Energy for the Future
Electrochemical Energy Conversion and Storage
Persistence Pays off
The University of Ulm is developing its Electrochemistry Department, a strategic contribution to the field of electromobility

Shaping the Energy of the Future
Basic research, implementation, commercial collaboration, training

Worldwide Attention Is Guaranteed
The Helmholtz Institute is a great asset to the University of Ulm

Grasping the System as a Whole
It will not be possible to adapt energy storage processes until all the details have been fully understood

From Model Systems to Technical Electrodes
Electrochemical and electrocatalytic reactions with complex real electrodes under realistic conditions

Materials with Large Surface Areas
Chemical energy conversion reactions in batteries and fuel cells could run more efficiently

Theorists Can Get the Ball Rolling
What individual reaction steps occur in batteries and fuel cells? How could the processes be optimised?

Playing Catch-up – Closing the Production Gap in Battery Technology
Interview with Werner Tillmetz, member of the board at the Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW) and head of the Ulm ZSW branch, on current developments in technology transfer

Overview
The Basics – Persistence in Research • The Helmholtz Institute Ulm for Electrochemical Energy Storage – A Bridge into the Future • A Selection of Current Projects at the University of Ulm

A Strong Focus on Industry
The Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW)

High-Quality Training Is Their Trademark
The Fuel Cell Education and Training Centre e.V. (WBZU) is a registered non-profit organisation that focuses on training, continuing education and publicity work in the fields of renewable and innovative energy technologies.

Setting Sights on Materials with a Long Lifespan
At the ZSW, researchers are studying batteries and their components on a production line that reflects industrial production processes.

The Big Challenge – The Issue of Storage
Substitute natural gas could enable a 100% renewable energy supply

“There Is Nothing More Exciting than Developing Innovative Materials at the Moment”
Increasing the driving range – researchers from industry and academia are working together to find new solutions

“The Most Important Thing Is an Understanding of the ‘Other World’”
Interview with Christian Mohrdieck, director of Fuel Cell & Battery Drive Development at Daimler AG in Stuttgart, on the collaboration with Ulm

Delving Deeper into the “Nano Cosmos” of the Battery
The University of Ulm is backing low-voltage transmission electron microscopy – a new trend in electron microscopy with applications for battery research – the roots are in “Science City” Ulm

Fuel Cells with Ethanol?
Our researchers know which direction their research should take

“We Are Very Active in Helping Our Students”
Small groups, international study programmes, graduate advising – the programmes in energy sciences offer these advantages as well

Junior Researchers in Ulm Display Great Motivation
Research connects nationalities – Combination of experiment and theory – Interconnected thinking

Communication with Our Students Is the Foundation – Excellence in Research the Result
Interview with Dieter Kaufmann, chancellor of the University of Ulm, on securing a position for the University as a research university

Publishing Details
While many other institutions have been cutting professorships in the field of electrochemistry over the past few years, we are one of the few universities in Germany to have continued to pursue the basic science of battery technology with unwavering commitment. Although the technology is very attractive, interest has declined as battery production has moved out of Germany. The industrial environment has shifted to Asia because the devices that require lithium ion batteries – such as notebook computers, iPhones and tablet computers – are produced there.

There were good reasons to adhere to electrochemistry. The Ulm Electrochemistry Department had been filled with outstanding professors from the start, including the recently deceased father of German electrochemistry, Dieter M Kolb. Furthermore, the Ulm Centre for Solar Energy and Hydrogen Research (ZSW) had established itself as a leader in Europe with its notable success in research and development of battery and fuel cell technologies with an application focus. Thus, it was essential to reinforce this distinguished position by intensifying basic research at the University and training highly talented junior researchers.

The field of electrochemistry is now experiencing a rebirth. Batteries are the foundation of electromobility and the seed of the Internet of Things, even the Internet of Energy. In our visions, energy will be available without mass in the future. This means that energy will no longer be transported in tank lorries across the streets in the form of petrol or diesel fuel, but electrically distributed via high-voltage power lines. Every car and every household will then be able to access electrical energy by the kilowatt hour via the power network, store it in batteries and then use it for driving, washing or cooking as needed. Here battery performance will play a crucial role.

Modern battery systems are not efficient enough. There is a need for further breakthroughs, particularly in the area of basic research – which is why we intend to expand the range of electrochemical research being conducted in Ulm significantly. Establishing the new Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU) was only the first step. Over the next few years, we plan to invest approximately one million euros per year in new professorships. In addition, millions of euros in external funds will be coming in from industrial partners or public funding organisations for the new professorships and their research projects.

We aim to make a significant contribution toward establishing Germany as a lead market for, and leading supplier of, electromobility. This thematic dossier describes the University of Ulm’s activities and expertise in the field of electrochemical energy conversion and energy storage.

Karl Joachim Ebeling
President of the University of Ulm

Persistence Pays off
The University of Ulm is developing its Electrochemistry Department, a strategic contribution to the field of electromobility
According to the National Electromobility Platform (NPE), Germany is to become a lead market for electromobility. The advisory board to the federal government is comprised of representatives from the sectors of business, academia, politics and society. Their common objective is to have one million electric vehicles on the streets by the year 2020. The German energy transition has further demands, including researching other alternative drive systems, such as fuel cells, and expanding the infrastructure – power networks, for instance. Here researchers from Ulm make contributions on several different levels.

The Electrochemistry Department in Ulm was built up over decades and has traditionally been very strong. The University of Ulm has all-round expertise at its disposal in both basic research and research with an application focus. Furthermore, the University benefits from the experience drawn from collaboration with industrial partners – the Centre for Solar Energy and Hydrogen Research (ZSW) in particular. The ZSW conducts research along the entire value added chain of batteries and fuel cells and collaborates with nearly all the companies in Germany that are active in this field. Education is another of Ulm's strengths. In the field of energy engineering alone, the University offers two international
The central message is this: the mega-topic of electromobility is not just limited to the car. It pertains to all forms of energy conversion, storage and transport. A foundation is emerging from the University of Ulm, in cooperation with its partners, that is important for the entire value added chain: electrochemistry.

The battery is the focus of numerous research projects. It is not only the key component of electric cars, but also of potential decentralised energy storage systems in homes. First and foremost, researchers are focusing on increasing battery performance and service life while reducing production costs. The process of recharging a battery in an electric car by means of a normal electrical outlet, for instance, takes four to five hours at present. The driving range of the battery is currently at around 150 kilometres. Businesses, research institutes and universities are working hard at achieving a larger radius. BASF is involved in a research consortium addressing questions concerning an improved range.

Batteries and fuel cells were considered to be more in the domain of application-oriented research for decades, but now they are a topic in basic research once again. The new interest is due to the progress that has occurred in research over the last few years, which now makes it possible to explain electrochemical processes in detail. New developments have included theoretical models and computer programmes that are able to simulate processes at the atomic and molecular levels. In Ulm, theorists and experimentalists are working together to find out how processes at the nano-level influence the battery as a whole, which has enabled researchers to start some test planning. Researchers from Ulm are currently developing a special microscope – a low-voltage transmission electron microscope – in cooperation with commercial partner Zeiss, in order to detect even the smallest material defects. This microscope enables researchers to record structures with a size of less than 0.2 nanometres – which is tantamount to a research revolution. The structure of a material is so relevant because it determines the processes that are triggered by the respective material. Changes in the material also alter the reactions. Thus someone who wants to intervene in chemical processes will first need to know the exact composition of the material in order to carry out the modifications.

German companies are investing around 17 billion euros in electromobility research and development alone. One of their aims is to increase the quantity of batteries being produced in Germany, as car manufacturers prefer domestic suppliers. It is easier for car manufacturers to coordinate with suppliers who are close by. The Federal Ministry of Education and Research (BMBF) is also funding a pilot production line for lithium ion batteries in Ulm. The line will be set up at the ZSW and 25 companies will be involved, including BASF, VARTA, Evonik and various research institutions. One of the aims of this project is to transfer newly developed production procedures, materials, components and system parts into commercial serial production. “High-performing, affordable batteries are a central prerequisite for the electric vehicle suitable for daily use. The future pilot production line in Ulm is a big step in the direction of electromobility”, explains Federal Research Minister Annette Schavan.

The Ulm Municipal Utilities, in cooperation with Daimler, have started another pilot project of a completely different nature: car2go is a car sharing model, in which users can hire a car for single journeys for about the price of a bus ticket. Martin Müller, professor of sustainability at the University of Ulm, has studied the behaviour of people hiring cars: “We examined how people’s journeys and their mobility behaviour are changing, and we were pleasantly surprised. Particularly with younger people, a change in mentality can be observed. Young people, who perhaps just a few years ago placed value on having their own cars, are open to new ideas and are happy to become involved in car sharing.” With its high road performance and moderate driving ranges, the car2go project is predestined for electric battery vehicles. E-Smarts have now been added to the fleet in Ulm. Several other cities have expressed interest in sharing projects as well.

Kristin Mosch, editor
The new Helmholtz Institute Ulm for Electrochemical Energy Storage (HIU) was established with the aim of developing efficient battery systems to be used for energy supply and mobility of the future. The Karlsruhe Institute of Technology (KIT) founded the HIU in cooperation with the University of Ulm. Associated partners are the Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW) and the German Aerospace Centre (DLR). The HIU brings great advantages to the University of Ulm.

“The HIU provides us with access to programmes and funding through the Helmholtz Association”, explains Peter Bäuerle, professor of chemistry and vice president of research at the University of Ulm. “We also benefit from the greater visibility that comes with it, which has already led to successive investments.”

One example is the pilot production line for batteries that is going to be set up on Oberer Eselsberg, the location of Ulm’s “Science City”. The production line will be under the direction of the ZSW and funded by the Federal Ministry of Education and Research (BMBF), the state of Baden-Württemberg and business partners. The University of Ulm is investing a great deal in attracting external institutes to its campus. The major advantages for the University are not only the synergies that arise through joint projects, but also the fact that collaboration projects like these have become an important criterion for securing external funding. “The larger the networks, the better the chance at success”, Bäuerle explains. The HIU’s clear focus is on researching the basics for powerful batteries and battery systems pertaining to electromobility of the future. The Institute is concentrating on the fields of “basic electrochemical research”, “materials research”, “theory and modelling of (electro)chemical processes” and comprehensive “system analysis”. Furthermore, analytical methods are being developed for researching the charging and discharging processes.

As a Helmholtz Institute, the HIU receives 90 % of its funding from the BMBF via the KIT and 10 % from the state of Baden-Württemberg. The DLR share of the funding is through the Federal Ministry of Economics and Technology. The budget for the new institute is fixed at around 6.5 million euros per year. Part of the budget is intended for funding three new professorships – one of which is funded by the DLR- and the salaries of

“The HIU provides us with access to programmes and funding through the Helmholtz Association.”

Peter Bäuerle
more than 30 staff members. Approximately 50 additional researchers will be financed via third-party projects. The state is erecting a new twelve million euro building in the “Science City”, in cooperation with the University of Ulm, where approximately 80 to 90 staff members will be working from the end of 2013.

The Helmholtz Association sees its institutes as special instruments for fostering cooperation with universities. Each institute is established on the campus of a university as a branch of a regular Helmholtz Centre. An institute’s staff members are employed by the respective centre; in the case of the HIU, the employer is the KIT. The University and the KIT select the head researchers in cooperation with the associated partners. Filling professorships is generally a time-consuming process, and yet the HIU is to start operation immediately. Thus, additional, externally supervised teams have been established. This means that the staff members perform research at the HIU and the corresponding professor works either for the University, the KIT, the ZSW or the DLR.

The official start was in August 2009 when the University of Ulm, the KIT, the ZSW and the DLR signed a letter of intent on planned collaboration in the field of electrochemical energy storage. In November 2010, following a phase of preparation and application that lasted nearly two years, an international expert team evaluated both the scientific projects and the overall project in Ulm. Following a positive vote by the expert panel, the Helmholtz Association Senate decided to establish the HIU in December 2010, and it began operation in January 2011. At the opening ceremony in January, Federal Minister of Research Annette Schavan and then-Minister President of Baden-Württemberg Stefan Mappus emphasised the significance of the research planned at the HIU and the KIT for Germany, as a place of technology and commerce, and especially for Baden-Württemberg with its strong automotive sector.

The Helmholtz Association intends to establish new Helmholtz Institutes only in states where there are not yet any. Following the establishment of three first Helmholtz Institutes in Saarbrücken, Jena and Mainz, an exception was made for Ulm: the subject matter took precedence. In addition to the expertise available at the University and the fact that Ulm is recognised for its strength in electrochemical energy storage – and especially battery technology – there was another argument for Ulm: the range of courses offered. The well-established study programmes in the fields of natural sciences and engineering played an important role, as did the two master’s degree programmes offered in English: “Energy Science and Technology” and “Advanced Materials”. Educating highly qualified scientific and technical junior researchers is a matter of utmost importance to the Helmholtz Association. In view of the desperate need for junior researchers in battery research, the HIU is planning to set up a research training group.

When the HIU was founded in Ulm, it attracted international attention. “After the inauguration, we even received emails with applications from people from the US who wanted to join us immediately”, Bäuerle reports.

“Nowadays, the larger the size of the network in which one works, the better the chance at success.”
Peter Bäuerle
Multiscale modelling examines what occurs inside energy storage systems at all levels: from the tiniest sub-atomic dimensions to the nano and micro levels, up to real systems. Researchers assess the processes at the individual levels using various methods, subsequently linking them together. The aim is to find out how elementary processes determine the macroscopic properties of electrochemical systems, such as batteries.

Knowledge of these connections is important – directed interventions, beyond a simple trial-and-error approach, can only be achieved with an understanding of the details. “We aim to investigate the system as a whole”, explains Timo Jacob, professor at and head of the Institute of Electrochemistry at the University of Ulm, an institute that combines experimental and theoretical expertise. “This is an approach that has only become possible with the advancements in research over the past few years. It was first necessary to develop suitable theoretical methods, which could then be implemented into efficient computer programmes.”

During a research visit to the USA, Jacob developed an enthusiasm for answering questions related to electrochemical systems and battery technology by referring to the atomic level.

In Ulm, new theoretical models and computer programmes have been developed that are able to reproduce atomic and molecular levels with the aim of influencing processes in batteries at the nano level.
“After receiving my PhD in Germany, where I focused on the nano level, I went to the California Institute of Technology as a postdoc, where I worked on an industrial project. Research in the USA is often very focused on application. The advantage is that you do not lose touch with reality. On the other hand, projects do not usually run very long – typically one year. My project concerned fuel cell improvement. It became evident rather quickly that in order to optimize the technology, the first step would need to be unraveling the elementary processes at the atomic level, something that can only partially be realized in short-term projects. In this respect, we are in a unique position here in Germany – we have the time and the means to pursue long-term fundamental research projects, without any pressure from the university or external sponsors to attain quick results – in the form of patents, for instance. Nevertheless, interesting and promising innovations are often the result.”

The research field that Jacob and his colleagues are focusing on is the interface between electrodes and electrolytes – important components of both batteries and fuel cells. Applying an electric voltage between electrodes and electrolytes triggers electrochemical reactions in the battery to convert or store energy. What exactly happens remains to a large extent uninvestigated. However, an understanding of these specific processes is exactly what is important for a focused regulation of the whole system.

Once researchers have understood an elementary process at the nano level, the next step is to observe how the same process manifests itself at the next higher level, e.g. the micro level. The equations that adequately describe the processes within a certain time and length scale can change if there is a change of level. For instance, although nanoparticles are subject to the same physical laws as macroscopic parts of the same material, their properties as well as their interactions with their environment require different equations.

“The advantage of the atomic level is that you can study effects in great detail – without great approximation”, Jacob says. “The results we obtain then serve as input for calculations at the next higher level. And it goes the other way too – we can draw conclusions about the atomic dimension from the results of the next higher level, allowing us to carefully check and, if necessary, modify our multiscale method.” This research approach requires expertise at every level.

Each area essentially provides a sufficient number of questions in itself. “You can restrict yourself exclusively to processes on the nanoscale. If your questions concern the real system, however, then the knowledge of one single level will no longer be enough”, Jacob says. For research projects like the ones being carried out in Ulm, it is essential that experts for each level – nano, micro, meso and macro – come together, both theorists and experimentalists.

This expertise has been built up in Ulm over decades. “My predecessor at the Institute, Prof Dr Dieter M Kolb, was one of the most respected experimentalists in the field of electrochemistry and played a substantial role in shaping this field over the last few decades; I, myself, started out as a theorist, but I now deal with electrochemical experiments as well”, Jacob relates. “At the Institute, we aim for a fundamental understanding of electrochemical effects by connecting experimental measurements and multiscale simulations. This combination is very important, especially for such complex systems, if we want to draw conclusions on real applications based on the understanding of elementary processes in well-defined systems. Often the methods that Jacob’s team requires do not even exist yet – they still need to be developed by collaborating theorists and experimentalists. Jacob continues, “It only works if you talk to each other. Ulm sets itself apart from many other universities in this regard – it has a high concentration of scientists who work with and are interested in electrochemical systems.”

Only a few institutes in the world have similar conditions, with researchers working together on the system as a whole.
A long-term objective in the field of electrochemical research is to describe the course of electrochemical and electrocatalytic processes on complex realistic electrode surfaces. This should happen on an atomic and/or molecular scale. The basis is formed by studies on idealistic model electrodes with well-defined structures and under idealised conditions – which makes such insight possible; the researchers then gradually move on to more realistic materials and reaction conditions. The outcome is relevant for both battery and fuel cell technology.

“On the one hand, we want to achieve a total, fundamental understanding of the interaction between electrode materials and electrolytes, and on the other hand, we want to understand effects that occur when we gradually move on to real, technical materials and reaction conditions”, explains Jürgen Behm, professor of physical chemistry and head of the Institute of Surface Chemistry and Catalysis at the University of Ulm. “That is why our work ranges from studies on the atomic scale, which are carried out on model electrons with a known surface structure and under idealised conditions, to studies on real catalysts and under realistic reaction conditions, similar to those in a real battery or fuel cell.”

One example is the electrode in a fuel cell. The electrode surface is coated with a catalyst, the typical material being a combination of platinum and carbon particles. The carbon particles serve as a support material for the much smaller “nanoparticles” from catalytically active platinum.

In order to achieve an understanding of the size proportions, the carbon particles can be imagined as footballs, with little platinum marbles...
stuck to them. As the electrochemical reaction in the cell occurs via interaction with the catalytically active platinum surface, this surface should be as large as possible. Nanoparticles have the advantage that they consist, to a large extent, of surface area. If a particle has a diameter of three nanometres, then 30 per cent of its atoms are on the surface. By way of comparison: on a cube with an edge length of one millimetre, only every one-millionth atom will be on the surface, whereas the rest of the atoms are “buried” on the inside. Jürgen Behm continues, “If I take particles that are smaller than three nanometres, I will have even more atoms on the surface. These particles, however, are often unstable and can aggregate.”

Furthermore, the chemical and electrochemical properties of very small particles are different to those of larger particles – e.g. in their catalytic activity. “Catalytic activity” refers to the ability to accelerate a reaction process. The smaller the amount of a catalyst needed, for example, to reduce 20 litres of oxygen per minute, the more active it is. A platinum particle diameter of three to four nanometres has proven to be the most suitable for oxygen reduction on platinum catalysts. “Optimal activity and surface are attained at this size, a quintessence of two decades of basic research”, Behm says.

Behm’s research team is especially interested in what happens when complex materials that consist of several components are used as catalysts, for instance a platinum alloy – i.e. a compound consisting of platinum and another metal. For this purpose, experiments are not immediately performed under actual technical reaction conditions; instead, researchers first experiment on models, using crystals in which the atoms have a completely uniform arrangement. Behm’s team has developed procedures to produce perfect, ultrafine layers of these materials, which can then be examined with regard to their electrochemical and electrocatalytic properties. Besides the amount of the individual components, another important factor is their surface distribution. “We see how the atoms are distributed using special scanning tunneling microscopes that resolve the individual atoms and even the various types (see image)”, Behm explains. “For instance, we were able to determine that A atoms prefer to have other A’s as neighbours. Or mostly B neighbours. Or they mix evenly. From a chemical perspective, it is a different situation each time, because the atomic arrangement and neighbourhood determines the electrochemical properties.” By correlating surface distributions and electrochemical and electrocatalytic properties, the corresponding properties of individual atomic arrangements can be deduced.

The results of these very elaborate experiments can then serve as a basis for comparison with theoretical studies in which calculations are performed to determine the electrochemical and electrocatalytic properties of surfaces with these exact structures. This means that, for the first time, electrochemical and electrocatalytic processes are even accessible on complex electrode surfaces with several components.

This type of research aims to gradually transfer the understanding of the molecular processes in electrochemical and electrocatalytic reactions – which has been gained on idealised models and under simplified reaction conditions – onto technical materials and conditions. This provides the foundation for fully understanding the corresponding processes in real batteries and fuel cells, which, in turn, is a prerequisite for systematic advancements.

“Just as there will be a range of different drive systems – batteries, fuel cells, hybrid, natural gas, 3-litre motor –, user behaviour will also vary, ranging from car sharing models to the privately used vehicles more dominant today. The car of the future will be versatile”, Behm believes.
Materials with Large Surface Areas
Chemical energy conversion reactions in batteries and fuel cells could run more efficiently

Battery and fuel cell performance stands to benefit from the use of nanomaterials. Researchers see nanomaterials as having great potential for improving performance. However, there are several fundamental questions that have not yet been adequately researched. A research team in the Inorganic Chemistry Department at the University of Ulm is addressing this topic.

In general, the field of batteries and fuel cells has seen great progress over the last few years. A significant amount of development is still necessary, however, to ensure that the new technologies will enjoy lasting success. The next step requires the development of new materials. For the energy markets of the future, current research is not only focusing on effectiveness and long-term stability, but also on manufacturing procedures and materials that are affordable and environmentally friendly.

Along with chemical composition and crystallinity, material structure is playing an increasingly important role in the nanometre range in improving performance. “This is exactly where one of our research areas becomes relevant”, says Mika Lindén, professor of inorganic chemistry at the University of Ulm. “Our work focuses on the production of highly porous nanoparticle materials or materials structured in the nanometre range.”
“Along with chemical composition and crystallinity, material structure is playing an increasingly important role in the nanometre range in improving performance.”

Mika Lindén

range.” By employing various template procedures, it is possible to synthetically produce nanomaterials – with a metal oxide or carbon basis, for instance – which then often exhibit a very high specific surface area and a narrow pore size distribution.

In the field of energy storage, researchers see great potential in both materials. However, the nanostructured materials exhibit properties that are different from those of a typical solid material: an example that has recently been studied is the influence of crystal size on magnetic properties, melting behaviour and optical properties. However, at present, virtually nothing is known about the effects that changes in the nanometre range have on electrical properties of these materials – something that is particularly relevant for use in batteries.

The groundbreaking questions of current research include: What effect does crystal size have on the chemical reactivity of nanomaterials? How do particle size and size distribution affect the charge transport and the optimum flow of charge?

A further aspect is the distribution of nanoparticles in composite materials. This is particularly relevant when considering to what extent the distribution in composite materials can be altered in a controlled manner.

Nanomaterials have a large specific surface area, which leads to a high surface energy. Nature always strives to minimise energy, so the result is often a distinct clustering of nanoparticles. In the worst-case scenario, this could result in a loss of the advantages associated with nanomaterials. “These are some of the most burning questions that I intend to investigate with my colleagues here in Ulm”, Lindén summarises.

“At the University of Ulm, we are fortunate enough to have several important conditions already in place to facilitate swift progress in this interdisciplinary research field: a wide range of lab equipment is available, distances are short and cooperation with other institutes is very straightforward.”
The interface between electrode and electrolyte is an important subject of research in the field of electrochemistry. The processes that occur at this boundary play a significant role in energy conversion and storage in batteries and fuel cells. Theorists and experimentalists are working together on new developments.

“A few years ago, collaboration went something like this: the experimentalists performed measurements, then approached the theorists and said, ‘We did this and this, and the results were this and this: Now explain it to us’”, says Axel Groß, professor of theoretical chemistry and spokesperson for the DFG research unit “Elementary Reaction Steps in Electrocatalysis” at the University of Ulm. “Now the impetus can come from the other direction as well. Theorists can make the first step by defining the central questions and modelling corresponding systems, thereby defining the line of research. In the experimental phase, the predictions are then tested. Here it is especially important to find suitable parameters in order to be able to compare the theory and the experiments.”

Researchers are studying the individual steps that occur in batteries and fuel cells during electrochemical energy storage and conversion, in which the release of energy creates electricity. Despite the fact that batteries and fuel cells have been objects of research for decades, numerous processes have yet to be explained at the molecular level. Even with very simple intermediate steps, there are differing models that are the subject of controversial discussion. It was difficult to explain the elementary steps due to a lack of sound theories and suitable technologies. Today, however, we have the necessary computer programmes as well as a range of new microscopic and spectroscopic experimental techniques. With scanning tunnelling microscopy, for example, it has become possible to image molecules on electrode surfaces. Scanning tunnelling microscopes are employed for dimensions in which light microscopes can no longer be of use. This is always the case when dealing with particles that are smaller than the wavelength of light. Without light, the human eye is not able to see – not even with the best microscope. These tiniest of particles have to be measured in a different way. A scanning tunnelling microscope maps structures via a form of scanning, without any direct physical contact. The tip of the microscope, which is only a few atoms wide at its foremost end, floats one nanometre (one billionth of a metre) above the sample in question. A current is applied between the sample and the tip, and this current changes as it moves along the arrangement of molecules. These changes are then mapped by the scanning tunnelling microscope as an image of the surface. Another procedure is spectroscopy, which allows the movements of individual molecules to be traced. Spectroscopy allows researchers to identify particles according to their vibrations, which in turn enables them to track particle interaction with the electrolyte and the electrode.

“We know what happens in batteries and fuel cells in general. Now it is important to calculate the steps the individual atoms and molecules take and what reactions occur in the process. For instance, we create a model of how a hydrogen molecule emerges from the inside of the electrolyte and appears on the electrode surface”, Groß relates. “In order to do this, we need to model both the electrolyte and the electric current that triggers protons to wander from one electrode through the electrolyte to the opposite electrode. Difficulties arise due to the fact that movements within a liquid – in this case the electrolyte – require complicated simulation methods. Many teams around the world are reluctant to face the large computational challenge.”

Creating a model of these processes is comparable to producing an animated film: a sequence of snapshots is produced and the images are then connected in series. One single image corresponds to a process that lasts approximately one femtosecond, i.e. 0.000 000 000 001 seconds. “It takes us several hours to model a step like this on the computer. We work on several computers simultaneously, which allows us to simulate about 50 steps per day”, Groß explains. “The programme tells us which configurations – which arrangements of molecules and
atoms – we have, and what forces are affecting them. The important thing is to take an average of many configurations. A liquid electrolyte, for instance, moves differently each time, so the molecular paths can only be traced as an average of numerous variants. We are among the first to use exact quantum chemical procedures to do so.”

The researchers do not include all the processes that occur in electrochemical cells when creating their models – that would be far too broad. Instead, they include a set of approximately 150 atoms each time. The start is generally an artificial collision created by the researchers in order to initiate the process. “We create a collision that is typical of a real impact. Then we follow what happens in real time.” One objective is to find out where reaction barriers are for the crucial processes. “What we want to trace can be thought of as a map. If I want to go to the Mediterranean Sea, I look for the path over the Alps with the lowest elevation gain and drive over the Brenner Pass. Similarly, we look at the potential mountain range and identify the easiest way that the atoms and molecules could take.”

Axel Groß

Electrocatalysis

Modelling and visualising elementary structures and processes on electrode surfaces

The business world is paying close attention to the research being conducted in Ulm. The worldwide scientific community is also familiar with the research activities here. Representatives from Ulm get invited to present their research findings at international conferences on a regular basis.
The ZSW’s main objective is to act as a liaison between the fields of basic research, which is conducted at the University, and industrial research, which has more of an application focus. How does that work? Should we imagine that you go into the labs, look over the researchers’ shoulders and say, ‘Oh, that would be something for Daimler’?

Werner Tillmetz: No, that’s not really how it works. Research projects with an application focus need to be explicitly set up as such – by the Federal Ministry of Education and Research, for instance. The findings that result from the basic research at the University then flow into these projects.

In your opinion, what else needs to be done to encourage the transfer between research and industry?

Tillmetz: In general, this knowledge transfer works very well. One thing that could possibly be set up at the University of Ulm would be process engineering, which does not yet exist there. Another project, which we hope will help to better establish us in the business world as a first point of contact, is the planned Energy Materials Competence Center – EMC² Ulm. Activities in the
Technology Transfer

field of energy materials, as well as their applications, will be coordinated and communicated under this umbrella. Another important step is the pilot production line for lithium ion batteries, which we, as a member of the Competence Network Lithium Ion Batteries e.V. (KLiB), would like to set up at the ZSW.

As we all know, there are already lithium ion batteries on the market. What is the difference between the existing batteries and the ones you are developing on the pilot production line?

Tillmetz: Germany has a lot of catching up to do when it comes to battery technology. Today’s commercial lithium ion batteries are used in the entertainment industry, in mobile phones, notebooks, etc., and they all come from Asia – primarily from China, Japan and Korea. Now, however, the automotive industry requires batteries for electric and hybrid vehicles. These applications demand a lot more from the batteries, such as much greater storage capacity, a longer service life and functional reliability under conditions of extreme cold or heat.

How exactly do the requirements differ?

Tillmetz: In Germany, a great interest in plug-in hybrids appears to be emerging. A “plug-in hybrid” refers to the combination of a medium-sized battery, which can be charged via an electrical outlet (plug), and an internal combustion engine. With these cars, the battery can be used for travel within the cities and the traditional engine for longer journeys. The longer journeys do not appear to be that important for Asian mega-cities. A battery in a hybrid car needs to fulfill different requirements than a battery in a purely electric vehicle. It is considerably smaller, yet needs to be very powerful.

Does Germany even stand a chance with battery technology in the global market or are the Asian countries going to overtake us anyway?

Tillmetz: We have a really good chance at breaking into the global battery technology market because we are very strong in several key areas, such as specialty chemistry, production line development and electrical engineering. What we are missing is the knowledge: How do I make a really good battery out of the various components? Asian countries are ahead of us where this question is concerned, but we are working hard on it. Our advantage is the strong and very committed local automotive and supplier industry.

Why are the car manufacturers waiting for your pilot production line? Why don’t they develop one themselves?

Tillmetz: The financial risk involved in setting up a battery production line is immense. For the players out in the industry, it makes a lot of sense to reduce the risk via joint research and development activities as well as external funding. This key technology may then come from Germany in the future as well, not only from manufacturers in the US or Japan.

Where do you see a need for change in funding policy?

Tillmetz: With regard to fuel cells and hydrogen production via electrolysis. Both technologies play a key role in shaping our future energy supply and mobility. There is still a lot of work to be done in materials research, especially in terms of meeting cost targets.

“...This key technology may come from Germany in the future as well, not only from manufacturers in the US or Japan.” Werner Tillmetz
Over the past few decades, a centre of competence has emerged in the “Science City” Ulm in the field of basic process research in batteries, and it is attracting worldwide attention. Research topics include fuel cell technology and, in a broader sense, electromobility. These fields of research are considered to be the foundation for developing sustainable, environmentally friendly mobility for the future.

Several factors have played a role in establishing the expertise at the University of Ulm in the field of electrochemical energy conversion and energy storage, including: founding institutions, appointing competent individuals to design the research and creating a living culture of cooperation.

A brief overview of the highlights:

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<th>Year</th>
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<td>1988</td>
<td>Founding of the “Centre for Solar Energy and Hydrogen Research Baden-Württemberg” (ZSW), founding member from the University of Ulm: Prof Dr Wolfgang Witschel; head of the Electrochemical Energy Technologies Division at the ZSW in Ulm, from 1991 to 2004: Prof Dr Jürgen Garche</td>
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<td>1990</td>
<td>Prof Dr Dieter M Kolb appointed head of the Institute of Electrochemistry</td>
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<td>1996-2005</td>
<td>German Research Foundation (DFG) Doctoral Research Training Group (Graduiertenkolleg GK 328) “Molecular Organisation and Dynamics at Interfaces and on Surfaces”, spokesperson: Prof Dr Dieter M Kolb</td>
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<td>2004</td>
<td>Prof Dr Werner Tillmetz appointed head of Electrochemical Energy Storage and Conversion at the University of Ulm and head of the Electrochemical Energy Technologies Division at the ZSW in Ulm</td>
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<tr>
<td>Since 2010</td>
<td>DFG Research Unit (FOR 1376) “Elementary Steps in Electrocatalysis: Theory meets experiment”, spokesperson: Prof Dr Axel Groß</td>
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Energy conversion and storage at a glance: four broad topics provide the structure for the research work conducted in Ulm. Current research results flow directly into the classroom – into teaching materials for the international master's degree programmes “Energy Science and Technology” and “Advanced Materials”.

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<th>Energy conversion and storage</th>
<th>Electrochemical Processes</th>
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<td>Materials</td>
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The Helmholtz Institute Ulm’s (HIU) focus is a very current topic in the fields of electrochemistry and electromobility. It concerns basic research for electrochemical energy storage. The field of battery technology, which is the central building block of energy storage, benefits in particular from the HIU’s research.

The HIU is being managed by renowned funding partners: the Karlsruhe Institute of Technology (KIT), the University of Ulm, the Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW) and the German Aerospace Centre (DLR). The Institute has been in operation since the beginning of 2011. In addition to expanding existing fields of competence, the objectives of this collaboration are: to integrate and improve education for young researchers and to predominantly exploit project results in Germany.

The federal government provided 10 million euros in funding for this collaboration within the framework of its Economic Stimulus Plan II. As a recognised top location for research in electromobility, the University received 2.75 million euros and the ZSW 2.5 million euros for investments out of the Federal Ministry of Education and Research’s (BMBF) budget – through the special programme “Electrochemistry for Electromobility”.

A research facility is in planning for the University of Ulm campus – the “Science City”. The costs of around 12 million euros will be covered by the Helmholtz Association, the BMBF, the state of Baden-Württemberg and the University of Ulm.
A Strong Focus on Industry
The Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW)

“The ZSW was founded more than 20 years ago at the University of Ulm, motivated by the desire to increase collaboration with the business world”, explains Werner Tillmetz, professor of electrochemical energy storage and conversion at the University of Ulm and ZSW board member. The ZSW is set up as a non-profit foundation; the founding members include the University of Ulm, the University of Stuttgart, the state of Baden-Württemberg, the German Aerospace Centre (DLR) and several commercial enterprises. The foundation’s goal is to conduct and promote research and development in the field of solar energy and hydrogen technology in cooperation with academic and applied research, transferring the results into industrial application.

“We work with a strong focus on industry – according to our by-laws, that is our job, and it is very important for securing funding for the Institute. We collaborate with almost all the companies in Germany that operate in the fields of fuel cells or batteries, as well as several companies abroad”, Tillmetz says. “Of course, on the other hand, we are reliant on collaboration with the university institutes as well. They pick up fundamental, new technologies, which we then translate for industrial applications.”
The ZSW's range of competence spans the entire value added chain of batteries and fuel cells: from modelling and simulation of electrochemical processes to synthesis and characterisation of active materials, from optimisation of components to demonstrating complete systems. Modern test benches enable our researchers to thoroughly evaluate and qualify components and systems in terms of performance, lifetime and safety. "We are the only ones in Europe who cover this entire spectrum", Tillmetz explains.

The ZSW has business partners from many different fields, including specialty chemistry, energy supply and the automotive industry along with its suppliers. At the same time, the ZSW works with a large network of research institutes both on and off the university campus.

The ZSW's main competences

The ZSW, with its branches in Stuttgart, Widderstall and Ulm, conducts research and development in the areas of energy management systems, photovoltaics, regenerative fuels, energy storage and energy conversion in batteries and fuel cells. Furthermore, the Centre focuses on transferring knowledge and technology into industry applications.

The research topics in Ulm are: batteries – new active materials, cell opening and post-mortem analysis, reference cells and cell production technologies, battery systems technology, battery safety and failure analysis; fuel cells – modelling and simulation, components and systems, lifetime and qualifications, new energy storage concepts and materials for the next generation.

High-Quality Training Is Their Trademark

The Fuel Cell Education and Training Centre e.V. (WBZU) is a registered non-profit organisation that focuses on training, continuing education and publicity work in the fields of renewable and innovative energy technologies.

In Germany, training and continuing education are important tools in ensuring that specialist business and administrative knowledge is updated in various sectors on a regular basis. Continuing education is gaining importance in view of demographic developments and the potential shortage of qualified professionals. Thus the WBZU has an important position: a registered non-profit organisation that focuses on training, continuing education and publicity work in the fields of renewable and innovative energy technologies.

The WBZU specialises in training in the fields of: fuel cells, hydrogen, batteries and mobility, CHP technologies and energy management and policy.

Courses are designed to meet the needs of the specific target groups: professionals from the areas of industry, trade, research and teaching. Other formats include presentations and informational sessions for pupils, teachers and the public. With its test stands, model experiments and exhibits, the technical school for practical training complements the WBZU's course offerings.

The WBZU offers practical training and continuing education with the following concentrations: fuel cells and hydrogen, batteries and electrification, CHP technologies and energy management and policy.

In addition to regular seminar rooms, the Centre has a specially designed technical school at its disposal for training and educational purposes. The attractive new building, the choice of topics and the on-site technical school lend the WBZU its unique character.

The WBZU offers practical training and continuing education with the following concentrations:
At the Centre for Solar Energy and Hydrogen Research (ZSW) in Ulm, battery research focuses on electromobility, stationary temporary buffer stores and material development for new batteries. Our researchers are searching for new materials or material combinations and examining these materials under real operating conditions in order to determine their suitability at the earliest stage possible.

“We want to be able to assess the potential of new materials as early on as possible”, explains Margaret Wohlfahrt-Mehrens, head of the Accumulators Materials Research Division at the ZSW. “A battery is an extremely complex structure comprising many different components. It is not enough to simply analyse the properties of individual materials; it is important to understand the interactions that occur in the complete system.” This pertains to the way components interact with each other and the changes that arise through battery operation. Charging and discharging a battery, for example, has consequences for the morphology of individual particles. The particles first expand and then contract again – what is known as the “breathing effect”. Another central factor is the aging process. How do the various components behave when they are in operation for a long period of time? “It generally takes 15 to 20 years until new materials can be implemented. Our aim is to shorten this timeframe. One of our current projects is developing methods for simulating aging in materials.”

Setting Sights on Materials with a Long Lifespan
At the ZSW, researchers are studying batteries and their components on a production line that reflects industrial production processes.

Electrode coating line: the eLaB’s state-of-the-art machines and lab equipment ensure progress and successful research toward the goal of high-powered batteries.
of the paste onto a plastic sheet, from which the electrodes are then produced. During the entire procedure, the researchers make sure to comply with the requirements of the industrial production process. This includes applying a uniform coating as well as maintaining a certain speed. Other relevant properties are adhesion, electrical conductivity and porosity of a material. A material that has high energy density as a powder could lose this quality during the course of the manufacturing process and ultimately produce only a small amount of energy in the finished battery cell. This is the case, for instance, when the material proves to be too porous during the coating procedure.

“We have found two different material combinations that are very suitable, one for the positive electrode and one for the negative electrode. The first cells with these material combinations are currently being produced at the ZSW.”

Margret Wohlfahrt-Mehrens

“We have found two different material combinations that are very suitable, one for the positive electrode and one for the negative electrode”, Margret Wohlfahrt-Mehrens says. “For the positive electrode, we use lithium manganese phosphate, which exhibits very good energy density and is much safer than standard materials. It has proved to be especially resistant at high temperatures and in the event of a crash. For the negative side, we use mesoporous titanium dioxide, which has outstanding properties, including the ability to charge quickly and a load capacity at low temperatures, even down to minus 40 degrees. It is also a material that is readily available, non toxic and relatively affordable to produce.” The first cells with these material combinations are currently being produced at the ZSW. The targeted field of application is stationary buffer storage, i.e. decentralised storing of energy in households. The use of mesoporous titanium dioxide resulted from a close cooperation with researchers from the University of Ulm.

Battery research requires a whole range of competencies, which is why it is a multidisciplinary field at the ZSW. Chemists, electrochemists, materials scientists and electrical engineers all work together in the individual teams, each bringing their own perspectives. Wohlfahrt-Mehrens sums up the benefit of researching in Ulm, saying, “Ulm’s unique advantage is that here many disciplines come together in very close quarters.” She continues, “A lot is done, as well, to promote and increase cooperation. There is an animated exchange between the ZSW and the individual departments at the University.” Various institutes are involved with the new Helmholtz Institute (see pages 6 and 19), which means that different research institutions are all pursuing the same aim: energy storage. Wohlfahrt-Mehrens says, “At the ZSW, we too benefit from the University’s specialised study programmes – we get master’s students and doctoral candidates with outstanding educational backgrounds.”

Wohlfahrt-Mehrens is confident about the application potential for her research projects: “I think that the next few years will be very exciting in terms of energy supply. Germany is a forerunner in the fields of regenerative energies such as wind power and photovoltaics. If renewable energy installation continues to progress as quickly as it has in the last few years, there will soon be a need for decentralised storage systems.” In terms of her personal energy use, Margret Wohlfahrt-Mehrens plans to purchase an electric car in the near future. “I live 25 kilometres from my work – exactly the right distance.”
The Big Challenge – The Issue of Storage
Substitute natural gas could enable a 100% renewable energy supply

A core problem for the energy transition is the issue of storage. The wind and the sun provide energy erratically – sometimes too much, sometimes too little. Storage systems are necessary to balance out these fluctuations. Such storage systems make it possible to store electricity and then access it on dark days without wind. Researchers at the Centre for Solar Energy and Hydrogen Research Baden-Württemberg (ZSW) and the Fraunhofer Institute of Wind Energy and Energy System Technology have developed a suitable means of storage: synthetically produced natural gas, or substitute natural gas.

The process of stockpiling energy currently involves storing fossil fuels such as coal, crude oil and natural gas. If conventional energy sources are to be replaced by renewable sources, however, then an alternative means of storage must be found. There is no other way to make a 100 per cent environmentally friendly power system feasible. It is easiest to store energy in the form of hydropower and biomass. The use of hydropower, however, is dependent on geographic conditions, and energy crops can only be produced in limited quantities, as agricultural areas are needed for other purposes. One option for energy storage that will surely be implemented in the future is battery systems in the home. However, this type of energy can only be available for a number of hours, never in large quantities or for long periods of time. “For long-term storage, the only option is chemical secondary energy sources”, explains Michael Specht, head of the Renewable Fuels and Processes Department at the ZSW. “We use surplus electricity, for example from wind farms or photovoltaic systems, to produce hydrogen, which we then transform into methane, using carbon dioxide. Methane is the main component of natural gas. The synthetically produced substitute natural gas has the same combustion properties as natural gas.” The novel element in this process is the combination of hydrogen electrolysis technology with methanisation technology. Another novel aspect is the installation technology; a basic requirement on systems that are intended to collect and balance out fluctuations in the electricity network is sporadic operability: as opposed to conventional power plants, which run constantly, they must be able to start and shut down quickly.

The biggest advantage of the substitute natural gas is that an existing infrastructure – gas pipelines – is already in place. Whereas a high-voltage power line in Germany transports less than one gigawatt of electricity, a gas pipeline can transport up to 30 gigawatts. The power network in Germany has a capacity of 0.04 terawatt hours (a gigawatt is one billion watts, a terawatt is one trillion watts). With this capacity, the entire energy requirement in Germany can be met for approximately one hour. The storage reservoir of the German natural gas network, in comparison, comprises more than 200 terawatt hours, which corresponds to the energy consumption for a period of several months. Gas makes long-term energy storage possible and provides a reliable energy supply. The gas is converted back into electricity in gas power plants. Alternatively, it can also be used as fuel for cars. Natural gas cars emit very little CO2, produce marginal particulate matter and are quieter than diesel vehicles.

“We have given the license for our procedures to the company SolarFuel GmbH, which is now building a large pilot facility for producing and storing substitute natural gas. Audi is contracting the pilot facility; they intend to use the gas as fuel for cars. The facility is located in Northern Germany, where wind farms frequently produce surplus electricity, which is then either sold at a minimal price or disposed of”, Specht reports. Changes to the system are necessary if storage technology is to advance. “We require a system of incentives for storing energy”, Specht believes. “At present, there is no incentive for renewable energy producers to consider the time factor. They simply receive money for each kilowatt hour. It makes a considerable difference, however, if electricity is fed into the network at peak times or at slack times. We need a financial incentive system, which would connect a financial impact to the time of feed-in.”

Scientists are currently focusing on improving gas production facilities, to conform to the demands of the energy market. Not only does synthetic gas need to have the same properties as fossil gas; the conversion back to electricity must also occur in such a way that electricity production invariably corresponds to consumption.

Specht is convinced that renewable energies are a viable alternative for the future, that it is possible to completely forgo fossil fuels. He has a solar thermal system and solar panels on his roof at home and reports, “I produce half of my electricity myself.”

Dr Michael Specht
How far can my car go on one battery charge? To work? To Munich? To Italy? These are key questions that researchers are attempting to answer from many fronts. With batteries of the third and fourth generation, the aim is now to drastically increase the driving range.

“In order to improve the battery, it is necessary to improve the performance of the cathode. That is why BASF is working hard on cathode materials of the third generation, the so-called high-voltage spinels and high-energy NCMs”, explains Rüdiger Oesten of BASF Future Business GmbH. Spinels are oxides with a lithium-manganese base and cubic structure; high-energy NCMs are NCMs – i.e. combinations of lithium, nickel, cobalt and manganese – with special stoichiometry (i.e. composition). “We are simultaneously conducting research on the fourth generation as well, including lithium sulphur technology, which can extend the driving range to 400 kilometres.”

Oesten is heading the “HE-Lion” project, a consortium of businesses and universities that acts as a framework for testing and developing new materials. The HE-Lion project is part of LIB (Lithium-Ion Batteries) 2015, a network of approximately 60 partners from the sectors of industry, research and academia. The Ulm Centre for Solar Energy and Hydrogen Research (ZSW) is also a member of this network, which is receiving 60 million euros in funding from the Federal Ministry of Education and Research.

One of HE-Lion’s objectives is to study NCM layered oxides of the second and third generation. Compared to standard materials for batteries in mobile phones and laptops, these new materials are superior in terms of cost, safety and service life. “The first results show that the cathode material is easy to handle and that it can be used to build robust, powerful batteries. Even after 1,000 charge and discharge cycles, these batteries still retain more than 80 per cent of their original capacity”, Oesten says. “There is nothing more exciting than developing good materials at the moment. The transfer from the lab to pilot scale went smoothly, which means that we can now supply quantities of more than 100 kilos without any problems.”

Oesten combines an understanding for the researcher’s perspective and knowledge from the business world. Before he joined BASF, he was also a scientist at the ZSW. “Ulm stands out in Germany in terms of junior researchers in the field of electrochemistry. In general, however, there is a massive shortage in this area. It is not enough to simply spend money; the experts must be there in order to conduct the research.”

Part of the HE-Lion project is an annual “Battery School”, where employees from businesses as well as universities can take advantage of training opportunities.
Christian Mohrdieck: Our largest projects concern fuel cells and batteries, for instance the tests that we are carrying out on battery service life in cooperation with the ZSW. We have also had a close cooperation for several years that concerns developing infrastructures and supplier structures. Furthermore, we have a collaborative project with the ZSW and twelve other partners within the framework of the EU project “AutoStack – Automotive Fuel Cell Stack Cluster Initiative for Europe”. One of our tasks here is to set up the requirements from the industry while the research institutes check what is feasible in terms of research.

Those projects are more focused on applications. What is your collaboration with the University of Ulm like?

Mohrdieck: We have PhD and diplom thesis projects at the University of Ulm, in cooperation with Jürgen Behm, for instance, who is a member of the Physical Chemistry Department and head of the Institute of Surface Chemistry and Catalysis (see page 10). Furthermore, I give a lecture myself in the international master’s degree programme “Energy Science and Technology” on the topic of “Hydrogen as Energy Carrier”. Numerous students have already joined our company because of these lectures. Several of my colleagues also give lectures at universities. The idea has become entrenched at our company: We’re the Daimler Lecturers.

Daimler has its own large development departments. Why do you need partners from academia?

Mohrdieck: One reason is that the ZSW has testing facilities that we do not have ourselves, and another reason is that we are often working to capacity. Regarding the University, we would like to work together on basic research because it is an area in which we need substantiated knowledge. That is why we are discussing options such as a joint lab for doctoral students, which both sides would have access to and in which doctoral students could pursue projects in the field of basic research.

The transfer of technology from academia to the business world is one of the declared objectives in political circles. What would you like to have from research partners in order to improve the collaboration?

Mohrdieck: The most important thing is more mutual understanding for the “other world”. For our partners in research institutes, this especially means an understanding for the aspects that do not have priority in science. For instance, it is sometimes difficult to convey the message to researchers that, from our point of view, it is not sufficient to simply show that something works. It is also necessary to prove that it works under all possible conditions in a vehicle. All the parts of the car must withstand various influences, such as temperature differences between minus 40°C and plus 80°C. The latter could easily occur if a car sits on asphalt under the blazing sun for a long period of time. For these purposes, it is necessary to conduct comprehensive studies that can take a several years to be completed. Scientists generally consider their work accomplished as soon as they have demonstrated that something essentially works. On the other hand, scientists probably see our perspective as very pragmatic and perhaps too narrow. At the ZSW and the University of Ulm, however, this is not generally the case. They have a very good understanding of our perspective.

How has your experience with the German scientific system been in general?

Mohrdieck: Compared to the US, Germany has a lot of untapped potential in terms of collaboration between science and business. In the US, the National Labs have a closer commercial...
connection. For instance, they have set up roadmaps for fuel cell and battery development in cooperation with representatives from industry and politics – with the US Department of Energy, to be precise. These roadmaps have attracted worldwide attention. There has not yet been anything comparable in Germany, unfortunately. We would be more than happy to discuss such an approach with the German research institutes.

How is it at the University of Ulm?

Mohrdieck: According to the information I have, for instance, researchers at the University and the ZSW asked themselves how they should react to the topic of e-mobility. There were a number of round table discussions, which we were invited to join at a certain stage, and at which I was able to present our ideas. I found it very positive. Perhaps it also has something to do with the fact that many members of the University have industrial experience, including the president; they can better understand the “other side”. At the University of Ulm, I also value the competence, the honesty and the consistent attention to quality. We often encounter partners who initially say that they can do everything, and then you slowly start to realise that that is not the case after all. Every project is discussed openly in Ulm, so there are no surprises about what individual strengths are or where no competence or know-how is available. This leads to very focused, pleasant and reliable collaboration.

Perhaps it is also the case that research partners expect relatively quick, marketable results from their collaboration projects with business partners, and are disappointed when the financial return is a long-term result. How long does it usually take until actual products come out of your projects?

Mohrdieck: It takes approximately three to five years to develop a car, depending on the level of innovation. This means that as early as five years before a car goes on the market, all of the key technical questions have to be answered. For example, if I have a new combustion system for a car that is scheduled to go into serial production in 2016, I already need to know today if it is going to work. There are three steps to the development process, each of which requires approximately one year: the principle feasibility, the conceptual feasibility and the serial production feasibility. The principle feasibility test is passed when everything essentially – or in principle – works. Once this has been achieved, we check the conceptual feasibility. This includes determining if the parts in question will not only work at the start of the car’s life, but also several years later. The final step is the serial production feasibility. At this point, it is necessary to create a product requirements document that includes all of the parameters to be met. All of the work that universities or research institutes do for us in terms of basics research needs to be completed by the time the principle feasibility has been achieved. People are not always aware of these boundary conditions.

You have been working with your research partners on developing electric cars for years. What is the current status on that?

Mohrdieck: The second generation of Smarts is already on the streets – that is more than 2,000 cars that are driving on the streets worldwide. Starting with our next generation in 2012, it will be a five-digit number. The third generation will also have a longer driving range, considerably surpassing the 100 kilometres of the first generation.

At the moment, electric cars are being leased rather than purchased, as their service life is not long enough to make them affordable. How do you decide whom you will lease the cars to? Are they mainly VIPs?

Mohrdieck: Essentially, we are aiming for a cross section of the population in order to collect as many driving profiles as possible. That means that we lease the cars to companies as well as private customers, including VIPs, thereby taking advantage of these multipliers to make the public aware of how suitable electric cars are for daily use.

What is the overall response?

Mohrdieck: People are generally very enthusiastic. There are three main reasons: first, the high torque – i.e. the acceleration behaviour the first few metres. People just want to speed away from traffic lights. That shows us that it is not necessarily sufficient to simply consider the horsepower. The sporty feeling has more to do with the torque than with the horsepower. The second positive discovery is: “It’s so quiet”, and the third: “It drives just like any other car”.

What kind of car do you drive personally?

Mohrdieck: As often as possible, I drive a fuel cell-powered car.

Do you always have a list with you of possibilities for filling up on hydrogen?

Mohrdieck: I can fill up at the company. For longer trips, I currently have a Mercedes GLK. As announced last summer, we will be setting up a network of hydrogen filling stations for areas of high population density, in cooperation with the company Linde.
Electron Microscopy

In order to develop new high-energy storage systems with high-energy density, new concepts of battery characterisation are required. Another current long-term objective is the atomic imaging of structural processes during the course of a battery’s charging and discharging cycles and the defect-related changes in situ in a transmission electron microscope. Researchers in Ulm are striving for advancements in research and development in the area of low-voltage transmission electron microscopy.

Ute Kaiser, professor and head of the group of Electron Microscopy in the Material Sciences Department at the University of Ulm, begins with the basics: “The nano science of materials is characterised by the atomic and molecular structure of the materials.” She and her team focus on addressing “nano questions”: What is the location of which atom? What is the appearance of the chemical bonds? Are there intrinsic electric, magnetic or mechanical fields? How do structural processes work in situ at the atomic level?

Structure-property relationships can be explained and modelled using the knowledge of a material’s atomic and molecular structure, which determines its mechanical, optical and electric properties. It is then possible to produce customised materials for the key technologies of today and optimise existing technologies.

One of the most efficient methods of analysis in materials science is transmission electron microscopy (TEM). This has been particularly true since aberration correctors for electron lenses became commercially available in 2005 (an aberration corrector is a pair of “glasses” for the electron lens). Aberration correction has enabled researchers to obtain images sharper than ever possible before. The University of Ulm faced the challenge of the new technology at an early stage, acquiring one of the first commercial devices of its kind worldwide. Since then, electron microscopists in Ulm have been pursuing the quantitative answers to the “nano questions”.

In contrast to a light microscope, an electron microscope does not use beams of light to capture images; instead, it uses rapid electrons with a wavelength millions of times smaller than that of light. The fast electrons (they nearly reach light speed at an acceleration voltage of 300kV) go through the specimen being studied and interact with its atoms as they pass through. As a result, they are diverted from their trajectory or even slowed down. Information about the specimen’s atomic structure can be ascertained from the arrangements and intensity of the electrons once they exit the specimen and following their imaging on the electron detector. It must be considered, however, that the lenses used for the experiment have a further influence on the trajectories of the electrons. Aberration correction now makes it possible to correct these errors. But what can be done when the atoms are displaced by the high energy of the electrons used to image them? This is the case with the lightweight materials important for batteries, such as carbon and lithium, whose displacement thresholds are significantly below 80kV, the current low-voltage limit of commercial aberration correction devices.

How exciting it would be, says Ute Kaiser, if we could image individual lithium atoms, for...
example, and explain their function throughout the charging and discharging cycles of a lithium ion battery at the atomic level. “Our motivation in developing low-voltage electron microscopy is to be able to study radiation-sensitive materials with atomic resolution”, explains the scientist who is also head of the SALVE project – Sub-Angstrom Low Voltage Transmission Electron Microscopy. “We want to use much slower electrons (‘only’ approximately a third of the speed of light) for imaging, diffracting and spectroscopic analysis.”

The SALVE project team is developing a microscope that will increase the resolution for lower voltages. Carl Zeiss NTS and CEOS GmbH, both companies from the state of Baden-Württemberg, are partners in this project. Kaiser continues, “The microscope is receiving much stronger ‘glasses’ that are optimised for the low-voltage area of 20kV to 80 kV!” This project is receiving funding in the amount of 17 million euros from the German Research Foundation, the state of Baden-Württemberg, both business partners and the University of Ulm.

The group of Electron Microscopy in the Materials Science Department in Ulm has been addressing the topic of electromobility for several years, focusing on questions concerning high-energy efficiency and a long lifespan. Why? Transmission electron microscopy enables researchers to obtain a wide range of information; a broad methodical palette can be applied in Ulm. From just one image or a series of images and the corresponding image calculations, electron microscopists here are able to determine the three-dimensional morphology, the two-dimensional atomic crystal structure and its tension, or, in special cases, the charge transfers (see image 1) at the atomic level. The researchers are also working on locally – and very precisely – determining the lattice constant from convergent electron diffraction patterns (see image 2) as well as ascertaining the local element distribution and electron structure using spatially resolved spectroscopy.

The hope is that TEM analysis, applied with its whole spectrum of methods, will enable researchers to delve much deeper into the processes inside battery materials in the future. Especially with the SALVE Initiative, researchers in Ulm are hoping to gain insights into the charging and discharging cycle, aging processes, diffusion and segregation processes at the atomic level.

“Low-voltage transmission electron microscopy is a brand new trend in microscopy, and we are in a position to say that we have an influence on it. There are now two big projects pursuing similar aims, in Japan and in the US. With its SALVE project, the University of Ulm is one of the lighthouses in this field.”

Ute Kaiser
Fuel Cells with Ethanol?
Our researchers know which direction their research should take

In electrochemical energy storage and conversion systems, be it batteries or fuel cells, reactions need to occur quickly, to ensure that the energy can either be withdrawn or stored effectively and without any loss. Extremely active electrodes, called electrocatalysts, are required for this purpose. Until a few years ago, developing new catalysts was a complicated process that involved a mixture of experience and intuition, and that necessitated countless, often unsuccessful, trials. A few years ago, however, a fundamental shift began to emerge: a transition to developing electrocatalysts with a rational, strategic approach. The results of this new approach are also being applied to catalyst research in the field of batteries.

This has all become possible due to great advances in experimental and theoretical electrochemistry. On the experimental side, various methods have been developed to investigate the course of a reaction on the atomic scale. Many of these methods are accessible in Ulm. Theorists have developed models on how the electronic properties of the electrodes influence the course and the speed of the reactions. Through the mixture of experimentation and theory, it is becoming evident which requirements a good catalyst needs to fill and which materials and structures show promise. Here quantum chemical calculations, first made possible through the development of faster and bigger computers, play a significant role. These computers enable scientists to calculate many chemical and physical properties that regulate electrocatalysis.

“Our group mainly works in the field of theoretical electrochemistry. In the last few years, we have been concentrating on hydrogen reactions, which play an important role in fuel cells. The fact that this reaction only comprises two steps makes it a very attractive subject of research for new theories”, explains Wolfgang Schmickler, professor of theoretical chemistry at the University of Ulm. “When we first began addressing this topic, we were initially attempting to explain established experimental results; you could say we were lagging behind the experiments. Our theoretical side has now flourished to such an extent that we even venture to predict which materials would make particularly good catalysts for this reaction before they have been tested. We now hope that the experimentalists will seize our suggestions!”

Electrochemists have been searching for good, affordable catalysts for more than a hundred years. All the simple metals and alloys were studied a long time ago, and no one was able to

Experiments and theories prove that often a single layer of active atoms on a low-cost substrate is enough to achieve a great catalytic effect: here the method is to substitute “cheaper” gold for the expensive platinum. This image shows the focus of work for theoretical chemists in Ulm; even from a purely scientific perspective, the electrocatalytic “cost advantage” is a great contribution to fuel cell technology.
Theoretical Chemistry

Intensive discussions are the breeding ground for great science. Argentinian PhD student German Soldano received a prize this year for his dissertation from the Applied Electrochemistry Division of the GDCh.

Prof Dr Wolfgang Schmickler

find anything better than expensive platinum. Researchers are now placing their hopes on nanotechnology, a field in which it is possible to modify electrodes at the atomic level. Both experiments and theory show that often a single layer of active atoms on a low-cost substrate is sufficient to achieve a large catalytic effect. From a purely scientific perspective, this is already a monumental success for the field of electrocatalysis. These findings also imply that just a small amount of active material in electrochemical cells could be enough. Only longitudinal studies will be able to show if these nano-structured electrodes prove successful in practice, i.e. if they are stable enough in the long term.

Transporting and storing hydrogen is problematic, which is why researchers have been pursuing alternatives for some time. Ethanol is a promising fuel: it is already being added to petrol and we have had access to proven methods of production and processing for years. “Instead of burning ethanol in motors, it would be much more effective to convert it directly into electricity in fuel cells”, Schmickler says. “After all, the degree of efficiency for a motor is restricted by the second law of thermodynamics, but that of a fuel cell is not.” Unfortunately all attempts to operate a fuel cell with ethanol have been unsuccessful to date. This is due to a seemingly simple, but elusive problem: “In order to convert ethanol, you have to break the bond between two carbon atoms. That should not actually be too difficult – our own bodies do it very effectively whenever we consume alcohol. However, it is rare that these bonds are broken in electrochemical cells and a large portion of the energy stored in ethanol is lost.” There are clues, however, about where to look in order to find a solution: for instance, it has been discovered that carbon bonds are easier to break in an alkaline solution than in an acidic solution. Furthermore, certain electrode structures, such as steps or surface alloys, are effective. “In this and related fields – for instance methanol fuel cells and new types of lithium batteries – there is a great need for research combining the areas of theory and experimentation. This is what we will be focusing on for the next few years”, Schmickler says.

Such fundamental problems cannot be solved single-handedly. That is why research associations like the Ulm GRF Electroanalysis Research Unit, the new Helmholtz Institute or the various other networks supported by the European Union are so important. Schmickler’s team has been participating in an intense exchange with Latin American countries for years as well, especially with Argentina and Brazil. Both of these countries have invested a substantial amount in education over the last few years, producing very well educated students – especially in electrochemistry. It is not just by chance that these countries show a big interest in electrochemistry. Brazil is one of the biggest producers of bio-ethanol, whereas in relatively low-populated Argentina, the constant winds of Patagonia are a potential reliable source of energy. Progress in fuel cell technology could make a substantial contribution to our future energy supply. “We have various exchange programmes, mostly with Argentina. So many staff members come from Latin America that Spanish has become the dominant language and we only switch to English or German when one of the few German PhD students enters the room who has not spent a few months in Buenos Aires, Córdoba or Santa Fe”, Schmickler says. “Good science flourishes best in an international atmosphere, in which different cultures, ideas and ways of thinking come together.”

“Our group mainly works in the field of theoretical electrochemistry. In the last few years, we have been concentrating on hydrogen reactions, which play an important role in fuel cells. The fact that this reaction only comprises two steps makes it a very attractive subject of research for new theories.”

Wolfgang Schmickler
“We do not have customers; we have young people who we deal with on a partner-like basis”, says Vice President of Studies and Teaching Ulrich Stadtmüller, explaining the University of Ulm’s self-image. “Customers get served. What we want is cooperation.”

Stadtmüller, who is a professor of mathematics, is proud of his university: “Here we seldom have mass lectures. Teaching takes place in small groups, in seminars and tutorials. We do a lot to help students because we do not want to lose anyone. We want young people to be successful in their studies, according to their abilities and needs.”

At small universities, distances are short and conversation flows easily. This is an advantage in the interdisciplinary study programmes, where representatives from different fields must come together. Ulm has created two such study programmes with an international focus and a third one is in planning. The University has thereby secured itself a leading position in the field of energy sciences. “Energy Science and Technology” and “Advanced Materials” are two international study programmes that integrate several disciplines. Requirements from the business world have even been incorporated into the curricula. Energy Science and Technology combines the subjects of chemistry, materials science and electrical engineering. Our graduates work in research or in industry, addressing questions of energy conversion and storage. The Advanced Materials Programme combines biology, chemistry, engineering, medicine and physics. Advanced Materials concerns developing new materials, such as those used in the field of energy engineering. All of the lectures are held in English and the majority of the students are from abroad. A further bachelor's degree programme – a mixture of chemistry and engineering – is in planning and there are bachelor's and master's degree programmes in the chemistry and physics departments that provide a good basis for studying problems related to energy.

Video lectures on the subject of electrochemistry are receiving a positive response too – they are organised in cooperation with the TU Darmstadt and the Karlsruhe Institute of Technology (KIT). These digitally recorded lessons are part of a teaching project involving nine universities and research institutes that work together in the “Electrochemistry Competence Network South”. The network is funded by the Federal Ministry for Education and Research (BMBF) and organises research projects as well as lectures for multiple locations. Video lectures are generally well received by the students. “They like it”, Stadtmüller says. That is why the University of Ulm is planning to record more lectures in the future and make them available on the internet. Students can then load lectures onto their iPods and listen to them at home – a good way to complement textbook learning. “However, a video lecture cannot replace the live lecture, with an instructor who stands up front and is enthusiastic about his field”, Stadtmüller believes.

Ulm has been very successful in the BMBF “Teaching Quality Pact” competition. Over the next six years, the University will be receiving more than six million euros to be used for improving studying conditions. The focus of the local concept is on transitional phases: the transition to university and the transition to the workforce. In the subjects of mathematics, computer science, natural sciences, engineering and medicine, incoming students can participate in a preparatory study programme and will even be able to conduct their own short research projects in the future. For graduates, the University plans to organise programmes in continuing education that can be taken parallel to working. “We are working on expanding training options for working professionals”, Stadtmüller says.

“The live lecture, with an instructor who stands up front and is enthusiastic about his field, cannot be replaced by an electronic tool.”

Ulrich Stadtmüller

“Someone who completes his bachelor's degree at our university and then pursues his profession for a few years can return for his master's degree without having to interrupt his career.”
Junior Researchers in Ulm Display Great Motivation

Research connects nationalities

I have studied in many countries. I did my bachelor’s degree in the Philippines, but a year of that I spent in Singapore. Then I went to Japan to pursue my master’s degree and my PhD. At a conference in Japan, I met Axel Groß, who is a professor here in Ulm in the field of theoretical chemistry (see page 14). We had a lot to talk about because he performs research in the field that I find the most interesting: theoretical modelling of electrochemical processes. He told me about the work being done at his institute and invited me to come to Ulm as a postdoc. At the time, I had a second offer from Vancouver, Canada, so I had to think about it first. What made Ulm appealing was its excellent reputation in the field of theoretical chemistry, but the language was a drawback. I didn’t know any German. But ultimately I threw all caution to the wind and decided on Germany. I have been here for a year now and I really like it. There are six different nationalities in my research group and we discuss in English while I am learning German through language courses. After my postdoc, I will definitely stay in research. I intend to set up my own research group at home, at a university in the Philippines.

Dr Tanglaw Roman, postdoc at the Institute of Theoretical Chemistry at the University of Ulm

Combination of experiment and theory

I have been working on my PhD for three and a half years. My topic is electrocatalysis on bimetallic electrodes. Bimetallic alloys often show higher catalytic activities than the corresponding pure metals. This can be ascribed to the ideal atomic arrangements or electronic surface structures for a certain reaction. I am studying the impact of certain electrode surface structures on the catalytic activity for an electrochemical reaction. Thus, structure-activity relations can be revealed that can contribute to the development of new and improved catalysts. The best aspect of my work is the variety: experiments in the lab and analysis and literature research on the computer. I particularly appreciate the mixture of experiment and theory at the Institute of Electrochemistry. It is pleasant studying at the University of Ulm because it is relatively small. The other students and professors are very approachable. Work-study jobs are easy to find at the University as well. I personally have a part-time position at the Institute, supervise lab courses and give seminars. I spend the other half of my time on my research. After I have completed my PhD, I could imagine either doing a postdoc at a university abroad or going directly into the industry.

Yvonne Pluntke, PhD student at the Institute of Electrochemistry at the University of Ulm

Interconnected thinking

I have never required much time to make decisions concerning my future. I wanted to study chemistry because I knew that that would enable me to contribute to the field of energy research and that this, in turn, would mean progress for the human race. Many people warned me that it would be difficult, but I found the challenges to be attractive rather than deterrent.

As a chemist, your thoughts have to essentially be interconnected: you acquire specialised knowledge and learn to think logically, because subjects like mathematics or physical chemistry are also part of your courses. The variety of subjects is so great that there is something for everyone. For anyone interested in battery development or the transition to renewable energies, I can wholeheartedly recommend studying in Ulm.

As it is a small university, the professors are very approachable – it is nearly always possible to have a chat with them. I enjoy research; however, if interesting industrial opportunities arise, I would not be opposed. There are not that many job opportunities for theoretical chemists as of yet. Especially in the business world, everything is experimental at the moment. That will change, however. In the future, when theories and technologies are more mature, it will become more common to postpone experimenting until it is known that something will work in theory – for purely economical reasons. Then theoretical chemists will be in demand in the business world as well.

Markus Jäckle is in the Chemistry master’s degree programme at the University of Ulm
Communication with Our Students Is the Foundation – Excellence in Research the Result

Interview with Dieter Kaufmann, chancellor of the University of Ulm, on securing a position for the University as a research university

What role does electrochemistry play in the University of Ulm's strategic planning?

Dieter Kaufmann: We are not a traditional comprehensive university; rather, we aim to specialise in specific areas, even within the fields of natural sciences and engineering. In expanding our Electrochemistry Department, we are focusing on an area that will become very significant over the next few years for society as a whole. This subject is already in high demand and we believe that students will become even more interested in electrochemical research and basic study programmes in the future. Excellent graduates are sought after in industry. We also need to offer opportunities for continuing education and life-long learning – i.e. working professionals, who have been in the work force for years, need to be given the opportunity to return to the University and learn about the newest procedures and research results.

Will you be allocating more funding for electrochemical science?

Kaufmann: Strategically important subjects have to be supported in terms of budgeting as well. We will be expanding these areas in close consultation with the faculties, as well as becoming innovative with our financing. An example of this would be early succession: if a professor will be retiring in three to five years, we can already appoint a successor now.

The Excellence Initiative is in the process of changing the university landscape in Germany; what is the University of Ulm’s position in this situation?

Kaufmann: The Excellence Initiative will result in a reorganisation of the university system; there will probably be some federal universities, research universities and teaching universities. The federal universities will require funding, which could mean that other universities will have less access to funds. We want to remain a research university and are therefore taking action to position ourselves in this field early on, for instance by covering specific topics.

In order to strengthen your own position, it is important to have a sufficient number of students. What is the current situation in Ulm in this regard?

Kaufmann: We do see a risk that many good students may transfer to an “Excellence University” in the future after completing their bachelor’s degrees. However, as universities, we depend on attracting good master’s degree students to secure sufficient junior researchers for the next generation.

What makes the University of Ulm attractive to students?

Kaufmann: We believe that our outstanding research, for example in electrochemistry, must already in itself be interesting for master’s degree students and PhD students. We can also offer advantages in comparison to the large universities: every professor knows his students personally and is approachable. In general, we try to stay in close contact with the students – even at the university management level – in order to best meet their needs. Student representatives were involved in all the committees in which decisions were made on the appropriation of tuition fees, for instance. Students will continue to be an important group of decision-makers when the tuition fees cease to exist and decisions must be taken concerning the appropriation of state funds, which will most likely replace the discontinued tuition fees.

What have the tuition fees been used for?

Kaufmann: The money has gone toward improving the general teaching situation in many different areas; for instance, new workstations have been created in labs, more tutorials have been set up, printers have been purchased and a bus shuttle system has been arranged for our students. We negotiated with the public transport authorities that students can be allowed to use the busses driving through the University campus as shuttles to get from one end to the other. The library equipment has been updated and new studying areas have been installed – and that is just to name a few of the improvements made.
These dossiers offer additional insight into the strategic research focuses at the University of Ulm. The appropriate contact persons from the University give journalistic interviews. The researchers and members of university management do not write much of the text themselves, as the dossiers are not aimed at professional scientific associations; rather, the articles address the University’s reference groups – politicians, administrators, students, alumni and representatives from the areas of media and commerce as well as interested members of the public. The editor of the dossier writes the articles, as an intermediary between science and society. For the current publication, the editor is Kristin Mosch, scientific editor from Lemmens Medien. Editing, proofreading and project management Lemmens Medien GmbH, Bonn – Berlin

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