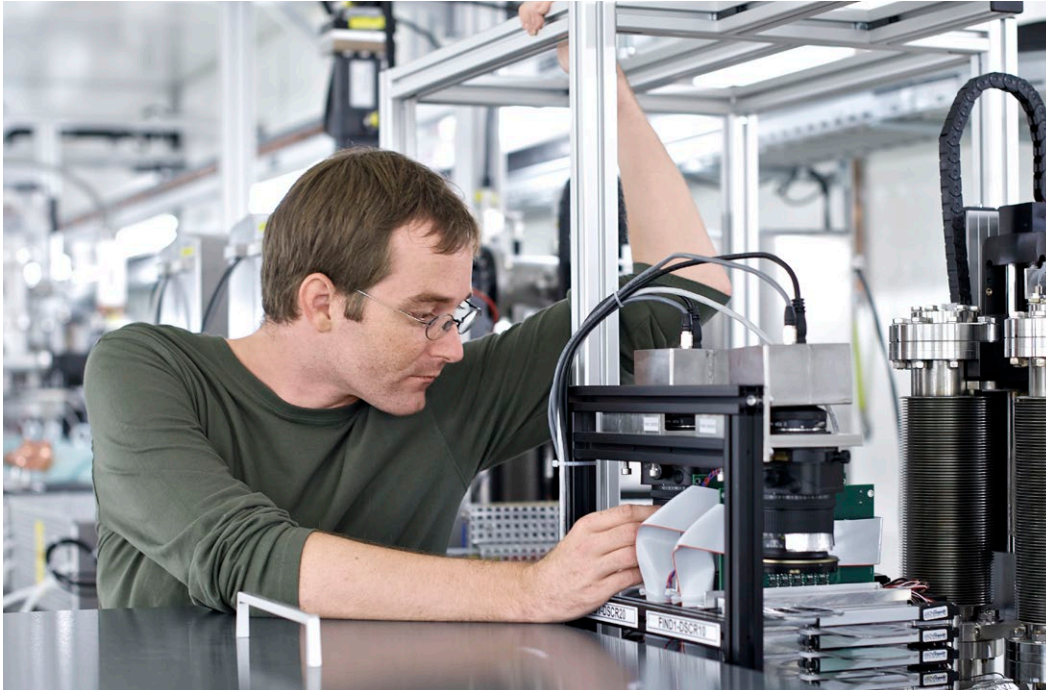


PAUL SCHERRER INSTITUT



# Materials for the Future

Research at the Paul Scherrer Institute



Materials are investigated at PSI using X-rays, for example, as shown here for the case of conducting polymers, which could be used in future transistors, solar cells or LED's.



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## Cover photo

At the new large research facility SwissFEL, PSI can pursue materials research with completely novel experiments.





How magnetic domains are ordered in a material plays an important role in magnetic data storage. At PSI, researchers use photo-emission electron microscopy to visualise domains – small regions in a material.

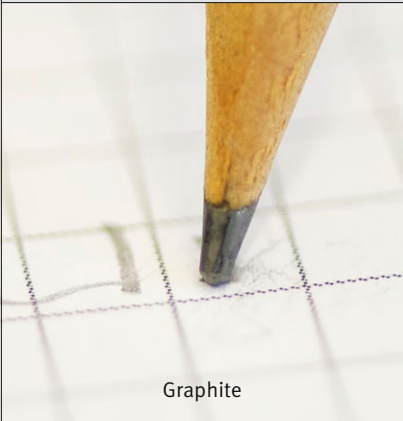
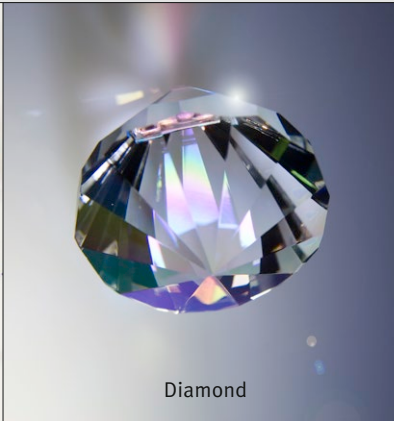
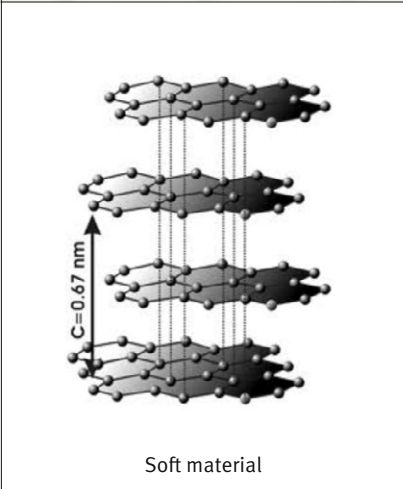
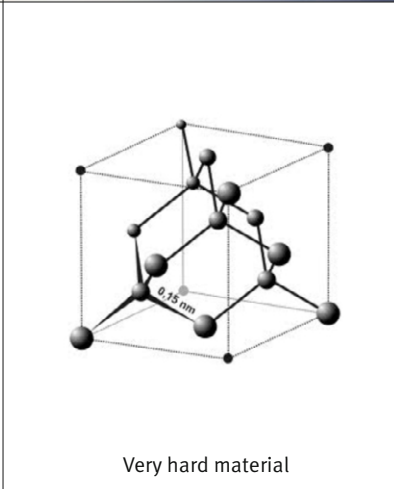
# Materials determine progress

Prehistory is divided into the Stone, Bronze and Iron Ages. With each new material, the human race took an important step forward in its development. In order to develop a computer chip or a battery for an electric car today, it is necessary to understand materials properly. Researchers at PSI are studying structures in the finest of detail, down to the scale of single atoms. In this way, the fundamental research of today will result in the technology of tomorrow.

Diamond is the hardest material that exists naturally on the earth. Graphite, on the other hand, is so soft that, when it is used as the lead in a pencil, it is rubbed off by the paper. The astonishing thing is that diamond and graphite are both made of carbon, i.e. from one and

the same substance. In the 18<sup>th</sup> century, no-one believed this until, in 1796, the English chemist Smithson Tennant burnt a diamond and thereby established that only carbon dioxide (CO<sub>2</sub>) was produced – the same gas that was also generated when graphite was burnt.

The difference in behaviour of the two materials depends on the interplay between the atoms in the material. Responsible for this interplay are the electrons, which therefore determine the properties of the material. And this is again reflected in the structure. In diamond, the carbon atoms bind together rigidly in all directions, whereas in graphite they are in loose layers, similar to slate rocks. These layers hardly stick together and it is consequently easy to rub graphite off. Tennant did not know this, however, as it is not possible to see the atoms using a normal light microscope. Only when the first X-rays were discovered did scientists begin to analyse materials in more detail. When X-rays strike a sample, they are scattered in well-defined directions, and the organisation of the atoms – the structure of the material – can be determined from the resulting pattern.

Pure carbon, C	
 <p>Graphite</p>	 <p>Diamond</p>
 <p>Soft material</p>	 <p>Very hard material</p>

In spite of their completely different properties, graphite and diamond both consist of carbon. The difference between them lies solely in the manner in which their atoms are joined together – that is, in the structures of the materials. 1nm (nanometre) is equal to one millionth of a millimetre.





PSI scientists at a facility where thin layers of different materials can be manufactured, using laser technology.

## X-rays as a microscope

Materials are still being examined at PSI by means of X-rays. The equipment is, however, larger than that used by a dentist. The X-ray facility at PSI – the storage ring of the Swiss Light Source SLS – has a circumference of close to 300 metres and is correspondingly powerful. X-ray radiation (or “light”) is not suitable, though, for all materials. For example, the structures of samples are studied in another large research facility by bombarding them with neutrons. While X-rays are strongly attenuated by metals, certain metals are almost transparent to neutrons. Water, on the other hand, slows neutrons down. The most exotic particle used by PSI scientists for materials research is the muon, which is used to study mag-

netic materials. PSI is one of only two research institutes in the world where all three of these methods can be used – X-rays, neutrons and muons.

Scientists come from all over the world to study materials in Switzerland at PSI. Of particular current interest are research projects in the field of energy; for example, lithium ion batteries must be improved for application in electric cars of the future. The materials for new batteries are being tested and analysed at PSI, with the goal of increasing the range of electric cars and the lifetime of the batteries. This does not mean, however, that PSI will produce and sell marketable batteries. In the laboratory only the smallest of samples are studied and new materials are developed. It remains the province of industry to fabricate complete batteries.

## Catalysts accelerate

Another example from the automobile industry is the catalyser. The combustion process within an engine produces carbon monoxide, as well as nitrogen oxide and sulphur dioxide, with the latter leading to the creation of acid rain. The catalyser in an automobile converts these materials into non-toxic gases before they emerge into the environment through the exhaust pipe. Thanks to the catalyser, and to catalytic pre-treatment of the fuel, there is no longer acid rain in Switzerland and in most parts of Europe. In spite of this, the catalyser is still being optimised at PSI, because precious metals, such as platinum, or rare earths are contained within it. The fewer of these are used, the cheaper will be the product.

At best, a new material for catalysers might even be found.

However, catalysts are not only found in cars. These are basically materials which accelerate a chemical process but which are not themselves consumed by it. They are used in many chemical processes, even in a widespread manufacturing process for producing diamonds (!), as there is a high demand by industry for diamonds, for cutting, drilling and polishing. Graphite changes into synthetic diamond at high pressure and temperature. However, if a catalyst is used, both the pressure and the temperature can be reduced. Thus the production process will use less energy and be more cost-effective.

### Long time-scale

The examples mentioned above from materials research serve to improve an existing product or manufacturing process. These technologies are almost at the stage of being marketable products, even if it often takes several years before the customer benefits. In other research projects, scientists are not working directly on concrete products but have ideas about how a new material could one day be used. Here, the fundamentals are being researched. An example of this is graphene, which is composed of carbon, as are diamond and graphite, but has a different structure consisting of a single layer of carbon atoms. This layer is extremely tear-resistant – a hundred times tougher than steel– and the electrons move around so quickly that a computer with a graphene chip would be

ten to one hundred times faster than current processors.

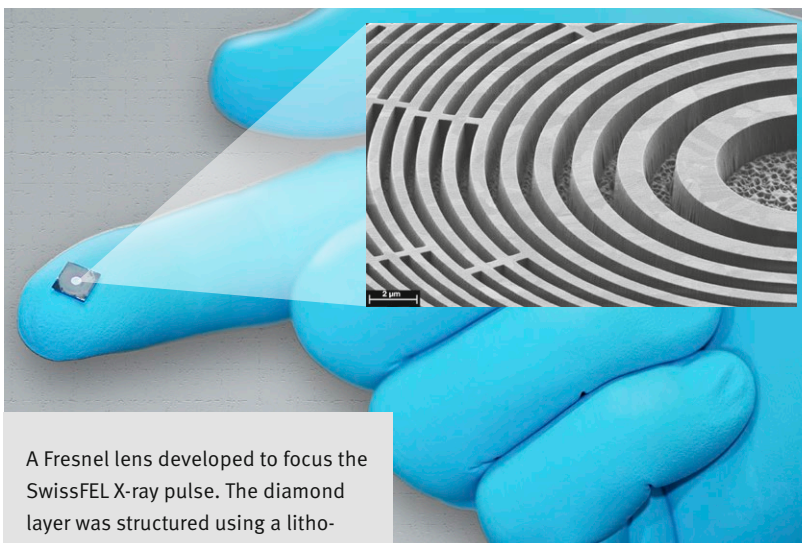
Whether a graphene computer will ever be produced, however, is unknown. At the moment, scientists are working on single transistors, but a computer chip consists of billions of them. Going from the first idea to a finished product often takes decades in materials research. For example, the transistors that are in today's computers were developed in the 1950's.

### Observing reactions

There is something, however, that PSI researchers can't do yet: They can't follow how the molecular structure or the positions of the atoms in a material move in real time. They are nevertheless dreaming about this as a way to follow artificial photosynthesis. Plants show us how it could be possible to use

energy from sunlight. The chemical reactions, however, occur too rapidly for them to be observed. Also, there are biological samples that are simply too small to be analysed in existing facilities. A new large research facility should solve both of these problems: the SwissFEL. This piece of equipment will function with short X-ray pulses that are focussed onto a point and will allow scientists to see how complex molecules in a human cell function. With this knowledge, doctors hope to be able to develop new pharmaceuticals.

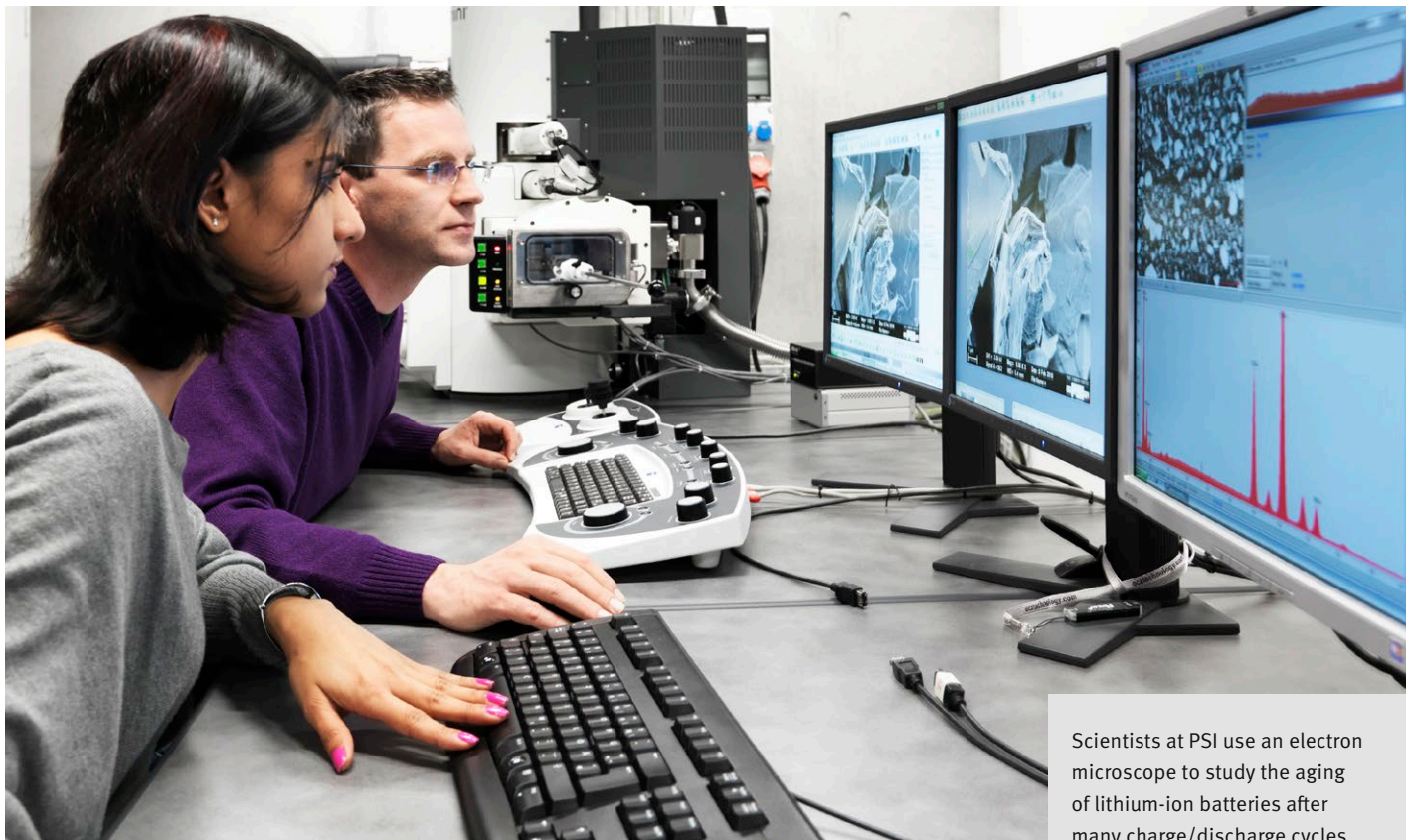
The circle of materials research will be closed with the construction of the SwissFEL, as the lenses that focus the X-rays must be extremely robust, and a good material for this is diamond.



A Fresnel lens developed to focus the SwissFEL X-ray pulse. The diamond layer was structured using a lithographic process in order to make the focussing possible. 1  $\mu\text{m}$  (micrometre) is equal to one thousandth of a millimetre.



# Lithium ion batteries



Scientists at PSI use an electron microscope to study the aging of lithium-ion batteries after many charge/discharge cycles.

**The electric cars of the future will be powered by lithium ion batteries. Researchers at PSI are improving the materials for these and are helping companies from the automobile industry to analyse and test prototype batteries.**

Around 1900, twice as many cars in New York ran on electricity than on petrol. The lead batteries for electric powered cars were heavy, however, and only gave a range of 50 km a day. At that time this was sufficient, as the roads outside cities were bad. Only as the suburbs became better linked and the petrol

engine was mass produced did the petrol engine gain the upper hand. Due to climate warming and the limited reserves of petroleum oil, the electric car has once again become an important topic of conversation. But not using lead batteries, as in the old days, since they would be too heavy to achieve the desired driving distances. Lithium ion batteries have established themselves in mobile phones and laptops. Lithium is a light metal that, chemically, has the greatest potential for storing electrical energy. In its pure form, however, it reacts vigorously with water and must not be allowed to come

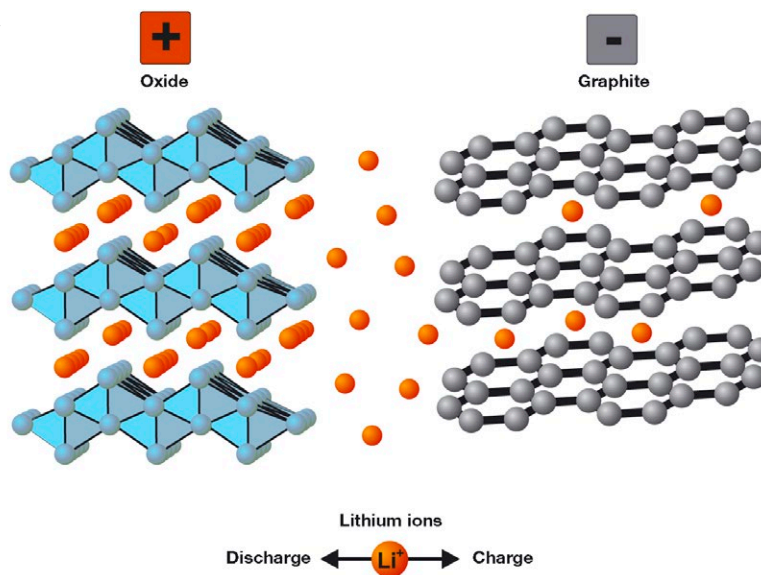
into contact with oxygen. In laptop batteries, it is therefore found in the form of lithium metallic oxide in one of the two electrodes. The other electrode consists of graphite. When the battery is charged, lithium ions migrate through a salt solution to the graphite electrode, where they collect. When the battery discharges, the ions migrate in the reverse direction.

## Limited lifetime

During the charging process, the graphite electrode expands by about 10%.



When a battery is being charged, lithium ions migrate from the positive electrode to the negative, graphite electrode. The reverse process takes place when the battery discharges.



Until a few years ago, this continual expansion and contraction limited the lifetime of lithium ion batteries to a few hundred charge/discharge cycles. Only as scientists became aware of this behaviour and stabilised the graphite electrode was a sufficient lifetime, as required for electric cars, possible.

Scientists at PSI are still working on new materials for lithium ion batteries. The aging of the materials used for the electrodes is being studied with the aid of scanning electron microscopy. A fine beam of electrons probes the electrode surface and the monitor shows where and how many electrons are ejected from the surface. A conventional microscope could not be used because the wavelength of normal light is far too long to be able to see the fine structure in the material. It would be like using a large spray can to write a postcard—the stream of paint would be simply too

wide. The electrons that are “shot” onto the battery samples are much smaller than the wavelength of visible light.

### Unique combination

PSI is one of very few laboratories in the world that can X-ray lithium ion batteries during the charging and discharging processes. Researchers there-

fore come from all over the world to PSI to study how the lithium ions migrate in the layers and are stored there. This is done, on the one hand, with X-ray beams at the Swiss Light Source SLS and, on the other hand, with neutrons at the Swiss Spallation Neutron Source SINQ. Lithium ions, in particular, are practically transparent to X-rays, whereas lithium is clearly visible to neutrons.

PSI is working on the improvement of battery concepts which are on the market today, and is also concerned with future technologies that could appear on the market in 10 or 20 years' time such as lithium-sulphur batteries, whose working principle can already be demonstrated in the laboratory. The technology with the greatest potential, however, is the lithium-air battery. Research has only just started, but storage capacities around a factor of 10 higher than those of the lithium ion batteries of today are theoretically possible. This would give an electric vehicle a driving distance of about 500 km.



A scientist manufactures a graphite electrode. The black graphite layer is applied in liquid form, spread over the surface and dried. During charging, this graphite electrode collects lithium ions, thereby storing energy.

# Fuel cells for cars

**Present-day electric cars can travel between 100 and 150 km on one battery charge. This driving distance can be increased by the use of fuel cells. Researchers at PSI are developing materials and concepts which are suitable for everyday use.**

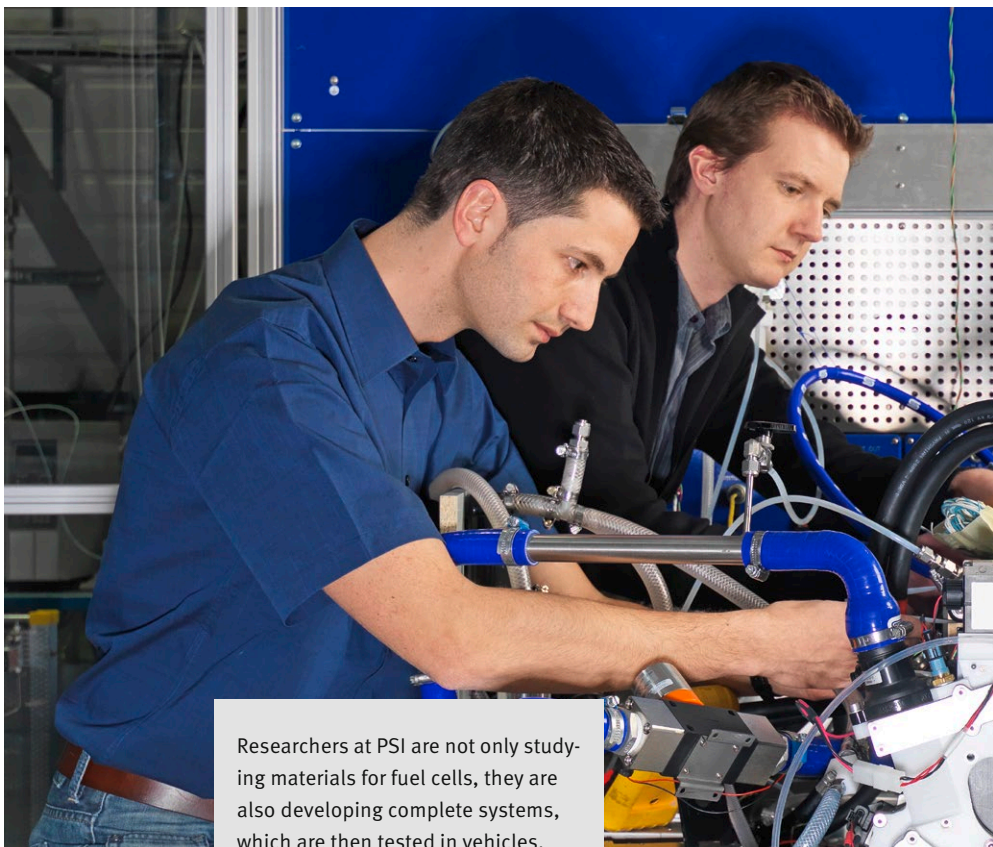
Around the year 2000, the fuel cell was heralded as the propulsion system of tomorrow for the automobile. Experts estimated that by 2005 the first fuel-cell powered cars would be available on the market. That has unfortunately not been the case. The system functioned reliably in the laboratory, but problems occurred under everyday conditions on the road. Repeated starting and stopping in city traffic taxed the system heavily. Instead of achieving a lifetime of at least 200,000 km, the fuel cell had to be exchanged prematurely. In addition, when the temperature dropped below freezing, the water that was produced as the end product froze. People who buy a car, however, also want to be able to drive it at  $-20^{\circ}\text{C}$  when going on their skiing holiday. Hydrogen is the fuel of the fuel cell. It is not burnt in the same way as in a conventional combustion engine, but reacts with oxygen in a controlled manner. Firstly, the hydrogen ( $\text{H}_2$ ) is separated into single atoms. In this process, each atom loses an electron. The naked nucleus of the hydrogen atom ( $\text{H}^+$ ), a so-called proton, then passes through a synthetic membrane. On the other side of the membrane, it comes into contact with oxygen ( $\text{O}_2$ ), producing water ( $\text{H}_2\text{O}$ ). The electrons cannot penetrate the insulating synthetic membrane and are carried away

through an electrode, flowing as an electric current to the other side. This current drives the motor of the car. The principle was first used technically in the 1960's, in space missions carried out by NASA.

## Synthetic membranes separate

The heart of the fuel cell is its synthetic membrane. Tiny channels within the membrane convey the protons, which are surrounded by water molecules.

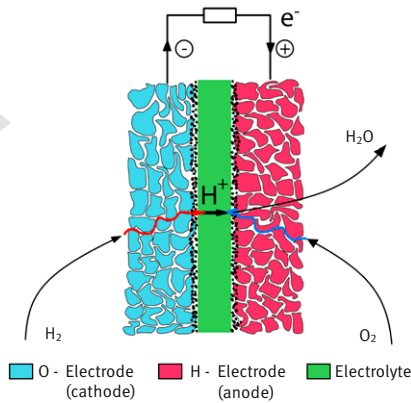
Thus the synthetic material acts as a sponge, but it only takes up the protons within their water mantle and lets them pass through when it is wet. A dry membrane cannot do this, which can be compared with trying to clean a dirty table with a dry cloth. The challenge is therefore to saturate the synthetic membrane in a fuel cell with 20% moisture, independent of whether the driver is travelling at full power or coasting. But a fuel cell consists of a stack of hundreds of membranes, and the saturation levels must be the same in each membrane.



Researchers at PSI are not only studying materials for fuel cells, they are also developing complete systems, which are then tested in vehicles.



Cross-section through a polymer electrolyte fuel cell: The hydrogen gas is used as fuel, and the moisture required to transport it through the membrane must be equally distributed throughout the fuel cell.



## Neutron imaging

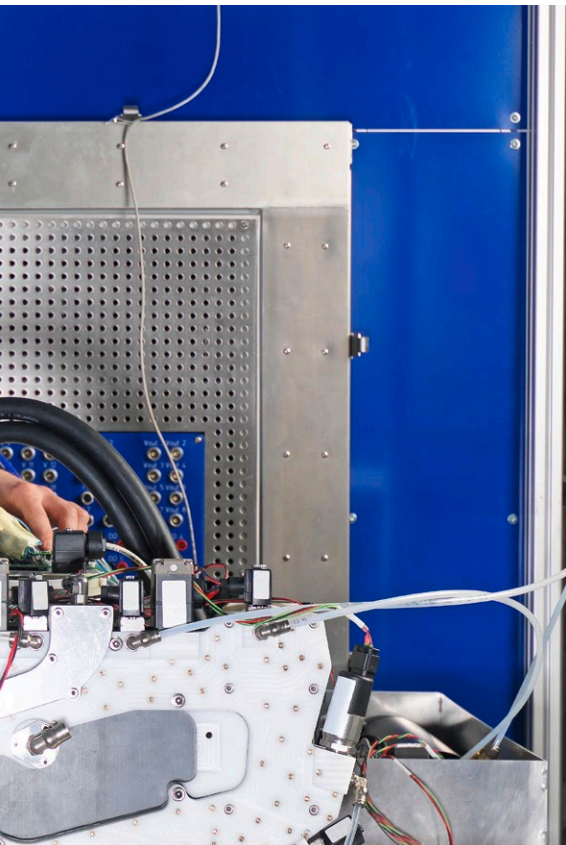
How can the humidity within a closed metallic container be seen? PSI has the right instrument for this. Scientists use “X-ray vision” to look through the complete fuel cell, but they do not use X-rays for this, they shine neutrons through the cell. If neutrons encounter water, they are slowed down and absorbed but, in contrast to X-rays, they have no difficulty passing through metals. From the resulting image, the development scientists can understand how the moisture is distributed within

the fuel cells. Therefore some of the world’s leading automobile concerns come to PSI to carry out this kind of research. Another question which is challenging scientists is the porosity of the fuel cell membrane. To find this out, they are analysing the atomic structure of membranes at the Swiss Light Source SLS.

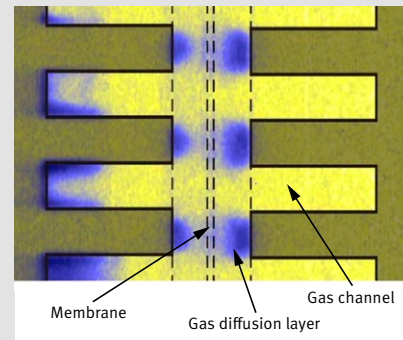
In order to optimise the fuel cell for practical applications, it is not only

energy from braking for a short time and use this energy to accelerate the vehicle afterwards. Researchers working on fuel cells at the Electrochemistry Laboratory at PSI are also developing technology and materials for super-condensers.

The reason that fuel-cell cars are not widely available on the market today is not primarily due to the technological challenges. It is rather due to the fact that the price is too high. Instead of producing the synthetic membrane using expensive, special processes, PSI is therefore working on a membrane of



The interior of a fuel cell: The picture shows the moisture distribution obtained using neutrons, which are strongly slowed down and absorbed by water (shown in blue).



necessary to improve the membrane. There is a problem with the water freezing, not that in the membrane but the water generated by the chemical process and given off as exhaust product. In order to solve this problem, the entire system must be considered. A further issue is the need for a rapid supply of energy in stop-start traffic, which is a problem for the fuel cell. This can be mitigated by using super-condensers. Like in batteries, these can store the

common plastic sheeting, as used in greenhouses. A few additional processing steps should make the foil appropriate for use as a fuel cell membrane. In the meantime, experts are agreed that affordable fuel-cell vehicles, suitable for everyday use, will be available within a few years.

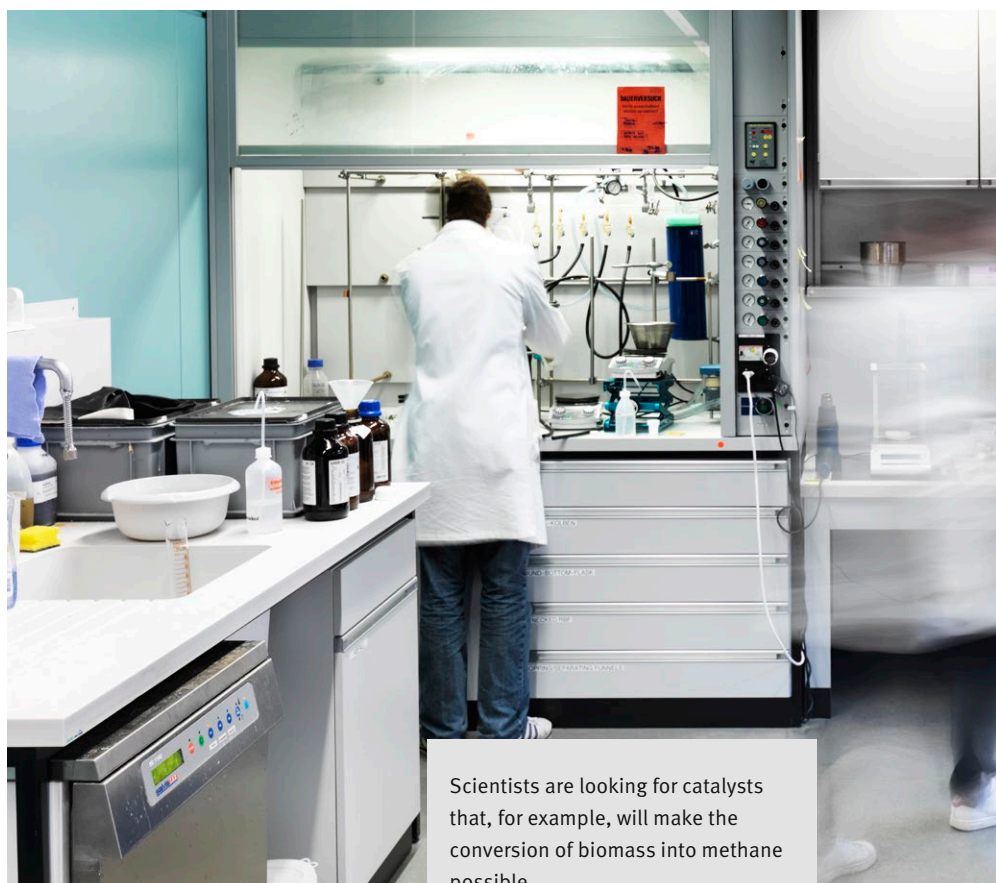
# Catalysts for energy and the environment

During recent years, strict emission level limits have resulted in the rapid development of exhaust gas catalysers. Indeed catalysers are not only responsible for cleaner air on our roads, but also improve many chemical processes.

Catalysts are known for their application in cars. Carbon monoxide and nitrogen oxide are produced during the combustion of petrol, diesel or other transport fuels and can be transformed by a catalyst into non-toxic substances. Less well-known is the fact that catalysts are also widely employed in the chemical industry. A catalyst is defined as a material which increases the rate of a chemical reaction without being consumed during it. It is estimated that a catalyst is used in the manufacture of more than 80% of all chemical products. For an ideal catalyst, the initial products should be completely converted into the end product with no undesirable by-products. In addition, as little energy as possible should be used. That would be the epitome of sustainable technology. Indeed some chemical processes are only technically possible with the use of catalysts.

## From power station to automobile

An active research field in the treatment of exhaust products is selective catalytic reduction – the so-called SCR Process – which is already applied in many commercial vehicles. In this process, ammonia is introduced into the hot exhaust gas, which reacts with the ni-



Scientists are looking for catalysts that, for example, will make the conversion of biomass into methane possible.

trogen oxide in the catalyser to become nitrogen. Initially, SRC catalysers were employed in power stations, whose exhaust gases had to be cleaned up. It was only at the end of the 1980's and the beginning of the 1990's that diesel vehicles became the focus of research. Today, this is the focal point of research, since the problem of nitrogen oxide is most acute and the requirements most severe. In vehicles, the ammonia is not introduced directly but is obtained from

urea, known by the name "AdBlue", which is put into the fuel tank in the form of a liquid solution. This process has been adopted for commercial vehicles since 2005. Scientists at PSI are conducting experiments on new catalyst materials and substances other than ammonia. The reason for this intensive research activity is the ever-stricter legal exhaust gas emission limits, which can only be met with larger diesel vehicles by using the SRC Process.





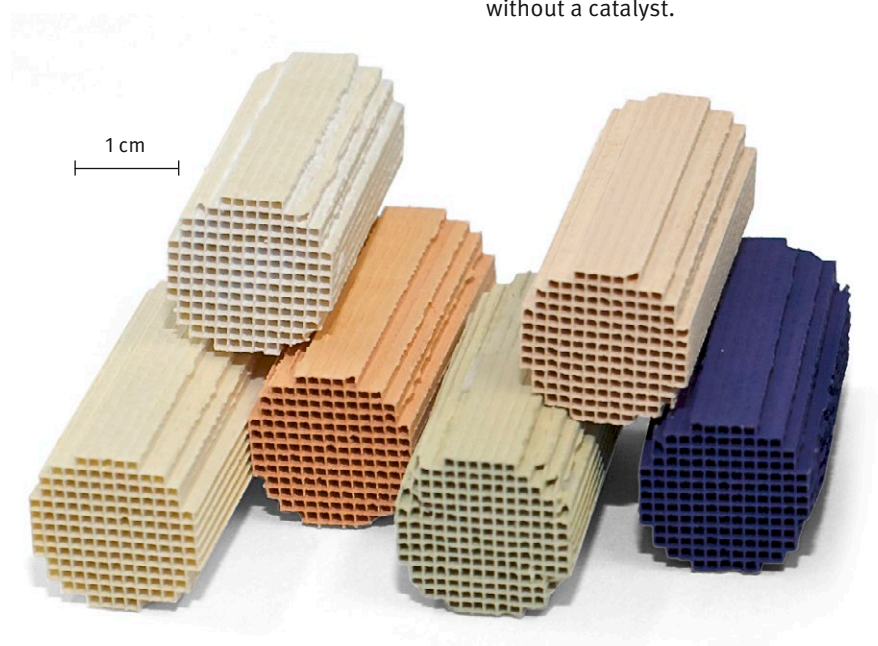
## The future belongs to bio-energy

Catalyst scientists at PSI are not only concerned about the post-treatment of exhaust emissions. Another of their goals is to obtain energy from biomass, i.e. continually growing raw material, but to avoid competing with the production of foodstuffs. For this, they are looking for catalysts that, for example, enable the efficient conversion of biomass into methane. No by-products should be produced and the reaction should take place at as low a temperature as possible, so that energy requirements are kept low.

At PSI the biomass is converted into methane by heating it up to 380 °C under high pressure and then passing it over a catalyst of ruthenium. Under these conditions, about 45% of it can be converted into methane. The remainder is turned into the by-products carbon dioxide, hydrogen and water. This conversion would not be possible without a catalyst.

Another way of producing energy is through photosynthesis. For this plants need water, carbon dioxide (CO<sub>2</sub>) and sunlight, and they produce carbohydrates, which act as energy carrier, and oxygen. Researchers are working throughout the world on how to reproduce photosynthesis artificially. For this, they are using nickel and cobalt that, with the help of sunlight, will enable water to be split into oxygen and hydrogen, which can then be converted in a fuel cell into electrical energy.

Nature is still a long way ahead of us and the efficiency of artificial photosynthesis is so far very modest. Nevertheless, bio-energy and artificial photosynthesis will without question become important topics once oil reserves begin to decrease. In the long term, biomass will become an important carbon source for producing chemical products and fuels. Intensive research has only been carried out in this field for the last 10 to 20 years, and as far as the potential of the method is concerned, scientists expect a number of surprises to emerge.



Different catalysts coated onto ceramic honeycomb bodies (far left: uncoated). The colour varies according to the chemical composition of the catalysts.

# Aging of steel

Steel holds bridges and buildings together and is widely employed from vehicle chassis to the pressure vessels of nuclear reactors. However, in order to guarantee their safety, steel constructions must be regularly tested, since steel also ages.

On 9 May 1985, the roof of the indoor swimming pool at Uster (ZH) collapsed, burying swimmers who were still in the water in the late evening. It turned out that a large proportion of the 207 steel shackles which held the concrete roof

had broken. Contrary to initial assumptions, it was not incompetent construction or poor maintenance that caused the collapse. The architect deliberately used non-rusting stainless steel, because it would be exposed to a humid atmosphere in the indoor swimming pool building. However, the chlorine in the air led to hairline cracks occurring

in the steel. Over the years, these cracks grew until about a quarter of the shackles were completely rusted through, without this being visible at the surface.

Hair-line cracks cannot be compared with the rust that is found in cars, for example. When normal steel rusts, its surface turns red and begins to flake off. In Uster, stress-crack corrosion led to collapse: very small cracks, which can only be seen under a microscope, grow when stainless steel is put under tension and chlorine attacks it.

Researchers at PSI examine the behaviour of steel under different ambient conditions.





Steel is tested in this facility under conditions which occur in nuclear power stations. The results are incorporated in mathematical models with which the safety, and therefore the lifetime, of a nuclear power plant can be estimated.



## Steel in nuclear power stations

Such invisible cracks are also of interest to scientists at PSI who are concerned with the safety of nuclear power stations. The steel used in a nuclear power station is exposed to hot cooling water and radioactive radiation, which can also lead to stress-crack corrosion as well as to stress-crack embrittlement of the steel. As at the indoor swimming pool at Uster, the condition of a reactor vessel cannot be assessed from its exterior. Hair-line cracks can often only be seen under the microscope in the laboratory after a steel sample has been taken from the vessel. Ultrasonic and eddy-current testing is therefore carried out regularly in a plant, in order to detect possible hair-line cracking before it reaches a critical extent beyond the safety limits.

PSI experts can judge the condition of the steels in the Swiss nuclear power stations very accurately. During construction, steel samples are placed inside the reactor, for example in the vicinity of the core. One after the other, these samples are extracted and tested on the Hot Lab at PSI. During this testing, notched metal specimens are bro-

ken with a hammer. These tests provide evidence of radiation damage in advance and the prospective degree of embrittlement of the pressure vessel. This basically simple test is, however, complicated by the radioactivity of the sample. To get around this, thick walls of concrete and windows made of leaded glass protect scientists from the radiation, and the samples are manipulated using a robotic arm.

### Cooling water must be clean

Corrosion occurs much more often in the welded seams of the cooling circuit than in the reactor vessel. One reason for this is that every weld leads to mechanical stress, because the metal melts during welding and contracts as it cools down. This tensile stress remains within the metal and, over the years, can lead to stress-crack corrosion. Just like what happened at the Uster swimming pool, chlorine atoms, amongst others, accelerate the pro-

cess. The chlorine comes from the salt which is present in very small quantities in the cooling water.

In the 1980's, scientists determined the link between stress-crack corrosion in nuclear power stations and the water. Since this time, the cooling water for nuclear power stations has been even more strictly purified and contains at least 1000 times fewer chlorine atoms than drinking water. Simultaneously, a new welding procedure has been adopted which results in compressive rather than tensile stress in the metal surface, so preventing subsequent stress-crack corrosion.

In order to avoid corrosion, the materials used today are not necessarily new. Careful operation, like taking care of the cooling water and temperature peaks in nuclear plants, and the appropriate and controlled preparation of the steel are crucial. Thus welding seams, for example, must be carefully ground and polished, as treatment has a decisive influence on whether cracks will appear after 30 years.

# Storing information



The finest of magnetic structures are investigated using X-ray beams from the Swiss Light Source, SLS.

**Computers, digital cameras, MP3 players and smartphones all belong to everyday life. They create vast quantities of data which must be stored – whether in a computer centre or at home on a hard disk.**

A computer stores information on a hard disk, which in principle functions in the same way as a tape cassette. A moving magnetic tape is read by a fixed audio head, while the magnetic material on a hard disk is on a spinning disk and the read head can be moved to the

desired position, without having to wind the tape forwards or backwards. The first commercially available hard disk from IBM in 1956 was as large as a cupboard and weighed half a ton. As the personal computer became more widely distributed in the 1980's, 15cm disks were already being built into PCs. These stored 10 megabytes of data, which is equivalent to one to three digital pictures taken by today's cameras. A modern hard disk is only half the diameter and can store more than one terabyte – i.e. 100,000 pictures.

With so much information being stored in such a small area, the amount of space in which a bit – that is, one single piece of information – can be stored must become ever smaller. The smaller this storage bit, however, the greater the danger that the magnetism can be spontaneously altered, such as by a magnetic field or even by the heat of the hard disk, since heat at the atomic level means nothing more than movement.



## Magnetic materials

Research centres, including PSI, are therefore working on new magnetic materials for hard disks. These should be produced in such a form that the highest possible magnetic field is needed to alter the magnetic structure on the hard disk – where the stored information is ultimately saved. Typically, this concerns materials composed of combinations of iron, cobalt and nickel, to which additional substances are added. Several layers in the form of thin films are stacked together in order to influence their magnetic properties in a targeted way. In this way, the single layers can behave completely differently to the stacked system as a whole. Thus the contribution of the different atoms also varies, depending on whether they are iron, cobalt or nickel. The speciality of

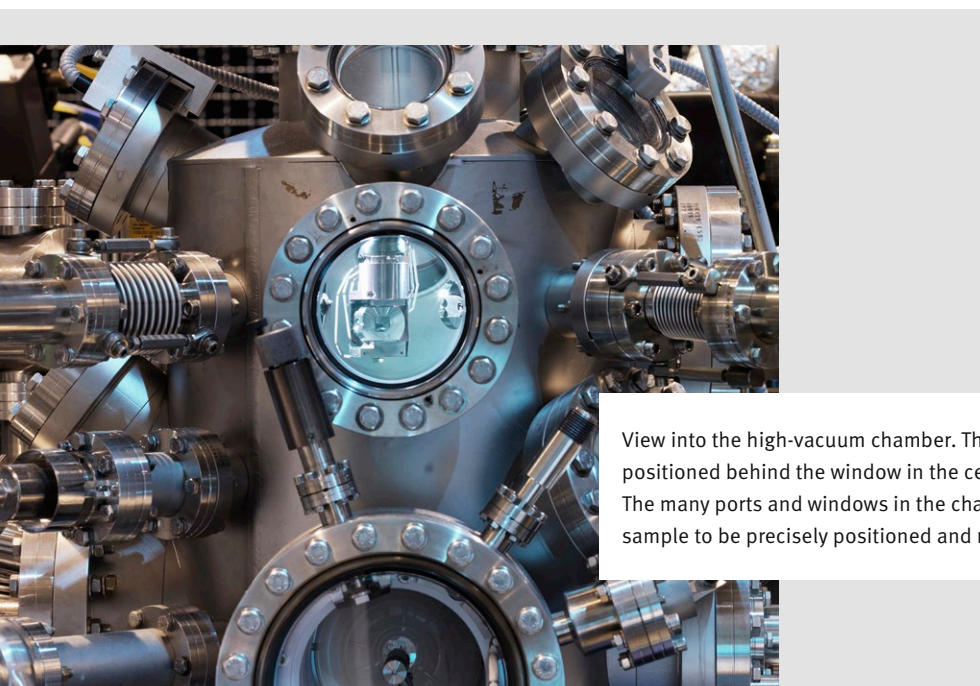
PSI researchers is to be able to measure the influence of individual metals in the various layers. In addition, they can create an image on a TV monitor of the detailed structures and their magnetic orientation.

For this, they use the X-ray beams from the Swiss Light Source, SLS. In order to be able to measure the thin layers, weak X-rays are used – so weak that they would be absorbed by only a few millimetres of air in the atmosphere. Experiments are therefore carried out in the absence of air, i.e. in a vacuum. The X-rays strike the material and release individual electrons from their atoms. These electrons are measured by a detector and evaluated with software, which produces an image of the magnetic regions.

## The finest of structures

X-rays interact with the atoms of different materials according to their wavelength. In this way, researchers can examine the magnetisation of either iron, cobalt or nickel by changing the wavelength. One of the difficulties in doing this is the fact that the structures are often only a few nanometres in size, and their shape influences the magnetic behaviour. For comparison: On average, our hair grows a few nanometres per second. In order to study these tiny structures, scientists at PSI have combined different microscopic methods and are using the most modern nano-lithographic processes.

The scientists are working not only to reduce the dimensions of the magnetic regions representing a single bit, but are also looking for ways to make the information faster to read or to store. The most up-to-date results show that a laser can change the magnetic orientation of a single magnetic region. These new developments offer unexpected possibilities, and the computers of the next generation will hardly remind us of the “good old PCs”.



View into the high-vacuum chamber. The sample is positioned behind the window in the centre. The many ports and windows in the chamber enable the sample to be precisely positioned and manipulated.

# Spintronics for fast computers

In the 1920's, physicists discovered the electron spin. Today, about 90 years later, this effect is now being used in hard disks. Scientists are toying with the idea of building complete computers using this effect, as spintronics is fast and uses very little energy.

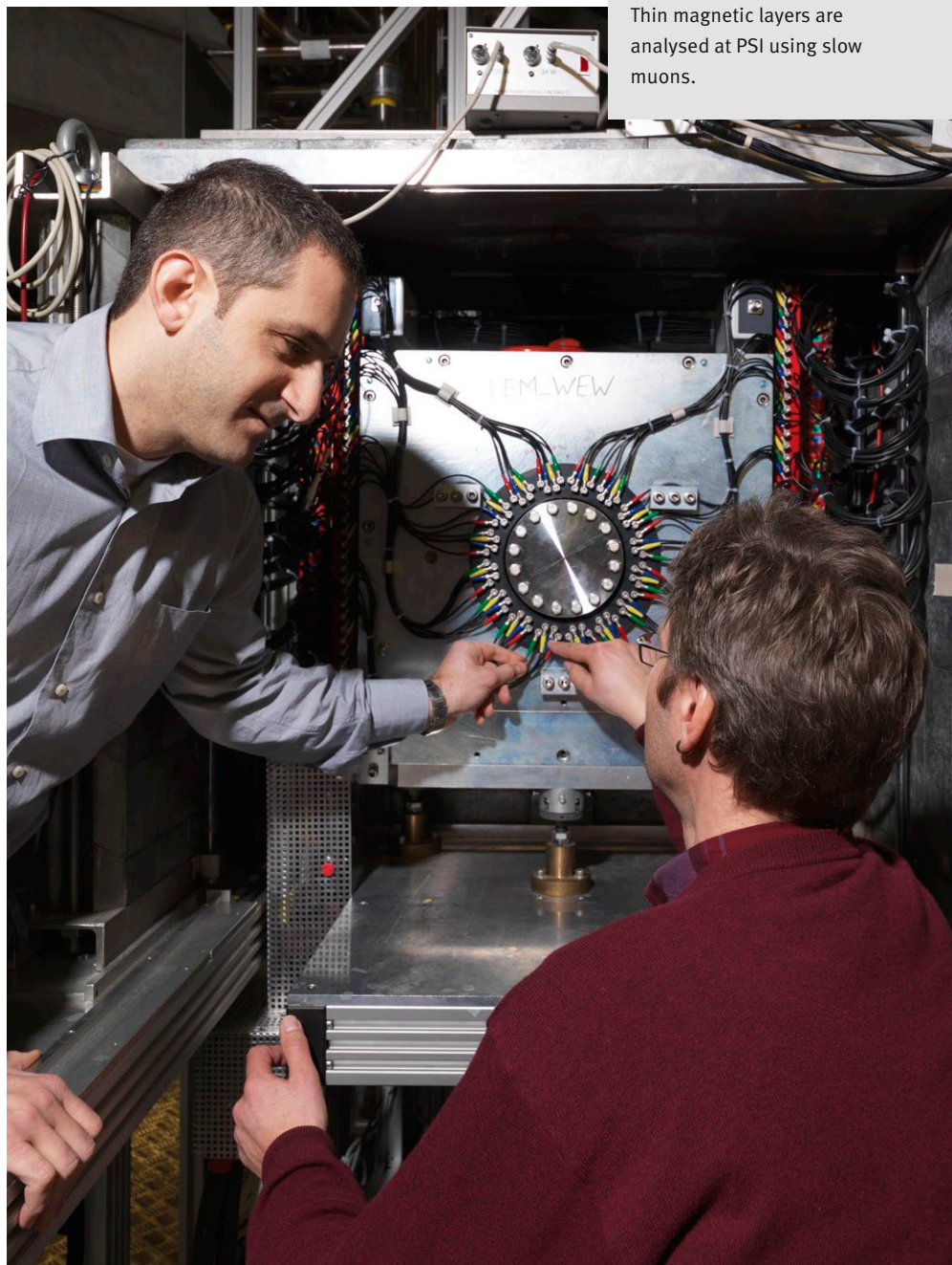
Information scientists sometimes talk of a pizza oven when they mean the 19-inch cabinet in which computers are conventionally stacked in a computer room. This is not only because the computers in it have the form of pizza boxes, but also because it is as hot inside as a pizza oven. A modern computer chip develops as much heat as the equivalent area on the hotplate in a kitchen.

Tomorrow's electronics should therefore not only be smaller and faster, but they should primarily use less energy. This cannot happen, however, without altering the fundamental principle of the computer, with the most important elements being transistors that switch currents. It is exactly these transistors that produce the heat. In order to interrupt a current, a transistor pushes aside the moving electrons into part of the conductor on the computer chip and current can then no longer flow. If the transistor behaves passively, the moving electrons reverse direction and the current flows again. Due to this continual coming and going of electrons, current losses occur, which are converted into heat and the chip becomes hot.

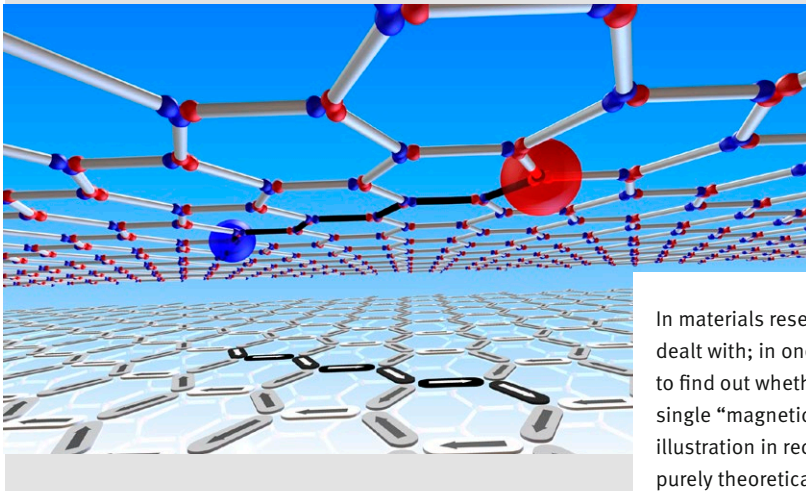
## Spin carries information

Instead of moving electrons around, in the computers of tomorrow scientists want to take advantage of a property of the electrons that has so far not been

Thin magnetic layers are analysed at PSI using slow muons.







In materials research, very basic questions are also being dealt with; in one international collaboration, for example, to find out whether magnetic monopoles exist and if these single “magnetic charges” can move freely (shown in the illustration in red and blue). These results are currently of purely theoretical interest, but could be the foundation for the development of future spintronics-based electronic equipment.



used: their spin. This can be visualised by thinking of the electron rotating about its own axis, either clockwise or anticlockwise. These two conditions are known as Spin-Up and Spin-Down. The decisive point is not only that the spin can be changed quickly but that the process uses much less energy than that needed to move the electron itself. Scientists call this “spintronics”.

The first components utilizing spintronics can already be found in every modern computer – in the read head of the hard disk. A small coil was originally used to read out the information from the magnetic domains. However, the smaller these domains became, the smaller were the voltages in the coils that had to be detected. Soon, measurements could no longer be made. Today, the electron spin is used instead of magnetic induction. The spin orients itself in line with the magnetic field of the material through which the electron passes. The electrons are initially aligned in the read head by a permanently magnetised layer. They then move through a layer which takes on the magnetic orientation of the magnetic region representing a single-bit. If the alignment in this layer is the same as the electrons, they can pass without significant resistance. On the other hand, if the alignment in the layer is in the opposite direction, the electrons are slightly impeded and must alter

their spin. In this way, the read head detects the magnetic alignment of the hard disk. This effect – called “giant magnetoresistance” – was discovered in 1988 by researchers in Germany and France, and in 2007 the Nobel Prize for Physics was awarded for the discovery.

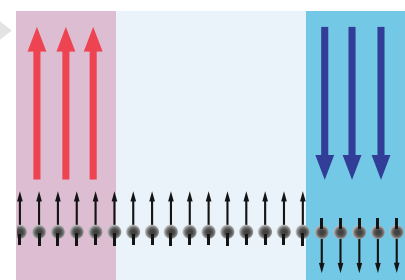
### Only slow enough at PSI

Scientists in the whole world are working on improving films for read heads and on transistor-like elements, which are important components needed to manufacture the computer of the future. One difficulty in this research is the analysis of the magnetisation orientation in such complex layered systems. PSI specializes in this, and researchers measure the magnetisation at a specific depths using slow muons. Muons are elementary particles which are created artificially. They decay after

a few microseconds, and it is exactly this decay which is used by scientists: The muon remains stuck inside the material and its spin aligns itself with the local magnetic field. Then it decays and, in a direction parallel to its spin, it emits a particle which can be detected.

A number of research groups in the world are working with muons. The difficulty in studying magnetic layers lies in generating muons which are slow enough. Normal sources produce fast muons, which penetrate too deep within a material. In addition, the penetration depth varies greatly. Researchers at PSI are the only ones in the world who can generate muons which are slow enough to analyse the thin layers in spintronics components. Consequently, groups from all over the world frequently visit Switzerland to carry out their research at this facility.

The interior of a spintronics device. Both outer layers are magnetised and the electric current flows from left to right. If layers on the right and on the left are magnetised in opposite directions, the spin of the electrons (represented as small spheres) rotates along their path, which slows down the flowing current and appears as electrical resistance.



# The cables of the future

Superconductors have been known for 100 years. However, because this phenomenon originally only occurred at very low temperatures, its application was, for a long time, used only in research. With the discovery of high-temperature superconductivity in 1986, however, hopes rose again for new industrial applications. Yet the mechanism which leads to high-temperature superconductivity is still not fully understood. Consequently, the important basic knowledge is missing, with which new and better superconductors can be searched for in a systematic way.

Superconducting materials carry current without resistance. For this, they must be cooled below their so-called transition temperature. Depending on the material, this can be as low as  $-269^{\circ}\text{C}$ . Such low temperatures can only be reached by cooling with liquid helium, which is complicated and expensive.

The first high-temperature superconductor was discovered in 1986, at the research laboratories of IBM Switzerland, in Rüschiikon. A well-known representative of this class of superconductor is yttrium-barium-copper oxide, which has a transition temperature of  $-180^{\circ}\text{C}$ . The interesting thing about

this temperature is that it lies above the boiling point of nitrogen ( $-196^{\circ}\text{C}$ ) and, as liquid nitrogen is cheaper than liquid helium to produce and is easier to handle, this opens up a broad new field of applications.

## Superconductors in action

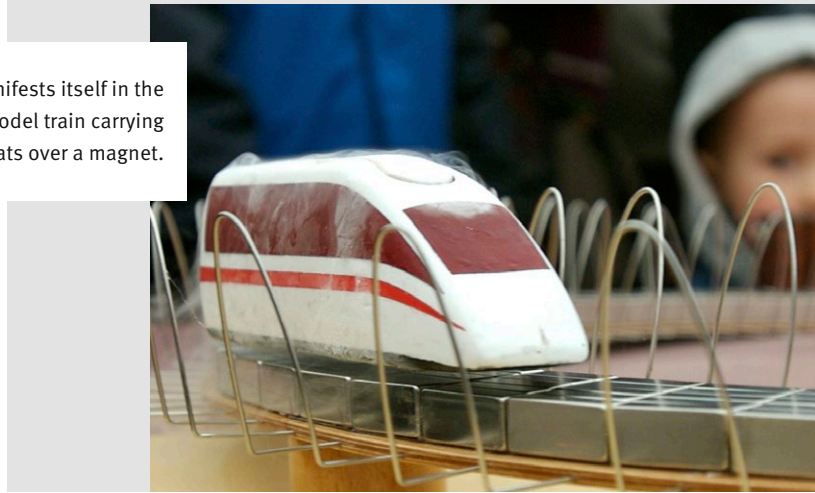
One important application area for superconductors is that of strong electromagnets, which are also used in a number of accelerator facilities at PSI, for example for the production of protons for the treatment of specific cancerous growths (proton therapy).

Researchers at PSI are trying to discover the secrets of high-temperature superconductors using neutrons.





Superconductivity also manifests itself in the Meissner Effect, through which a model train carrying a superconductor floats over a magnet.



The magnet coils used in these electromagnets are made of superconducting wires, which are kilometres long but only a few micrometres in diameter. High-temperature superconductors are, however, made of ceramic materials, which are brittle and difficult to process. For electromagnets, classical low-temperature superconductors are therefore used which are made of metallic alloys. The coils are closed on themselves and the current can indefinitely flow without loss. In order to charge the coils, a small segment is heated above its transition temperature and a current fed in through feeder cables. Once the desired current has been reached, the segment is cooled again and so the circuit is closed again. In order to maintain the magnetic field, liquid helium has to be regularly topped up. This is already the case in practice, for example, in facilities used for magnetic resonance tomography (MRI) in the medical field.

A further beneficial characteristic is the high current-density capacity of superconductors. In order to carry the same current as a copper wire, a superconductor with a much smaller cross-section can be used. Such cables made of high-temperature superconductors can be cooled by nitrogen. Taking into account both the cable insulation and the cooling, a superconducting cable can still carry five times as much current as a copper cable of the same diameter. Admittedly, however, they are between six and eight times more expensive. Since 2008, 660 metres of such cables form part of the electricity network in the USA – at Long Island, New York. In the inner-cities, there is often no room

available for additional copper cables. Here the implementation of superconducting cables can then make sense.

### Investigating the phenomenon

Although classical low-temperature superconductors are today well understood, the phenomenon of high-temperature superconductivity has not yet been conclusively explained. Researchers at PSI study superconductors in order to better understand what they consist of. To do this, they fire a beam of neutrons at a material sample to determine the positions of its atoms and the electronic properties of the superconductor. In normal conductors, electrical resistance occurs as the result of collisions of the electrons in the material. For this situation, a comparison can be drawn with what would happen on a main thoroughfare through Zurich with heavy traffic but without traffic signals. Again and again, the traffic lanes would have to be closed because of accidents and traffic jams would occur. This would look different if there were traffic signals, leading to “agreement”. Cars would all start off together and would be able to travel most efficiently as a group, profiting from the “green wave” at traffic lights. Similarly, in superconductors there is

a collective “agreement” between electrons, so that they can pass through the material without resistance. But in contrast to the case of low-temperature superconductors, it is still not clear how this group “agreement” is reached in high-temperature superconductors. Nevertheless researchers are almost certain that interaction between superconductivity and magnetism plays an important role here. In order to understand this better, researchers at PSI stack alternating layers of superconductors and magnets together. The properties of these samples are then examined using neutrons, muons or X-rays. With this new knowledge, scientists hope to find out how high-temperature superconductivity works and thereby establish the basis upon which the properties of such superconductors can be selectively improved. It is conceivable that materials exist with an even higher transition temperature, which can be more simply and cheaply cooled. As a distant vision the dream remains to be able to use superconductors everywhere to replace normal cables in use today where a great deal of energy is lost as heat. The current could then be transported without losses over great distances and simply stored, two aspects which constitute great challenges today in the application of renewable energy.

# Magnets under stress

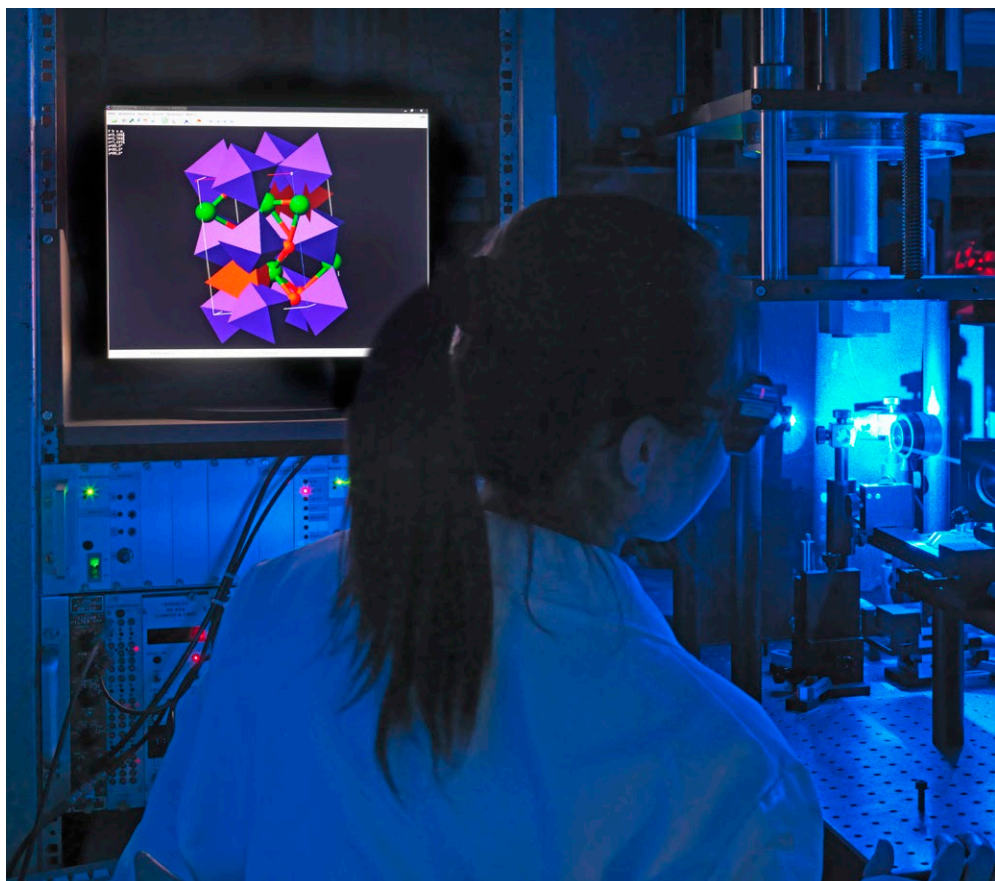
Computers of the future will possess immense storage capacity in the smallest space. It will be possible to access data much more quickly and, after a power loss, no data will be lost. Researchers are working today to understand the fundamental behaviour of such systems.

With the compass – one of the oldest applications – ferromagnetism was already known in ancient China. Ferromagnetic materials are of themselves not intrinsically magnetic, but they can be magnetised by a strong, external magnetic field. If this field is removed, a portion of the magnetisation remains in the material – and then the magnetised compass needle later aligns itself with the earth's magnetic field. The same effect is used in the hard disks of computers in order to store information and later retrieve it.

Along with magnetism, there are other ferroic phenomena, for example ferro- or piezoelectricity. One well-known application of the piezoelectric effect is the piezoelectric cigarette lighter: By pressing a button, a cam strikes a piezoelectric crystal, thereby deforming it and producing a voltage of up to 15 kilovolts, which discharges through two metal contacts joined to the crystal. This produces an electric spark, which ignites the gas flowing out of the lighter.

## Combined properties

Magnetism and ferroelectricity are two material properties which do not normally occur together in nature. Scien-



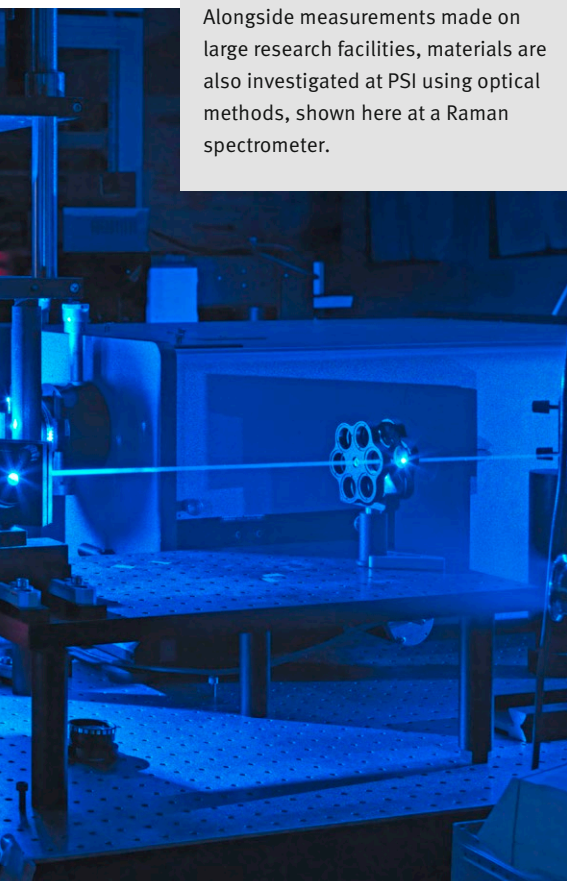
tists ask the following question: Are there nevertheless materials which have both properties – so-called multiferroics? If yes, then how strong is the effect and is it possible to use these for applications? Here the magneto-electric effect is of particular interest, because the magnetic orientation can be changed by applying an electric field. Conversely, a magnetic field can be used to reverse ferroelectric orientation. If the material is placed in a magnetic field, an electric field can be measured. The first research projects

already began 50 years ago in the Soviet Union, where physicists were studying materials in which magnetism and ferroelectricity occurred together. The effect that was found, however, was very small and not interesting enough for practical applications.

In general, data storage would be a possible application for these multiferroic materials. On a conventional hard disk information is stored in bits. One can think of each bit as a tiny bar magnet. When the north pole points upwards, this signifies a digital bit of in-



Alongside measurements made on large research facilities, materials are also investigated at PSI using optical methods, shown here at a Raman spectrometer.



ventional hard disk and requires less energy. In addition, the moving parts of a hard disk become redundant, and so a fast-rotating, vibration-sensitive disk is no longer necessary.

### Research in its infancy

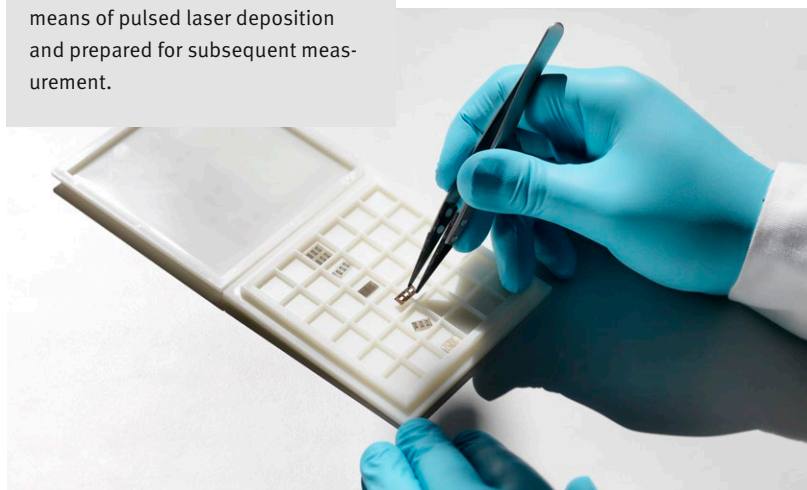
For their studies, scientists at PSI use thin films of multiferroic material as well as thick samples, depending on whether they can be manufactured in the one or other form and depending on which properties in each need to be studied. In the case of thin layers, the very small volume of material— around 100,000 times smaller than a drop of water— presents a great challenge to making measurements. Additionally, most of these materials are insulators,

which means that it is not easy to measure their electrical resistances. For this reason, this class of materials must also be studied at large research facilities with neutrons, muons or X-rays in order to obtain information about their electronic and magnetic properties.

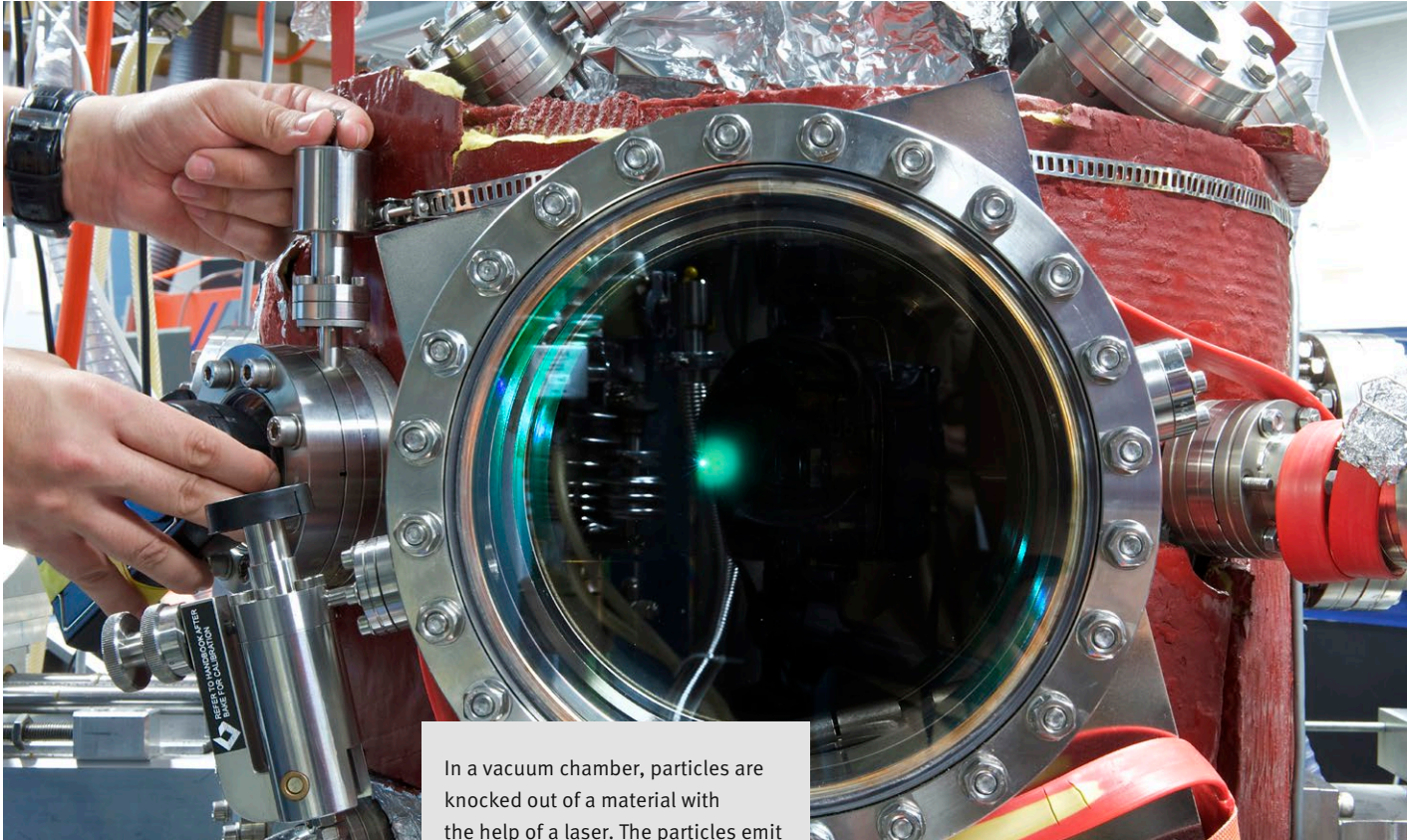
Research in this field is still young, but when the scientists understand in the near future how the multi-faceted interaction between magnetism and ferroelectricity takes place, they will be in a position to manufacture materials with new properties in a selective way. This could result in completely new applications.

formation corresponding to one; when it points downwards, it signifies a digital zero. On a hard disk, there are billions of such bits. The data is written or read by means of a current in a magnetic read-write head. Multiferroics possess the same basic structure, but with the difference that the magnetic bits here can be influenced by the application of an electric field. In this way, the storage medium can be directly written to, and read, without the need to create or detect a magnetic field. This works far faster than writing to a con-

Thin layers deposited on single crystals. The multiferroic materials are deposited on the substrate by means of pulsed laser deposition and prepared for subsequent measurement.



# It all depends on the internal details



In a vacuum chamber, particles are knocked out of a material with the help of a laser. The particles emit green light on their way from the material to the sample holder (from left to right).

To discover an interesting material property is one thing, but to understand it is another. In experiments aimed at investigating its properties, a material is required in pure form, as the slightest deviation from the ideal structure can lead to radical modifications. Samples must be able to be manufactured in which billion upon billion of material building blocks are exactly arranged according to the given building plan. And that is an art in itself!

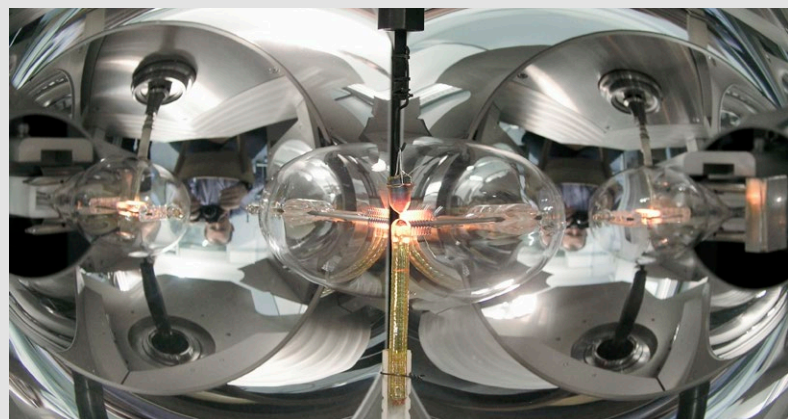
It is their novel properties that make new materials interesting for applica-

tions – such as the ability of superconductors to carry current without any electrical resistance. As useful as these properties are, it is often not clear how they come about. In order to unlock these secrets, researchers study the processes within materials and observe what happens at the level of their smallest building blocks – the individual atoms and electrons. Specialists

call this the determination of the static and dynamic structure of a material. And for this they need, in turn, an appropriate object to study – a sample. To produce one of these is really not easy, as it must only contain the material of interest. This is because only the properties of this material should be visible, and not those of any other substances which are mixed with it. It is therefore not only important to use the right constituent elements, they must also be arranged exactly according to the building plan, because every small deviation can give rise to an undesirable effect. At most, a few building



View into the 40-cm-wide interior of a mirror oven used for producing large single crystals. Focussed light is used to melt a polycrystalline cylinder fixed in the centre, from which a single crystal will be created.



blocks in a billion are allowed to be wrongly placed. This is like tolerating a few typing errors in a library containing many thousands of books. Otherwise the complete library would be unusable.

## Growing perfect crystals

Researchers have developed many processes for producing appropriate samples; for example, for fabricating crystals. Indeed, every material in which the building blocks are ordered in a regular and repeating pattern is called a crystal. Generally, crystalline materials consist of many small crystals which are oriented differently – this applies to metals from which many pieces of equipment are constructed. In order to produce such a “polycrystalline” material, researchers start off, as a rule, with a completely disordered condition – with the molten material, in which no atom is fixed in one place. When such a material cools down, its atoms order themselves according to their local environment into a crystalline structure. The tiny crystals that are created in different places all grow in different directions and when they join they are not uniformly aligned.

Such a polycrystalline sample is entirely adequate for many experiments, but sometimes disorder is detrimental, as it can obscure the real properties of the material. For example, the interfaces between the individual mini-crystals can provide resistance to electrical current and disguise the fact that the material itself conducts current extremely well. In this case, researchers

need single crystals; that is, larger pieces of material with uniform crystal structure. One method of producing such a single crystal consists of starting out with a small cylinder of polycrystalline material, about the size of a felt-tip pen. With the aid of very intense light, a thin layer at the end is melted and then allowed to solidify slowly. In this way, the atoms have enough time to orient themselves into the ideal crystalline structure. Then the adjacent layer above it is melted and its atoms fit into the preset structure of the lower layer. After the complete cylinder has been melted in this way and allowed to cool again, layer by layer, it will have an ideal continuous crystalline structure. This is an often tedious process that can last up to two weeks. At the end, however, an outstanding crystal, for example a superconductor or a multiferroic material, has been created. This will, as a rule, be cut into smaller slices, whose interior can be observed with neutrons or synchrotron light.

## Thin layers provide a remedy

Producing a large single crystal in this manner does not always work, as there are some materials whose molten form is too liquid, while others only melt at very high temperatures. For example,

gallium already melts at 30 °C, but tungsten needs to be heated above 3400 °C in order to melt it. Therefore, in order to be able to study crystal samples of these materials, researchers choose a different method – they make very thin layers.

Here, too, they begin from a state of maximum disorder: They vaporise the material. If a laser with a high enough power is available, any material can be vaporised, even tungsten. The vaporised material deposits onto a prepared, very flat substrate. If this is carried out correctly, the atoms organise themselves into a regular crystal structure on their own. All of this obviously takes place in a vacuum, to ensure that no air molecules get into the sample. The result is a very thin crystal – in the best case consisting of only 10,000 atomic layers – around a thousandth of a millimetre thick, but sometimes even a thousand times thinner. Not all conceivable experiments can be performed with this crystal, however, but tests with synchrotron light, neutrons or muons often work well and deliver insights into material properties that are important, for example, for spintronics or superconductors.

# The tools of science

**The smaller the structures, the bigger the equipment needed to examine them. On the campus of PSI there are now four unique large research facilities: the Swiss Light Source SLS, the Swiss Spallation Neutron Source SINQ, the Swiss Muon Source  $S\mu S$ , and – the newcomer in the bunch – the SwissFEL X-ray-free-electron laser.**

Materials scientists want to understand the fundamental mechanisms that give rise to very special materials properties. With this knowledge, they are able to develop new materials or improve existing ones. PSI scientists determine material properties using a variety of different tools, from an ohmmeter to measure the electrical resistance of a material to instruments for measuring the optical properties of a material. Alongside these, to some extent specialised, measuring devices available in many PSI laboratories, scientists also use large research facilities, similar to giant microscopes, with which they can look deep inside materials. This is because, ultimately, the properties of a material are determined by the ordering of its atoms and the balance of the forces existing between them. Specialists talk of the static and dynamic structure of a material.

## Synchrotron light

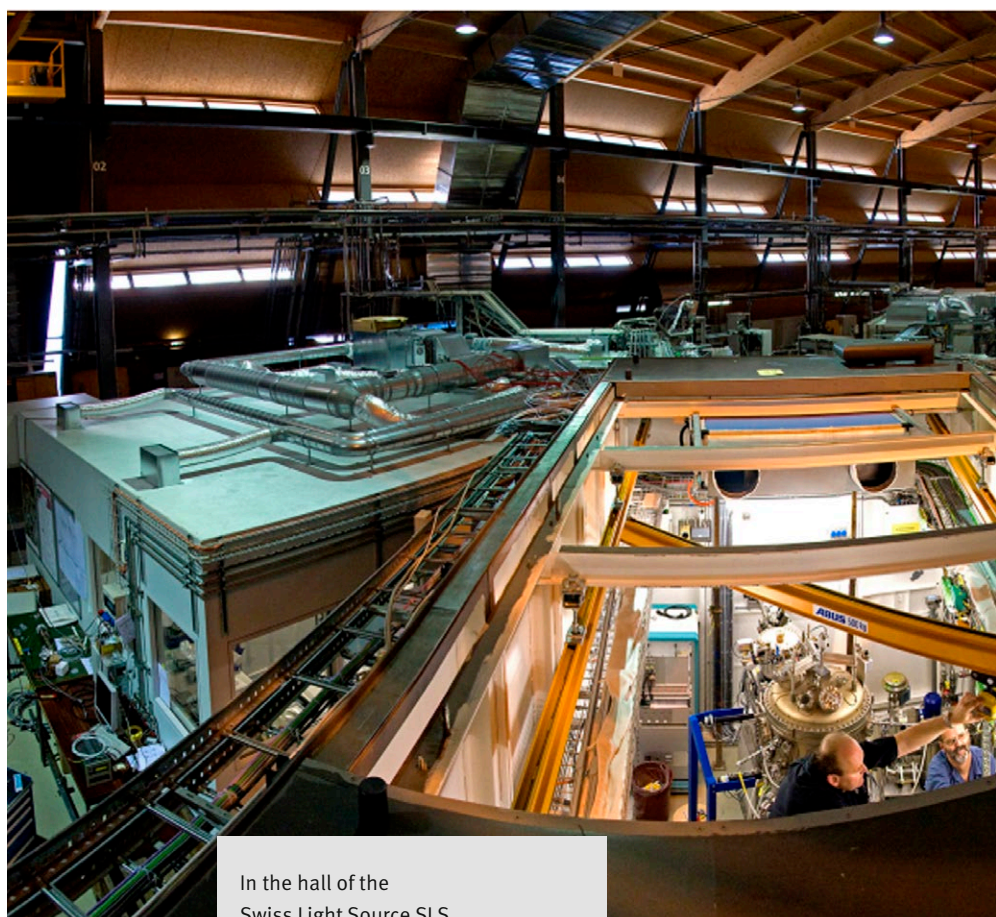
The wavelength of visible light is about a thousand times greater than the atomic distances found within a material. It is therefore impossible to see atoms using normal light, not even with the best magnifying lenses. Research-

ers at PSI therefore use a synchrotron light source. This generates light with a very short wavelength, which is invisible to the human eye – so-called X-ray radiation, or light.

X-rays are produced when electrons are rapidly decelerated. First of all, the electrons must be accelerated to a high speed. This takes place in the same way as in televisions with a cathode-ray tube: Electrons emanating from a glowing filament are accelerated by a high voltage between two metal plates. In such a television, this beam of electrons produces a picture on the screen.

In an X-ray device, the voltage is higher and the electrons strike a piece of metal. This decelerates them so strongly that X-rays are generated.

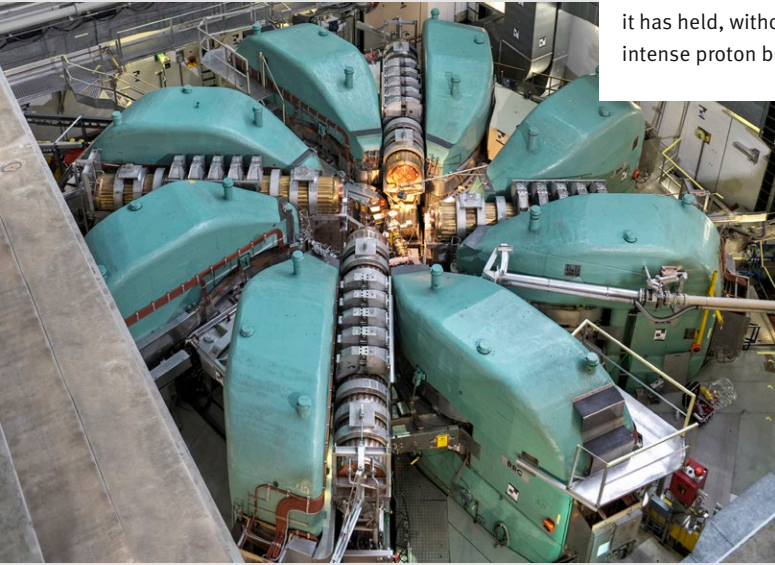
For materials research, the X-rays produced by a conventional machine, such as that used by doctors, are not intense enough for every purpose. They also do not cover a broad enough wavelength needed for many applications. Hence, electrons in the SLS are accelerated to almost the speed of light. Subsequently they are stored in a ring with a circumference of almost 300 metres. Here, they circulate inside a metal duct, in a



In the hall of the Swiss Light Source SLS.



The PSI proton accelerator, used for producing the muons and neutrons needed for experiments. Since the 1970's, it has held, without interruption, the world record for the most intense proton beam.



ments, they must continually re-adjust their instruments. At the SLS, on the other hand, lost electrons are replaced by new ones every four to five minutes, so that the intensity of the X-ray beam hardly changes.

## Neutrons

vacuum, so that they do not collide with air molecules. Every so often along their pathway there are short, straight

sections followed by magnets which force the electrons to move for a brief moment in another direction, so keeping them on the right circular path.

The electrons are so fast that the deflection by the magnets is sufficient to generate X-rays – called synchrotron light. This happens because the deflection is also an acceleration and – like the collisions of electrons with a piece of metal in a conventional X-ray machine – this leads to the generation of X-rays. For a few years, researchers at PSI have employed even more sophisticated acceleration sections – magnets with alternating polarity which force the electrons into a wavy path, thereby producing radiation which is particularly intense.

The synchrotron light source at PSI has the advantage that, compared to facilities in other research centres, it can provide scientists with a sustainable beam of high stability. In many other facilities, the electron beam is only fed into the storage ring once and then left there to circulate for about eight hours. During this time, the beam becomes weaker as it loses electrons and no more are fed in. This is problematic for scientists because, for many experi-

Alongside X-rays, scientists use other methods to give a complementary insight into materials. Light elements, such as hydrogen or lithium, are practically transparent to X-rays, as is also the case for organic materials, which are composed primarily of hydrogen and carbon. Also, the lithium in lithium ion batteries let X-rays pass through almost unhindered. In this case, scientists get around the problem by using neutrons, which interact with some very light elements. As neutrons are electrically neutral, the negatively charged shell of the atoms is transparent to them. Only when they hit the small, but heavy, atomic nucleus do they interact.

Neutrons, as well as protons, form the atomic nucleus. Since they only occur naturally in nuclei, PSI researchers must generate neutrons in an indirect way. They do this by accelerating the naked nucleus of a hydrogen atom – a single proton – and by shooting it into a block of lead. The proton collides there with the nucleus of a lead atom, which is composed of protons and neutrons. The nucleus then begins to vibrate so strongly that it loses a number of protons and neutrons, which is how researchers obtain neutrons.

These neutrons, however, are too fast





View into the neutron guide hall. With its total of 18 different instruments, some of which are the only ones of their kind in the world, materials can be studied at PSI with neutrons.



for experiments and for this reason the lead is placed inside a water tank. The heavy water ( $D_2O$ ) and, in a second stage, liquid heavy hydrogen ( $D_2$ ) slow the neutrons down to a speed which is suitable for experiments. In a similar way to X-rays, the neutrons are now directed onto the material to be analysed. Depending on the material structure, the neutrons are deflected and slowed down, thereby providing scientists with information about the material. And since neutrons behave like small magnets, conclusions can even be drawn about the magnetism in the material.

## Muons

Muons react even more sensitively than neutrons to the magnetic fields inside magnetic samples. They become stuck

inside the material and occupy empty spaces between the atoms. After a millionth of a second they decay and emit a particle that can be detected. Not only the direction but also the strength of the magnetic field in the material can therefore be measured at a desired depth, which depends on the speed of the muon.

In order to be measured, muons must first of all be artificially produced, although they do occur naturally when high-energy sunlight strikes the atmosphere and continuously produces muons, which even reach the earth's surface. These natural muons, however, cannot be captured and used, as they decay too rapidly. Muons are produced in the laboratory as decay products from the collision of protons with carbon nuclei.

Also here, the initially generated elementary particles are too fast and must

be decelerated. One speciality of PSI is the production of extremely slow muons and it is the only institute in the world that can produce such slow muons. These are first of all slowed down by a silver foil and then cross a layer of frozen inert gas; for example, argon. This works like a crowd at the main railway station during rush-hour. A pedestrian can only let himself or herself be carried along by the crowd, and can neither walk faster nor slower than the crowd. Thus muons which were initially moving along at different speeds are brought to the same speed, and researchers can thus fix the depth to which the muons should penetrate the sample.



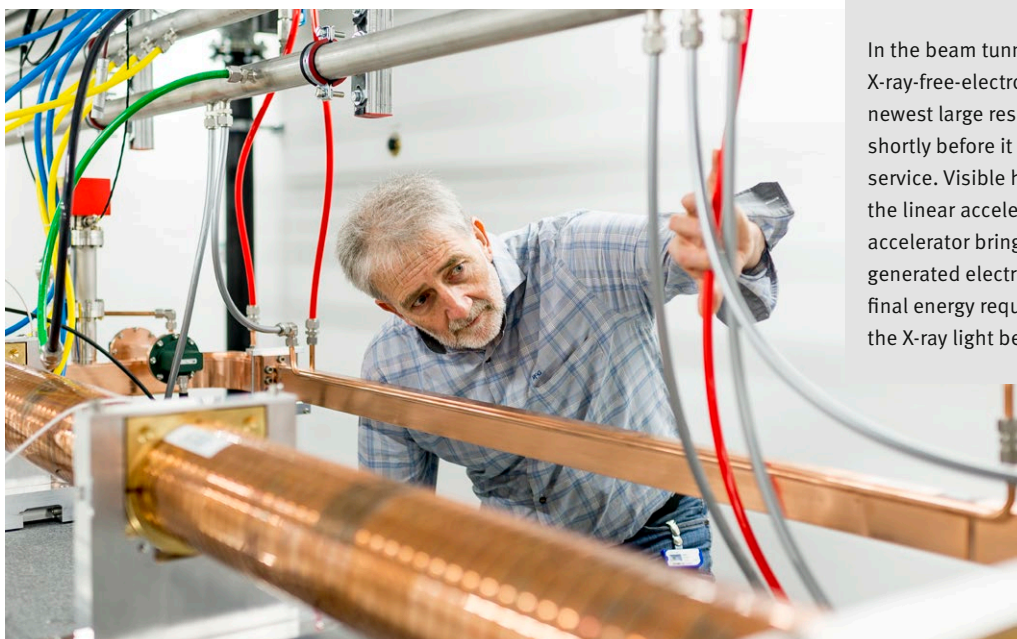
## SwissFEL

The SwissFEL X-ray-free-electron laser is the most recent addition to the large research facilities of PSI. Most materials can be characterised using the X-rays of SLS, the neutrons of SINQ, and the muons of S $\mu$ S. But there are limits. These apply, in particular, to some important molecules that determine the functionality of biological cells. Crystals of these so-called membrane proteins can be studied today at SLS, but only if they have a size of at least one-hundredth of a millimetre. Unfortunately, only a few of the membrane proteins occurring in nature and in human beings can be produced at this size. And it is just this knowledge of the structure of membrane proteins on which the pharmaceutical industry today is setting great hopes, in order to be able to develop new medications.

In addition, no ultrafast processes, such as those taking place during the rapid switching in multiferroics and spintronic devices, or in catalytic chemical reactions, can be observed in the three large research facilities SLS, SINQ, and S $\mu$ S. The “illumination times” are too long.

The problems encountered with small samples and ultrafast processes can be solved by the use of extremely intensive and very short X-ray pulses. These are exactly what the SwissFEL X-ray-free-electron laser, the fourth and newest large research facility at PSI, delivers. The electrons used for the production of the X-rays in this facility are obtained from a very short laser pulse striking a piece of metal. The resulting electron packets are fed into a linear accelerator to be brought up to the final energy required, and by means of sophisticated “tricks” the electrons

are compressed so tightly that they behave “collectively”. On sending them through an alternating series of magnets, as at SLS, they then emit X-rays. In contrast to a synchrotron light source, however, this will occur more or less “in harmony”. The X-rays in the pulse are thus about a billion times more intense than in the SLS beam and have characteristics that enable a sharp picture to be obtained from even the smallest sample. Due to the short pulse, snapshots can be taken of ultrafast physical, chemical, or biological processes. These can then be put together into a film that researchers can view in slow motion, in order to obtain new knowledge to create the materials of the future.



In the beam tunnel of the SwissFEL X-ray-free-electron laser, the newest large research facility of PSI, shortly before it was brought into service. Visible here is part of the linear accelerator. The linear accelerator brings the previously generated electrons up to the final energy required. Only then can the X-ray light be generated.



Bird's eye view of  
the Paul Scherrer Institute.





# PSI in brief

The Paul Scherrer Institute PSI is a research institute for natural and engineering sciences, conducting cutting-edge research in the fields of future technologies, energy and climate, health innovation and fundamentals of nature. By performing fundamental and applied research, we work on sustainable solutions for major challenges facing society, science and economy. PSI develops, constructs and operates complex large research facilities. Every year more than 2500 guest scientists from Switzerland and around the world come to us. Just like PSI's own researchers, they use our unique facilities to carry out experiments that are not possible anywhere else. PSI is committed to the training of future generations. Therefore about one quarter of our staff are post-docs, post-graduates or apprentices. Altogether PSI employs 2200 people, thus being the largest research institute in Switzerland.

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