution in front of a cell test stand.

Bavarian Center for Battery Technology (BayBatt)

Battery expertise – made in Bayreuth

The central importance of battery systems for the energy storage and use of the future is associated with an enormous need for qualified experts. Highly qualified graduates are needed to actively shape the development of sustainable, safe and networked battery technologies.

BayBatt has therefore launched two dedicated battery-related Master's programmes - the first of their kind at German speaking universities. The English-taught programme *Battery Materials and Technology (M.Sc.)* and the German-taught programme *Batterietechnik (M.Sc.)* train interdisciplinary experts who focus on the entire value chain of energy storage systems.

The new Master's programmes are geared towards graduates from both the natural sciences and engineering. We welcome excellent applicants from Germany and abroad who want to work on the energy transition to meet the demand for skilled workers.

With its graduate school, BayBatt is pursuing interdisciplinary doctoral training around the specific topic of batteries. Doctoral students can take advantage of the unique research, training and networking opportunities offered by the center and in turn increase the (international) visibility and scientific reputation of Bayreuth. All doctoral students of the Bavarian Center for Battery Technology's graduate school will be provided with a workplace in the center's building so that they are part of the interdisciplinary, international team from the very beginning.

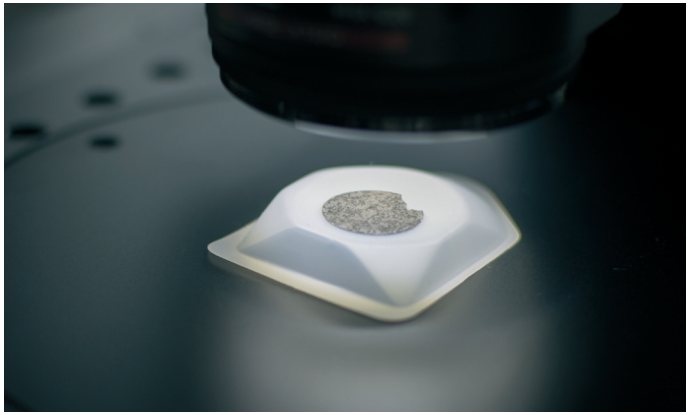
As a third pillar in the training concept, in future BayBatt will also qualify relevantly trained professionals for the field of battery technology through continuing education courses.

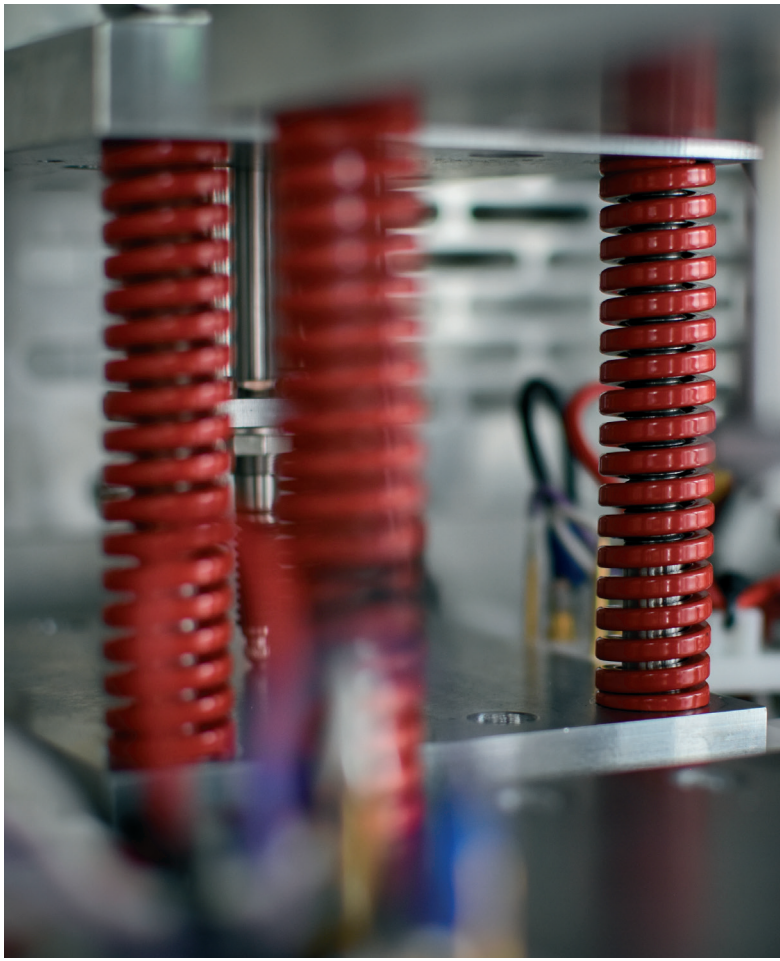
Bavarian Center for Battery Technology (BayBatt)

First point of contact for Bavaria's industry representatives

Bavaria has an excellent industrial structure with internationally competitive production, projection and services, with top positions in industrial research and development. This applies to the chemical industry, component manufacturers, suppliers and Original Equipment Manufacturers (OEMs) in the automotive and energy industries, as well as grid operators. BayBatt aims to be the number one player in battery technology.

We want to be the contact point for Bavarian industry by providing expert advice, by supporting R&D projects and by offering research services. We strive for a bidirectional transfer and lively exchange of ideas and concepts, know-how and employees between our research center and the relevant players in the Bavarian battery industry.





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