Faszination **Forschung**

TUM Research Highlights
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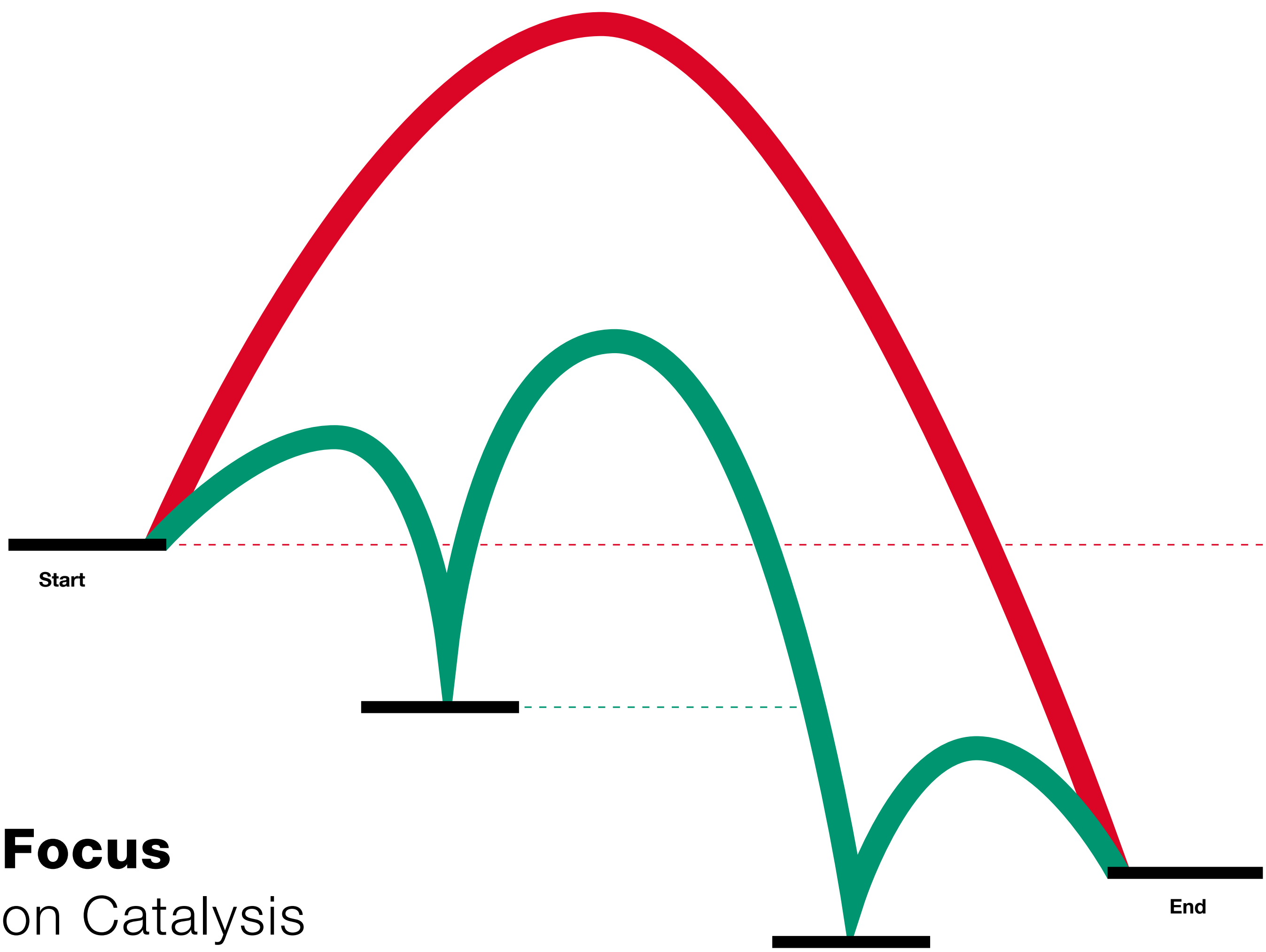

Focus
on Catalysis

Catalysis I: Small in Size, Big in Impact
Catalysis II: Millions at my Beck and Call!
Nanoscience: Magically Drawn to the Interface

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Dear TUM friends and associates,

Catalysis is one of the trending technologies in our high-tech society. New catalysts and catalytic processes are paving the way for energy-efficient, low-resource substance conversions with the ability to add value while saving money. They will also make it easier for us to use renewable raw materials. At TUM, we have been prioritizing research into catalysis for several years now. Today we are proud to present our new TUM Catalysis Research Center in Garching. The largest and most modern center for catalysis research in Europe, this interdisciplinary facility provides an excellent scientific platform for our continued endeavors in this area.

In Ulrich Heiz's lab, scientists are creating nanocatalysts with tailored properties comprising just a few atoms. This work is paving the way for the design of catalysts that behave in a specific way and are resource-efficient. Meanwhile, Thorsten Bach is developing catalysts to precisely control the products of photochemical reactions, thus laying the foundations for material-efficient production processes that use natural light as an energy source.

Thomas Brück's research focuses on algae, specifically on how to efficiently harness this sustainable natural resource to produce biokerosene and valuable chemical materials. To further this work, TUM, in cooperation with the Airbus Group, has built the world's first algae research facility at the Ludwig Bölkow Campus in Ottobrunn. The Werner Siemens Foundation recently provided EUR 11.5 million in funding to further research in synthetic biotechnology.

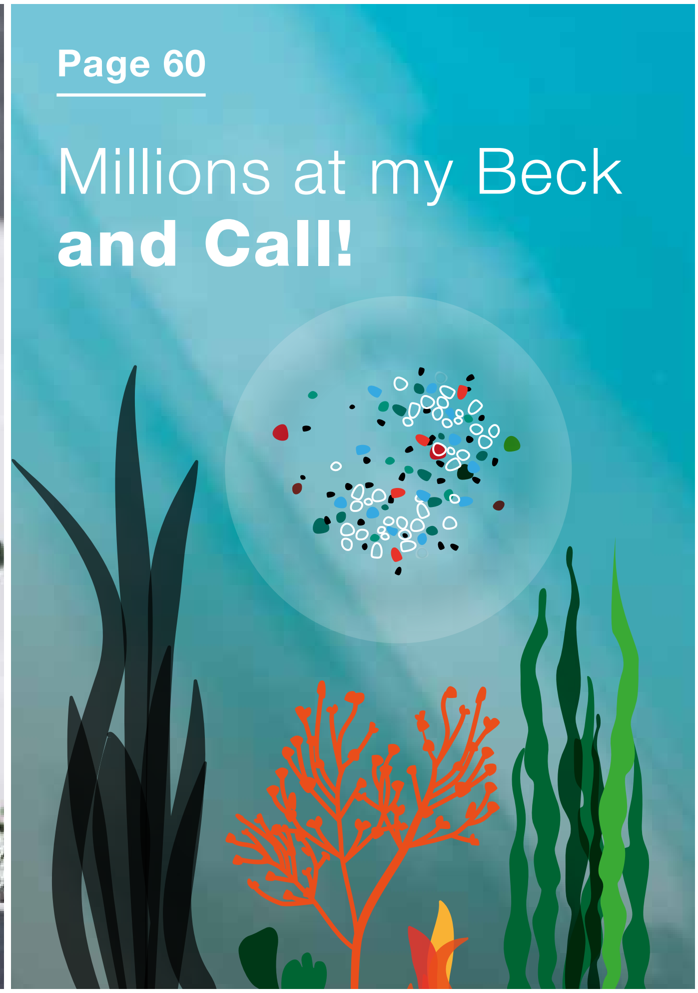
Physics researchers working with Johannes Barth are creating new nanostructures and molecular functional architectures on specially structured interfaces. Their work is, among other things, paving the way for new kinds of nanomaterials and future nanoelectronic systems. Thirty years have elapsed since the discovery of high-temperature superconductivity, and still the physics behind the phenomenon is not fully understood. Jitae Park and Astrid Schneidewind are managing two unique instruments at the Heinz Maier-Leibnitz neutron source research reactor (FRM II) that could contribute to a possible theory for this phenomenon. Scientists from all around the world are using these experiments to gain new insights. The infrastructure in place here is yet another jewel in Garching's catalysis crown.

As one of the world's top research universities, we are also involved in several other high-profile projects. The most accurate digital elevation model of the Earth yet produced is being compiled from data beamed down by the TanDEM-X radar satellites. Applications range from forecasting volcanic eruptions to creating digital maps for self-driving cars. With a team headed by Richard Bamler and Michael Eineder, TUM is one of the primary European scientific partners in this mission overseen by the German Aerospace Center (DLR).
Eckehard Steinbach is developing a robot that uses a small camera to control its movements and gripping pressure. This completely novel technology is already a viable alternative to today's more costly industrial robots. Steinbach's team is currently building an initial prototype for industrial applications.

I hope that you will be inspired by the work of these members of the TUM family who are striving to bring us the technologies that will make our world a better place, now and in the future!

Prof. Wolfgang A. Herrmann

Picture credit: Heddergott



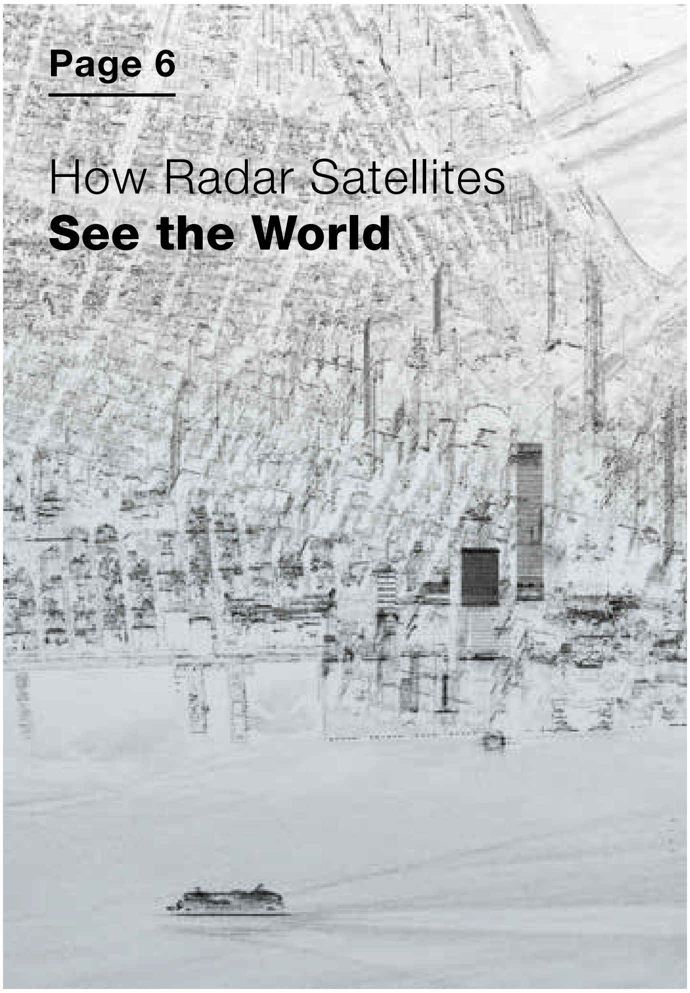
Cover Story

"Catalysis is at the top of today's scientific, economic, environmental and policy-making agenda."

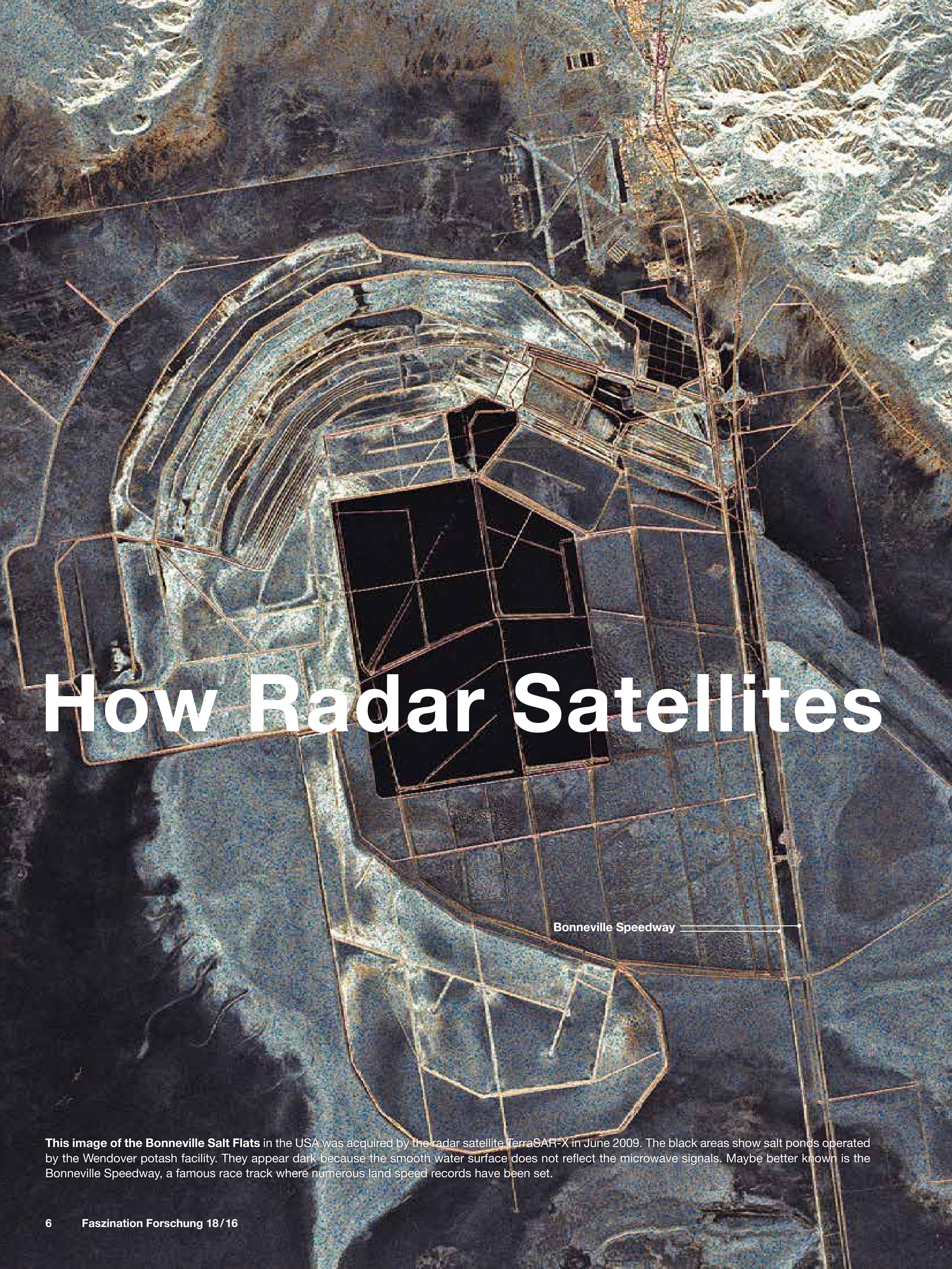
Wolfgang A. Herrmann

Research and Technology

Picture credits: Jooss, Bauer, DLR, Graphics: ediundsepp



In every Issue



How Radar Satellites

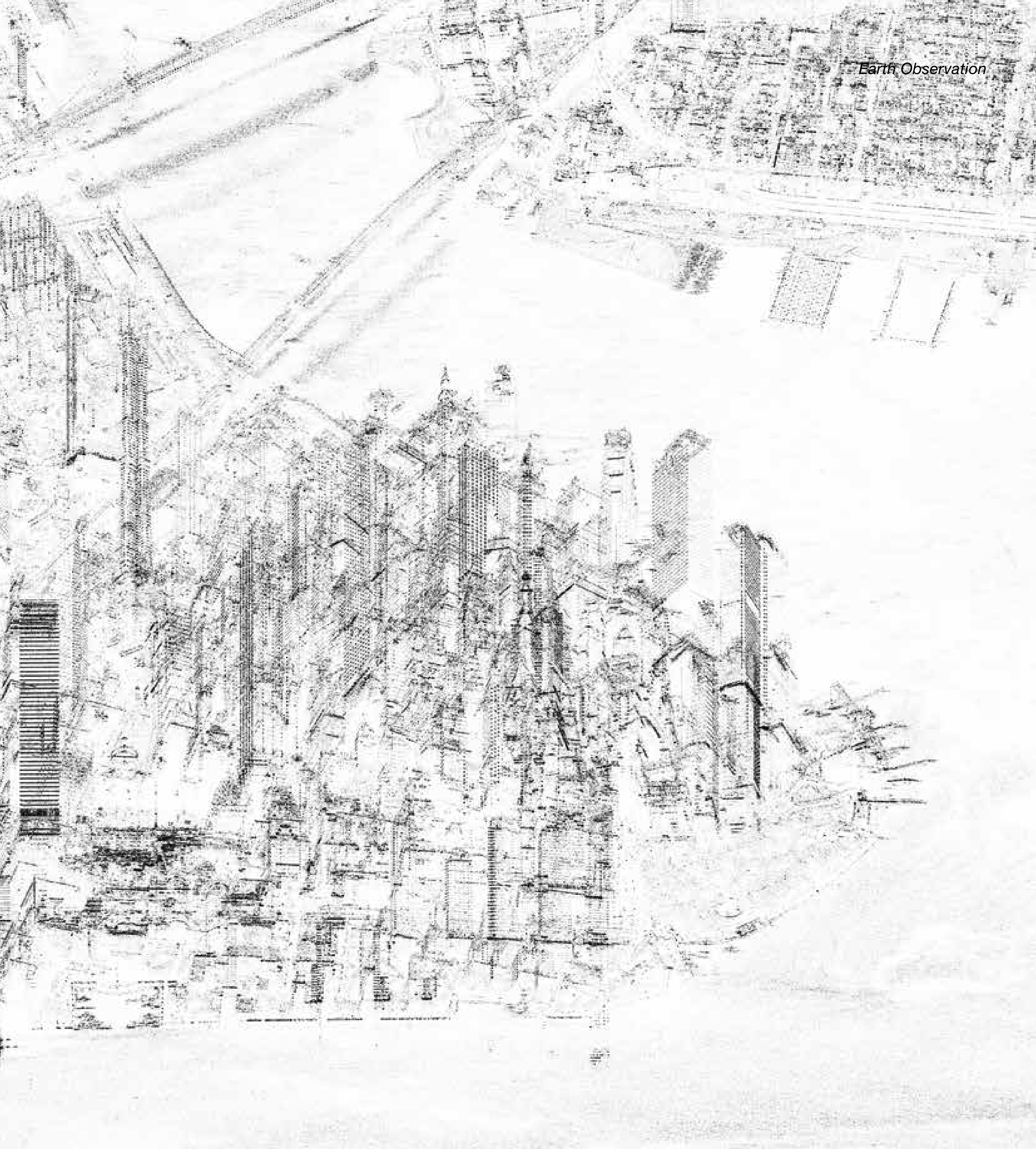
This image of the Bonneville Salt Flats in the USA was acquired by the radar satellite TerraSAR-X in June 2009. The black areas show salt ponds operated by the Wendover potash facility. They appear dark because the smooth water surface does not reflect the microwave signals. Maybe better known is the Bonneville Speedway, a famous race track where numerous land speed records have been set.

See the World

Space missions deliver global 3-D topography mapping and more.

Picture credit: DLR

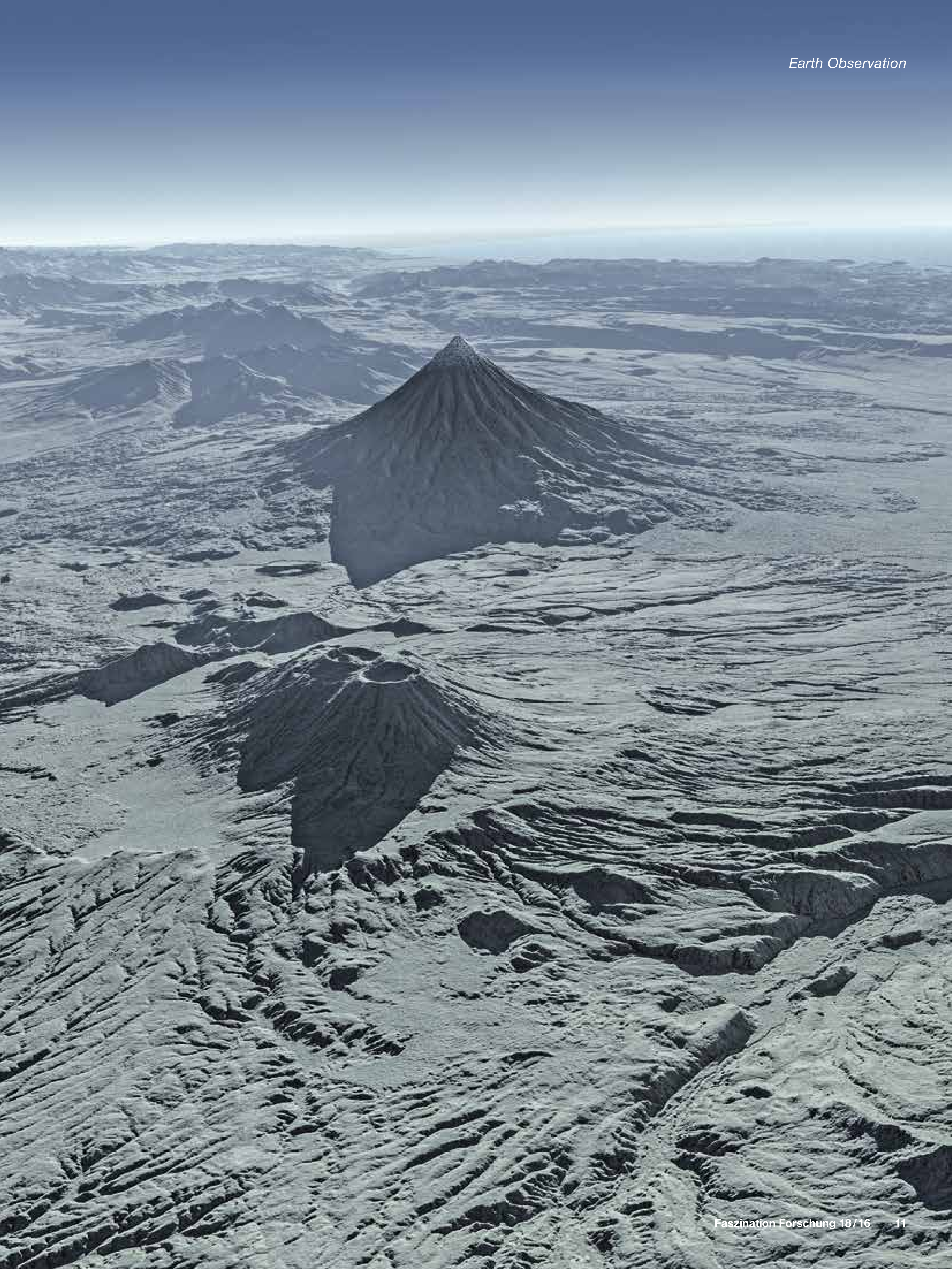
Picture credit: DLR

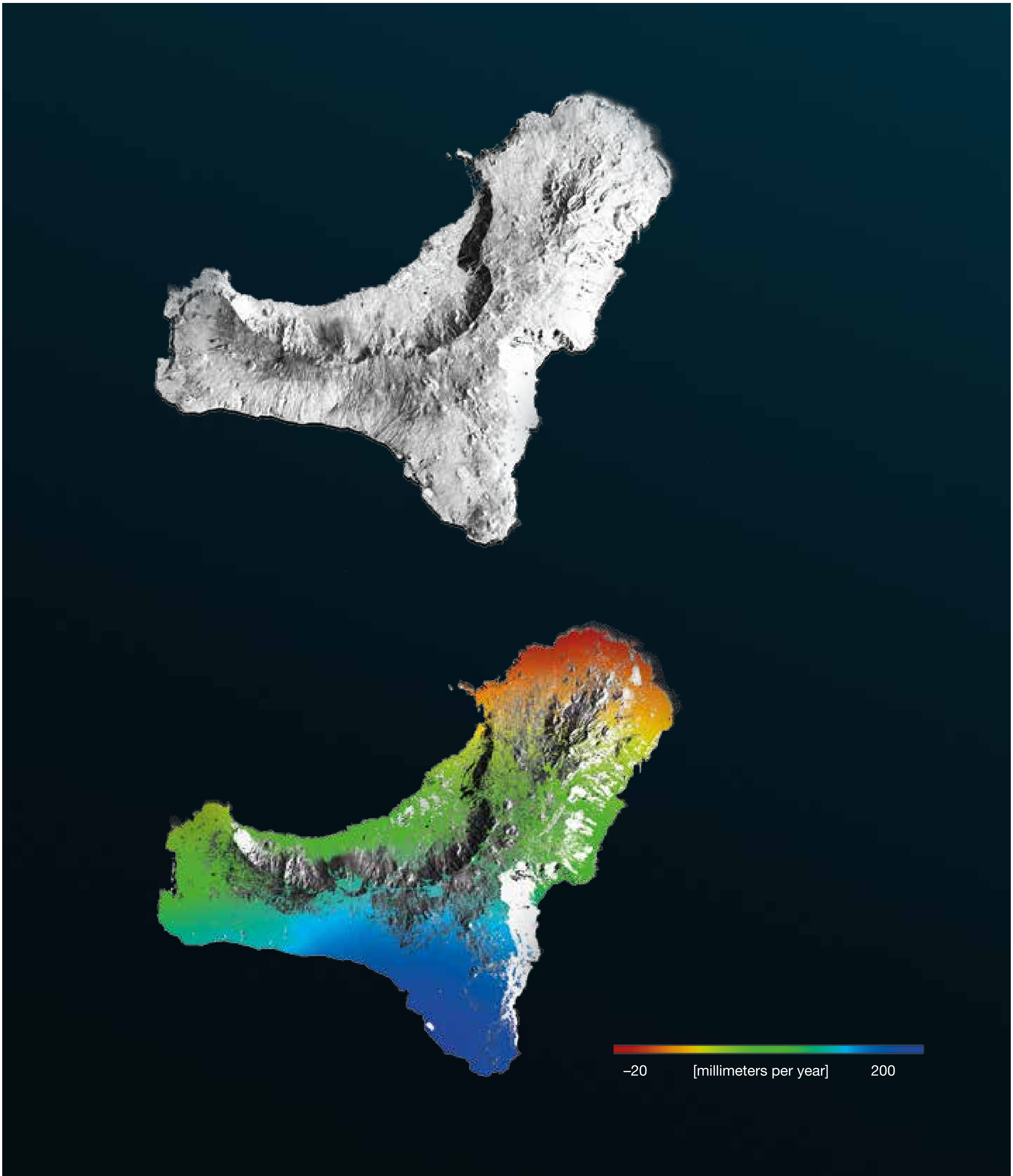


Radar Art: Image of Manhattan Island, New York with a ship cruising the Hudson River in the foreground. Due to the high resolution of TerraSAR-X, ships, docks and bridges, and even individual windows of high-rise buildings cause strong radar reflections. For esthetic reasons, the grey values are inverted – water appears white and windows appear dark. The image is presented in such a way that the geometric radar distortions – a common phenomenon in radar imaging – appear like a perspective view of the city.

SAR satellites are frequently used to monitor the activity of volcanoes worldwide. This artificial bird's eye view shows the volcanoes of Kamchatka peninsula in Russia. It is composed of millions of height measurements acquired by the TanDEM-X mission. Each data point represents an area of 12 m × 12 m with a height accuracy of 2 meters.

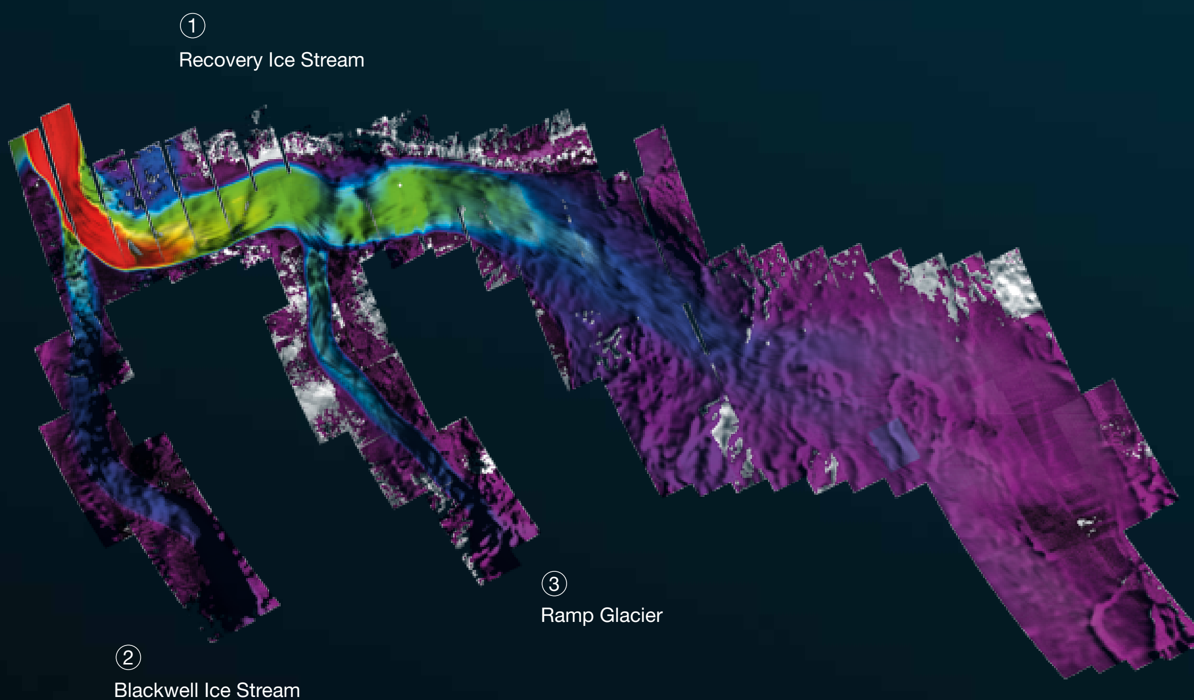
Picture credit: DLR





Volcanoes sometimes announce their activity or eruption days or weeks before by a small deformation of their surface, which is caused by pressure changes inside the magma chamber. Such small signals can be measured from space with radar interferometry. The top image shows a TerraSAR-X view of the Canary Island El Hierro. The bottom image shows several centimeters deformation (blue: uplift, red: subsidence) on the El Hierro volcano between 2011 and 2013 derived from 50 TerraSAR-X data sets. The actual eruption occurred underwater in the bottom left area of the image.

Picture credits: DLR, Graphics: ediundsepp (source: DLR)



Measuring the speed of the Recovery Ice Stream flowing into the Filchner-Ronne Ice Shelf in Antarctica. The ice mass transported to the ocean by Antarctic glaciers is an important climate indicator and contributes to sea-level rise. Ground-based measurements of the glaciers' velocity are demanding, time-consuming, and "point-wise." Radar satellites record the velocity patterns of whole ice streams with high resolution and thus can deliver much more complete data for climate research — any time of year, not only during the Antarctic summer.


DLR

DLR scientists and TUM professors Richard Bamler (right) and Michael Eineder are leading the data analysis work for the TerraSAR-X and TanDEM-X missions.

Picture credit: ediundsepp

Link
www.dlr.de/eoc

Patrick S. Regan

Wie Radarsatelliten die Welt sehen

Blickt man von einem Punkt einer polaren Umlaufbahn schräg nach unten, ist infolge der Erdrotation jeder einzelne Fleck unseres Planeten in regelmäßigen Abständen zu sehen. Wird nun die Szene mittels Radar im Mikrowellenfrequenzbereich ausgeleuchtet, lassen sich Objekte unabhängig von den Wetter- und Lichtverhältnissen sichtbar machen. Für das „Radar-Auge" der computergestützten SAR (Synthetic Aperture Radar)-Technologie, bei der aufgezeichnete Wellenfelder in gestochen scharfe Bilder umgewandelt werden, treten selbst kleinste Details so deutlich hervor wie in einer Großaufnahme. Verfügt man gar über zwei solcher Augen, lässt sich damit eine Entsprechung zum stereoskopischen, dreidimensionalen Sehen erreichen.

Damit ist im Kern beschrieben, was die Radarsatelliten TerraSAR-X und TanDEM-X in Verbindung mit einer ausgeklügelten Datenverarbeitung am Boden leisten. Wichtigstes Ergebnis ist ein digitales Höhenmodell (DHM) des gesamten Planeten, das für jeden beliebigen Punkt eine Höhenangabe liefert und 3D-Ansichten erlaubt. Diese Daten bzw. das DHM werden zum Beispiel für Kartographie, Hydrologie, Erdsystemforschung, Katastrophenschutz, aber auch für kommerzielle Anwendungen wie die Planung und das Management von baulicher Infrastruktur benötigt. In enger Kooperation mit Industriepartnern arbeitet das Deutsche Zentrum für Luft- und Raumfahrt (DLR) daran, entsprechende Missionen an den Start zu bringen. Die TUM ist dabei einer der wichtigsten Wissenschaftspartner, insbesondere in den Bereichen Algorithmenentwicklung, Datenverarbeitung und experimentelle Anwendungen. Geleitet werden die Arbeiten von Prof. Richard Bamler und Prof. Michael Eineder, die sowohl an der TUM als auch beim DLR tätig sind.
Wie die Ergebnisse belegen, liefert TanDEM-X nicht nur das umfassendste und konsistenteste Höhenmodell, das es gibt, sondern ist darüber hinaus 30-mal genauer als das beste bislang verfügbare DHM. Die Wissenschaftler des DLR planen bereits eine weitere Satellitenmission namens Tandem-L, die an die bisherigen Erfolge anknüpfen soll. Technologie und Einsatzpläne sind hier dahingehend weiterentwickelt, dass sich Veränderungsprozesse auf der Erdoberfläche bzw. in der Bio-, Geo-, Kryo- und Hydrosphäre kontinuierlich beobachten lassen. □

The twin satellites TerraSAR-X and TanDEM-X orbiting Earth at an altitude of around 500 kilometers. The TanDEM-X mission will survey all 150 million square kilometres of Earth's land surface several times over during its three-year mission, delivering a global elevation model that is homogeneous in quality and unprecedented in accuracy. It produces 3 petabytes of data and one trillion data points, each representing an area of 12 m^2 at a height accuracy of 2 meters.

Picture credits: DLR, ediundsepp


EARTH
OBSERVATION
CENTER
DLR
Eingeweiht am
20. Juli 2010

You can see a lot, looking back at the Earth from space. From a vantage point in orbit, on a path that crosses the poles, every square meter of the surface comes regularly into view as the planet turns on its axis. Illuminating the scene in microwave frequencies, radar makes objects visible day or night, regardless of the weather. Better still, with an "eye" of synthetic aperture radar or SAR – a computer-enabled technology that transforms long-distance measurements into sharp images – details become as clear as in a close-up. And with a pair of such eyes, you get the equivalent of stereo vision and three-dimensional sight, with extremely high resolution and global coverage.

This is essentially what the radar satellites TerraSAR-X and TanDEM-X, coupled with sophisticated data processing on the ground, are delivering. The main product is a digital elevation model (DEM) covering the entire planet, to be completed in the fall of 2016 and then further enhanced for selected regions. It will give a height for every point and enable 3-D views. Virtually all commercial and scientific activities that involve mapping depend in some way on digital elevation models. Applications run the gamut from navigation services and infrastructure engineering to Earth systems monitoring, hydrology, and disaster recovery. Results to date already confirm that this model – besides being the most complete and consistent – is more than 30 times more accurate than the best previously available.

The German Aerospace Center DLR has worked closely with industry partners – EADS Astrium and Infoterra, now both units of Airbus Defence & Space – to get these missions off the ground and to get data products into the hands of commercial users. TUM is one of the primary scientific partners, particularly in connection with algorithm development, data processing, and experimental applications. The circle of scientists using mission data – for studies ranging from land use to climate change impacts – is large and growing, with more than 200 researchers attending the latest user group meetings. A follow-on mission has already been proposed, building on this success and opening up new possibilities.

From 1-D measurements to 3-D images

The names alone, TerraSAR-X and TanDEM-X, tell part of the story: Terra emphasizes that Earth is the object of this remote sensing program, SAR highlights synthetic aperture radar, and X identifies a specific band of electromagnetic radiation, centered on a wavelength of around 3 cm, which partly determines what the radar can see in detail. TanDEM-X stands for "TerraSAR-X add-on for Digital Elevation Measurements." But the names can refer either to the individual satellites or to the missions as a whole, and TanDEM-X employs both satellites. To avoid confusion, let's call the satellites TSX and TDX respectively, reserving the full names for the overall missions.

The satellites are nearly identical twins, although TSX was launched three years earlier than TDX. Since 2010, they have been orbiting together in a tight, helical formation that allows them to fly safely – at around 25,000 kilometers per hour – as close to each other as 100 to 500 meters. To better understand why, consider how space-based radar measurements are transformed into images, models, and maps.

Radar, stripped to its essentials, is a technology for measuring distances. Transmit a short radio-frequency pulse, wait for the reflection that comes back from an object in its path, and the time interval provides the basis for determining the distance. In reality, that reflected pulse is more like a "wave package" that will have different peaks at different times, corresponding to multiple objects. Record the entire complex reflection, and the data could yield an image, not just a distance between two points. The next logical step might be flying the radar system on an airplane or a satellite to scan the land as it moves along, but physics presents a problem (the first of many): One of the limits to how sharply a radar

The radar satellite mission TanDEM-X yields a global digital elevation model over 30 times more accurate than the best previously available.

system can resolve an image is the size of its transmitting and receiving antenna; looking down from an orbital height of around 500 kilometers, achieving even meter-scale resolution would require an antenna several kilometers long.

This is where SAR comes in. The distance a radar satellite flies during the time it illuminates a point on the ground with its actual antenna becomes, in essence, the size of a virtual antenna: an appropriately large "synthetic aperture." Now the orbiting radar can scan the ground – at an inclined angle, to distinguish objects at different distances – recording many complete reflections together with precise temporal and spatial details. Such data, downlinked to a ground station and transferred to a computer center, will be the primary input for the intensive signal processing needed to produce two-dimensional images and bring out features including surface roughness. The synthetic aperture is like a lens that can only be brought into focus by algorithms running inside the computer. But with very good algorithms, that virtual lens can be focused with almost arbitrary resolution. This is a key strength of TerraSAR-X and TanDEM-X, according to TUM Professor Richard Bamler, who also heads the Remote Sensing Technology Institute at DLR: “Every bit of the raw data from these satellites runs through algorithms developed here by DLR and TUM scientists, because we want to make sure the quality of the images is optimal and quality controlled. No one else in the world has developed such a processing chain.”

After processing, data captured by TSX during the three years it orbited alone showed just how good one such eye in the sky can be. Resolution can be comparable to the best optical satellite imagery, with advantages including independence from weather conditions, global coverage every 11 days, and consistent quality. TerraSAR-X demonstrated resolution as high as 0.25 m × 0.5 m, together with geometric location accuracy as high as 1 to 2 cm, which is comparable to the best GPS technology.

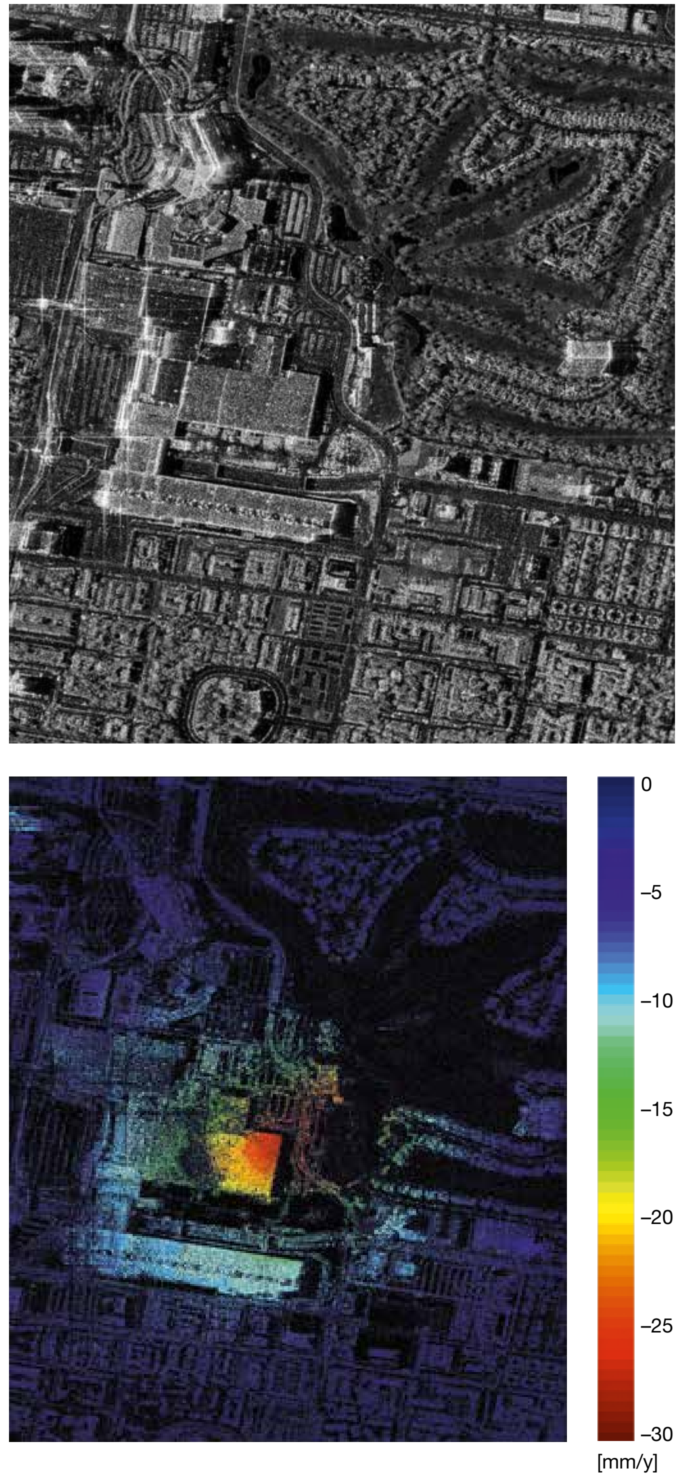
Once TDX joined TSX in space, they began to operate together as an even more powerful instrument: a SAR interferometer. “This is where we get something like a stereo view,” explains Prof. Michael Eineder, a department head in the DLR Earth Observation Center. “But unlike with optical stereo camera arrangements, we determine the 3-D position of a point by tiny differences in distance to the two SAR satellites. These differences are measured by finding the relative phase shifts of the two received wave packages. A map of these phase differences is called an interferogram. In X-band, an interferometric phase of 360 degrees corresponds to a wavelength of 31 mm.”

Fine tuning required

On a global scale, TanDEM-X has delivered 12-meter resolution for surface areas and height resolution of 2 meters. Considerable fine tuning was required to achieve this with the first-ever tight formation flight for stereo radar, while also dealing with an assortment of technical challenges.

Sometimes TSX and TDX fly parallel to each other, sometimes more or less in single file, depending on what kind of scanning is desired. Imaging can be done along or across the flight track, and in modes ranging from broad scans to a “spotlight.” Regardless of the flying formation or imaging mode, in TanDEM-X only one of the satellites is transmitting a radar signal while both are receiving and recording the reflections. Since differences between arrival times recorded for the two satellites will form the basis of the images – affecting every subsequent step in processing and analysis – a number of measures were designed-in or developed to account precisely for timing and position.

For example, a dedicated radio link between TSX and TDX is used to monitor any frequency difference in the two independent oscillators that “keep time” for their radars. This allows interferometric phase correction during processing on the ground to an accuracy of about 1 degree. Also, GPS and other means are employed to determine the relative posi- ▷



Monitoring subsidence: The top image is a TerraSAR-X view of Las Vegas Convention Center and an adjacent golf course. The bottom image shows ground subsidence of up to 3 centimeters per year caused by withdrawal of ground water near the Convention Center between 2009 and 2010. Radar interferometry is used to measure many subsidence phenomena, e.g. in former mining areas or the effects of gas extraction, oil pumping or subway construction.

Picture credits: DLR

“Every bit of the raw data from these satellites runs through algorithms developed here by DLR and TUM scientists.”

Richard Bamler

Richard Bamler and Michael Eineder

Teaming up for TanDEM-X

Richard Bamler (top) studied electrical engineering and communication theory at TUM, completing his doctoral work and habilitation here in the 1980s. He joined the German Remote Sensing Data Center (DFD) in 1989, where he was responsible for the development of signal processing algorithms as well as enabling technologies for synthetic aperture radar and atmospheric sounding. In the mid-1990s he spent time at NASA’s Jet Propulsion Laboratory as a visiting scientist and at the University of Innsbruck as a guest professor. Bamler served as co-director of the German Remote Sensing Data Center at the German Aerospace Center (DLR) from 1998 to 2000 and established the DLR Remote Sensing Technology Institute (IMF). As director of that institute, part of DLR’s Earth Observation Center, he is responsible for around 150 scientists and engineers working in a wide range of fields. At the same time, Bamler is a professor at TUM’s Department of Civil, Geo and Environmental Engineering, where he has headed the Chair for Remote Sensing Technology since 2003.

Upon receiving his diploma degree in electrical engineering and telecommunication science from TUM in 1990, Michael Eineder (right) joined the German Aerospace Center (DLR) to develop synthetic aperture radar (SAR) signal-processing algorithms for the SIR-C/X-SAR radar mission with NASA. While maintaining his affiliation with DLR, he completed his doctoral work at the University of Innsbruck in 2004. In 2013 he was appointed Honorary Professor at TUM. As a department head in the DLR Earth Observation Center, he leads algorithmic research and development of processing software for satellite missions that exploit synthetic aperture radar and SAR interferometry. One of Eineder’s current efforts focuses on expanding collaboration between the space agency and researchers in various disciplines of the geosciences.

Picture credits: ediundsepp

tions of the satellites – to within 1 millimeter. The distance between any point on the surface and TSX is minutely different from its distance to TDX, and obtaining accurate height measurements globally depends on precisely recording these distances in the first place. Given the extremely small baseline between satellites compared to the 500-some kilometers between the satellites and the ground, errors and uncertainties could otherwise be greatly magnified.
Further adjustments and processing steps of a more mathematical nature – such as phase unwrapping, atmospheric delay compensation, and geocoding – address unavoidable physical and technical artifacts in the data. Many of these essential algorithms have been developed by a joint team at TUM and DLR headed by Profs. Bamler and Eineder. They guarantee the world-leading accuracy and performance of the mission.

Erasing borders, pushing boundaries

TanDEM-X provides a geometrical basis for harmonizing all kinds of remote sensing data. This is information you can build on, literally, as it is needed for the planning of large construction projects, new rail lines, and the like. The new global DEM enables timely updating of existing maps and vastly more reliable mapping of poorly studied or inaccessible regions, including parts of Africa, Asia, and of course Antarctica.
In addition to producing the first seamless, borderless, high-resolution digital elevation model on a global scale – the primary mission goal – TanDEM-X is also enabling a wide range of scientific studies. Researchers at TUM and DLR are pushing the limits by generating even more accurate DEMs on local scales, and they are testing the feasibility of applications based on new interferometry and SAR techniques. A few striking examples illustrate the potential for monitoring Earth systems and our built environment. One doctoral candidate observed the growth of rice crops with decimeter accuracy. Another candidate is determining the ice loss of glaciers all over the world.
Within the TerraSAR-X mission alone, researchers demonstrated the possibility of precisely measuring changes in the land, whether due to tectonic, environmental, or human activity. A joint DLR/TUM research group sponsored by the German Helmholtz Association developed a new method called imaging geodesy. This method allows for centimeter-accuracy measurements from space, comparable to the capability of GPS receivers on the ground but without the need for such expensive devices. Using imaging geodesy, available maps and optical satellite imagery can be geometrically pin-pointed to the centimeter level – for example, to support self-driving cars with precision maps and landmarks.
Another experiment targeted remote monitoring of critical but relatively inaccessible infrastructure. This test focused on checking the structural integrity of an offshore platform, anchored to the sea floor and subject to tremendous forces, that houses AC-to-DC conversion equipment for a wind farm. Other DLR researchers use SAR to investigate parts of the Earth that are hardly accessible even via remote sensing, such as the polar regions and the oceans. They have charted the velocity of glacier flows in Antarctica, and the paths of drifting icebergs that could threaten shipping. By analyzing surface wave patterns in the ocean, they were able to produce bathymetric profiles of coastal areas where changes can occur relatively quickly, offering an alternative to time-consuming and expensive sonar surveys. Also proven was the power of SAR to clearly map the extent and mark the edges of an oil slick on the ocean, based on the contrast between oil-smoothed waters and the normal surface roughness. The same technology could help identify which ship spilled the oil, using specialized algorithms that fingerprint vessels according to structural features and their characteristic wakes.
By exploiting the interferometric phase of multi-temporal SAR images, researchers can measure slight geometric changes of Earth's surface and of urban infrastructure, on the millimeter scale and below. Studies have documented seasonal deformation in buildings and bridges, which swell slightly in warmer months and contract in winter, as well as one-time changes such as the compaction of recently completed steel-and-concrete skyscrapers.
A strong impetus for future missions comes from what TerraSAR-X and TanDEM-X have enabled scientists to see in relation to important areas of the Earth sciences: climate change impacts reflected in melting ice or altered ocean currents; the slight heaving of a volcano that hints at a coming eruption; ground deformations that show how a recent earthquake has rearranged the land; signs of potential hazards from flooding or landslides. This approach has also been successfully tested to characterize forests in different parts of the world, to measure the heights of the trees, and to chart the path of deforestation.
To do this even better, DLR and TUM researchers have proposed a future satellite mission – again using SAR interferometry with a pair of satellites orbiting in close formation, but equipped with larger antennas, L-band radars, and other technical innovations tested or inspired by TanDEM-X. The wave band is key. While the present missions have had some success with 3-D imaging of vegetation, most of the X-band signal reflects off the canopy. In the L band, with a central wavelength around 24 cm, all levels of a forest are illuminated, from the treetops to the ground. The technology and operational plans for the envisioned mission, named Tandem-L, are optimized for observing dynamic processes on Earth's surface: in the biosphere, geosphere, cryosphere, and hydrosphere. With this, Tandem-L is expected to achieve new heights in mapping, observing, and monitoring our living planet.

Patrick Regan

Neutrons Reveal the Secrets of Superconductivity

Thirty years into the investigation and the theory still has gaps – researchers worldwide are still attempting to fathom why some materials suddenly become superconductive at specific temperatures. The PUMA and PANDA experiments at the FRMII research neutron source are among the best in the world for investigating certain aspects of the phenomenon. There, scientists have spent the last ten years or so piecing together the picture.

Link
www.mlz-garching.de

Superconductors are crystalline solids with complex lattice structures. Especially high-temperature superconductivity is not yet fully understood. Neutron beam experiments at Heinz Maier-Leibnitz Zentrum (MLZ) in Garching shed light on the phenomenon.

Graphics: ediundsepp

Spin waves seem to be one key to the phenomenon of high temperature superconductivity. They can be measured by means of neutron scattering. The PUMA and PANDA experiments beam neutrons from one side into the crystal and measure how many are scattered by the electron spins and at what angles.

Brigitte Röthlein

Spinwellen als Auslöser für Supraleitung?

Seit vor 30 Jahren Materialien entdeckt wurden, die bei weit höheren Temperaturen supraleitend werden als die bis dahin bekannten Substanzen, versuchen Forscher die Mechanismen zu verstehen, die hinter diesem Verhalten stecken. Die Hoffnung ist, nicht nur endlich eine konsistente Theorie zu finden, sondern auch, weitere Stoffe zu entwickeln, die im besten Falle sogar bei Zimmertemperatur supraleitend werden. Die bisher gültige Theorie, die aber nur konventionelle Supraleiter erklären kann, geht davon aus, dass Gitterschwingungen – Phononen – im Kristall zur Bildung sogenannter Cooper-Paare beitragen, die den verlustfreien Stromtransport bewirken. Dies gilt aber nicht in Bezug auf die neu entdeckten Substanzen.

Da sich in den letzten Jahren herausstellte, dass bei den Hochtemperatur-Supraleitern magnetische Vorgänge im Inneren des Kristalls eine große Rolle spielen, hat sich Neutronenstreuung als das Forschungswerkzeug der Wahl etabliert. Dr. Astrid Schneidewind und Dr. Jitae Park betreuen am Heinz Maier-Leibnitz-Zentrum (MLZ) in Garching die beiden Spektrometer PANDA und PUMA, die als die weltbesten Instrumente ihrer Art gelten. „Neutronen sind elektrisch neutral und können deshalb ins Innere von Kristallen eindringen, haben aber gleichzeitig ein magnetisches Moment, das heißt, sie können an den Elektronen gestreut werden, die ebenfalls magnetische Dipole sind“, sagt Park. Damit lassen sich magnetische Strukturen im Inneren des Kristalls aufklären. Wissenschaftler aus aller Welt kommen seit Jahren ans MLZ und bestrahlen supraleitende Materialien mit den Neutronen aus dem Hochflussreaktor FRM II.

Unter der Mithilfe von Schneidewind und Park sind so inzwischen von Forschern aus der ganzen Welt eine Reihe von Puzzlesteinen gefunden worden, die zu einer kompletten Theorie der Supraleitung beitragen können. Vieles deutet darauf hin, dass dabei Spinwellen eine entscheidende Rolle spielen könnten. □

„Der Traum ist, Supraleiter zu entwickeln, die sogar bei Zimmertemperatur – also ohne aufwändige Kühlung – funktionieren. Aber bis dahin ist noch ein weiter Weg.“

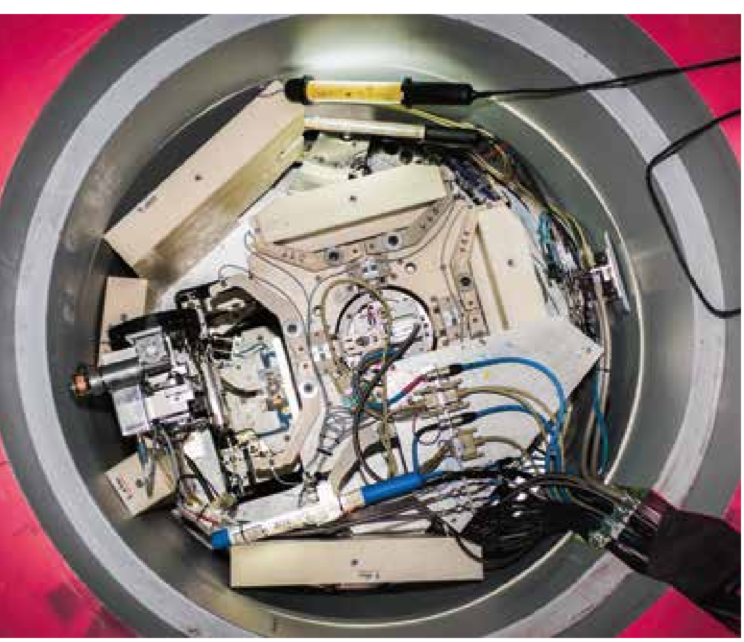
Jitae Park

Rarely are theory, basic physical research and practical applications so closely linked as in the case of superconductivity. If it were possible to explain the physical mechanisms that cause some compounds with complex crystal lattice structures to lose all electrical resistance at a particular critical temperature, we could then set about optimizing this superconductive capability or even identifying completely new contenders. “The dream is to develop superconductors that even work at room temperature – so no need for resource-intensive cooling,” explains Dr. Jitae Park, who is researching superconductivity alongside his colleague Dr. Astrid Schneidewind at the Heinz Maier-Leibnitz Zentrum (MLZ) in Garching, “but we have a long way to go.”

In 1911, Dutch physicist Heike Kammerlingh-Onnes encountered a strange phenomenon that he was unable to explain: if he cooled mercury to below – 269 degrees Celsius, its electrical resistance would drop abruptly to zero and it would conduct electric current without any losses. This discovery was known as superconductivity. Gradually, scientists established that around a dozen elements and well over a hundred alloys display similar behavior. However, the so-called critical temperature below which superconductivity takes place was always only a few degrees above absolute zero, which corresponds to around – 273 degrees Celsius. This is expressed as 0 kelvin and corresponds to the point at which all thermal motion of atoms and molecules stops.

Since the temperature required to induce superconductivity is so very low, liquid helium was required to cool the materials.

Astrid Schneidewind mounts a high temperature superconductor sample for the neuton scattering experiment. During the measurement itself, the sample is positioned in a cryostat and people are not allowed near the experiment.

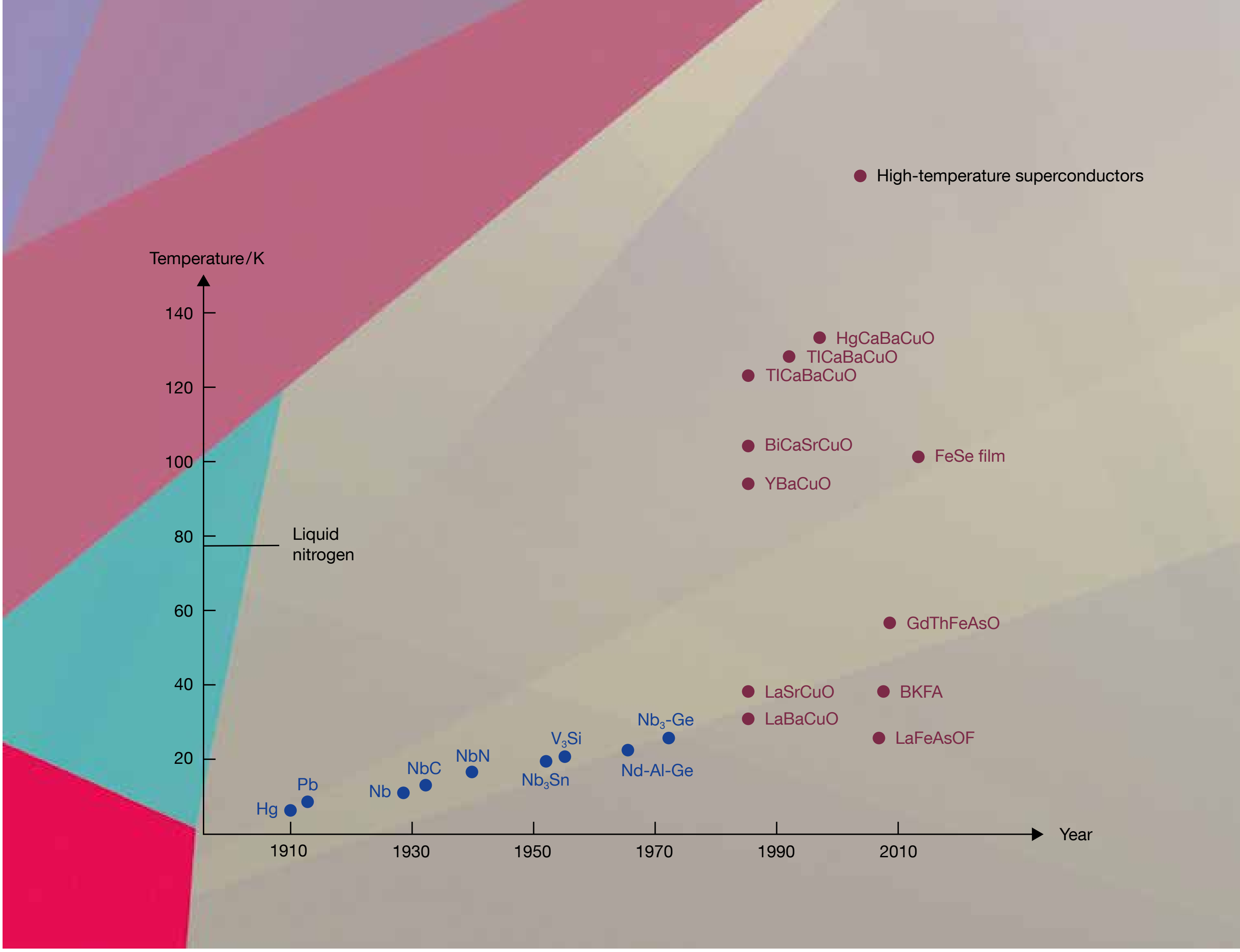


A look inside the monochromator. It offers four monochromators which allow the scientists to select neutrons with certain energy levels for the experiment.

The huge effort involved in supplying this gas meant that just a few practical applications were viable – such as superconducting coils to generate extremely strong magnetic fields for accelerator experiments, fusion devices and magnetic resonance imaging (MRI). And for many people, that was the extent of the superconductivity story.

Fresh discoveries widen horizons

It thus caused quite a stir when Swiss and German scientists K. Alexander Müller and J. Georg Bednorz made their announcement at a New York meeting of the American Physical Society in March 1987: they had discovered a material the year before that became superconductive at the relatively high temperature of 35 kelvin. This was the ceramic material lanthanum barium copper oxide (LBCO), which possesses a complex crystal lattice structure and belongs to the cuprate family. The two researchers were awarded the 1987 Nobel Prize in Physics for this breakthrough. This then opened up a new area of research, yielding a raft of new materials with ever-higher critical temperatures. These high-temperature superconductors (HTS) paved the way for totally new



Superconductivity was first discovered in 1911. For decades, all materials found had to be cooled with liquid helium to temperatures just above −273 Celsius, or absolute zero, to trigger superconductivity. Finally, in 1987 the first material was discovered that became superconductive at the relatively high temperature of 35 kelvin.

Picture credits: Filser, Graphics: ediundsepp (source: Keimer PIUZ 201291297 / TUM)

technical possibilities, inspiring utopian visions among engineers. They predicted a revolution in the transfer of energy if they could successfully transport electricity across long distances without losses and with no need for cooling. A pilot project has been running in the German city of Essen since 2014, with one kilometer of superconductive high-voltage cable spanning the distance between two substations, cooled only by liquid nitrogen – which requires a lot less effort than cooling with helium. In the telecommunications sector, too, HTS could play an important role: superconductive components could increase technical performance by enabling component miniaturization, reducing interference and thus dramatically improving transmission quality. Scientists assumed that if they could just work out how these high-temperature superconductors actually work, it should be possible to produce even better ones. But that is proving to be a lot more difficult than it sounds – even today, there is still no generally applicable theory that explains their behavior. The quantum mechanical theory proposed by US researchers John Bardeen, Leon Cooper and Robert Schrieffer towards the end of the 1950s was a significant milestone, explaining the mechanism underlying conventional superconductivity. Known by the initials of its three authors, this BCS theory gained them a Nobel Prize in 1972.

The BCS theory postulates that the electrons in a superconductor form Cooper pairs, which – unlike single electrons – do not collide with one another or interact with the conducting crystal or its defects, thus impeding scattering. They thus experience no resistance as they travel. The fact that electrons, which of course are negatively charged, are able to form pairs without repelling each other in the first place is attributable to a quantum mechanical effect that only arises in solid-state bodies – specifically crystals – and is caused by lattice vibrations (phonons).

The mysterious role of magnetism

The BCS theory may provide an adequate explanation for the processes in conventional superconductors, but it falls rather short when it comes to high-temperature superconductivity. One of the sticking points is behavior in the presence of magnetism. While normal impurity in the crystal lattice has virtually no effect on the conducting state, this ▷

“PANDA and PUMA are among the world’s best instruments in their field.”

Jitae Park on the reserach environment at MLZ

state is extremely sensitive to foreign atoms, which behave like tiny magnets and are known as dipoles. A small percentage of these atoms distributed in the crystal lattice is enough to suppress conventional superconductivity altogether in standard metals and alloys.
The story is very different when it comes to high-temperature superconductors. Here, researchers have discovered that they can even promote superconductive effects by doping magnetic materials in such a way that they partially lose their magnetism. The assumption today is therefore that the Cooper pairs – which are demonstrably also present in high-temperature superconductors – are held together not by phonons but by spin waves. These magnetic phenomena occur in crystals and are caused by the electromagnetic moment of electrons, known as spin. Many scientists view these spin waves as one of the keys to understanding the mechanism of high-temperature superconductivity. But how can we measure these spin waves? “Neutrons are a particularly good tool for this,” reveals Jitae Park. “They are electrically neutral and can thus penetrate the interior of crystals. At the same time, they have a magnetic moment, meaning that they can be scattered by the electrons that also possess magnetic dipole fields.” This sheds light on magnetic structures in the interior of the crystal.
Small wonder, then, that so many research groups from all over the world have made their way to the MLZ over the past few years, keen to irradiate all manner of exotic crystals with neutrons. The PUMA and PANDA experiments in particular are ideally suited to this type of investigation. Each of these involves beaming neutrons in from one side and counting how many of them are scattered by the electron spins in the crystal and at what angles. The amount of energy lost by each neutron in this process is also resolved. The models that emerge from these days or even weeks of measurements then enable the physicists to draw conclusions about the processes inside the crystals. Schneidewind and Park are on hand to advise and assist them in this endeavor, since it takes a great deal of experience to correctly assign and interpret the numerous measurements obtained.
Astrid Schneidewind, who has been looking after the PANDA spectrometer since 2004, talks about her “60 ton giant” with evident affection and emphasizes the importance of an experienced team that is familiar with every nut and bolt and knows what to tweak and where for any given outcome. Her young Korean colleague, Jitae Park, has been working in this field since his doctorate and has also become an internationally acknowledged expert in performing and interpreting such investigations at the MLZ, especially with PUMA. “We have made many discoveries over the ▷

Dr. Astrid Schneidewind and Dr. Jitae Park

Research groups come from all over the world to use their instruments

Two career paths that could hardly be more different have ultimately converged in superconductivity research roles at the MLZ. Dr. Astrid Schneidewind began her career at Technische Universität Dresden, where she initially focused on low temperature physics, having always been drawn to research “off the beaten track.” However, the turmoil surrounding German reunification meant she was unable to finish her doctorate. “The wall coming down threw a major spanner in the works, with only half of all positions staffed again afterwards.” She was also expecting the first of her two daughters at the time, so decided to focus on her family for the time being. Four years later she then returned to her old institute, essentially to undertake a second doctorate – which she successfully completed this time. “Doing another doctorate so late has kept me young,” reflects the 51-year-old physicist. “It’s meant I’ve almost always worked with colleagues at least ten years my junior.”
So Schneidewind was unperturbed when she finally arrived at the MLZ after her move to Munich and often found herself working with university graduates. “I see myself in an advising and supporting role where younger people are concerned,” she says. “I’m aware that I can contribute a lot of life experience that others have yet to gain.” She also has a very relaxed relationship with her 34-year-old colleague, Jitae Park.

Park, for his part, was already cultivating an interest in neutron scattering during his studies in Seoul. He therefore decided to pursue his doctorate at the Max Planck Institute for Solid State Research in Stuttgart, where he became interested in superconductivity. His two children were thus born in the heart of Germany’s Swabia region, meaning that his daughter “initially learnt Swabian dialect at kindergarten, while my son tends more towards Bavarian as a result of moving to Munich.” Both children now speak a mixture of German and Korean. Park’s wife also comes from Korea and hopes to resume her training as a fashion designer shortly.
Both Astrid Schneidewind and Jitae Park particularly value the outstanding research environment Munich has to offer. “PANDA and PUMA are among the world’s best instruments in their field,” declares Park – who would, however, also be ready to move elsewhere if conditions were even better. His colleague, though, now takes a more laid-back approach – she is happily settled in the north of Munich, having found a good balance between research, team work, administration and family life. And she doesn’t mind being on call in the evenings or at the weekends, which sometimes means hurrying back into work to rescue a baffled researcher.

Picture credits: Filser

Calls her PANDA experiment a “60 ton giant” with a touch of affection: Astrid Schneidewind and her team know every nut and bolt in their baby and know what to tweak to answer any question a scientist might have.

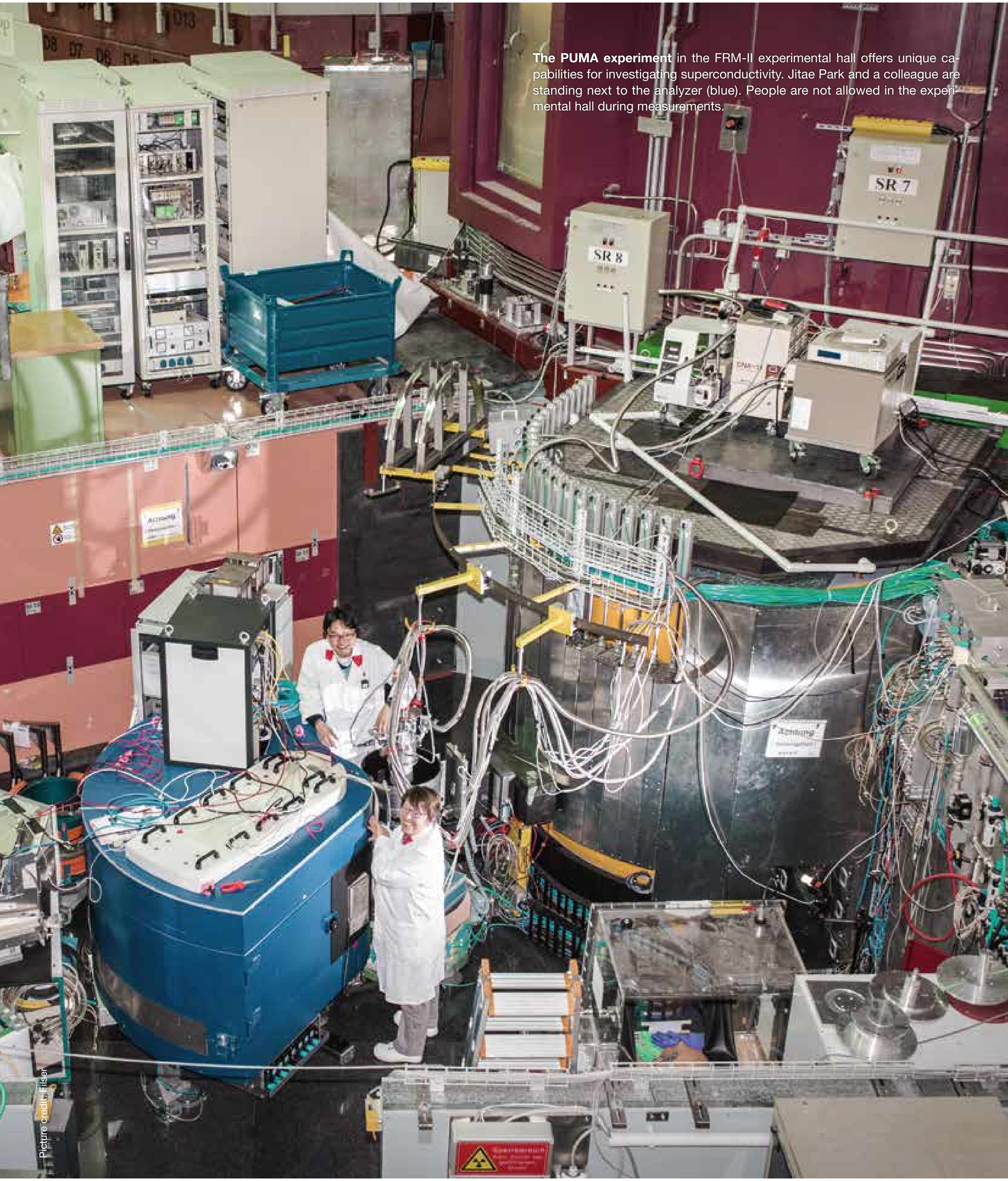
past few years, including specific energy loss patterns with the neutrons," he reports. "This is known as resonant mode and points to the formation of Cooper pairs." The assumption by both experimental and theoretical physicists is that spin waves play a crucial role in this. "All the materials we investigate here exhibit this type of resonance but we still don't have a precise explanation for it yet – unfortunately nature is just not that straightforward!"

Alongside their services at the MLZ, both scientists are also pursuing their own research interests. Crystal doping is high among them. Whether or not superconductivity can be induced at various temperatures depends on how many excess electrons or distortions the crystal contains. However, they are still some way from explaining this. "We are investigating three different types of material: cuprates, iron-based superconductors and heavy fermions," explains Astrid Schneidewind. "Our aim is to identify a pattern that applies to all three

"We are investigating three different types of material: cuprates, iron-based superconductors and heavy fermions. Our aim is to identify a pattern that applies to all three so we can finally find out how they work."

Astrid Schneidewind

so we can finally find out how they work." The latest measurements suggest that a transition in wave function symmetries might be a condition for the formation of Cooper pairs. "This might hold the key," muses Jitae Park. At just 34 years of age, there is a good chance that he will see the solution to this puzzle in the course of his active research career. Perhaps he himself will play a pivotal role. *Brigitte Röthlein*



The PUMA experiment in the FRM-II experimental hall offers unique capabilities for investigating superconductivity. Jitae Park and a colleague are standing next to the analyzer (blue). People are not allowed in the experimental hall during measurements.

Picture credit: Filser

Catalysis Research at TUM

Catalysis is a key technology, not only in the value generating, efficient conversion of raw materials, but also in transformation of our energy systems. To meet all these challenges, industrial societies need new catalysts and catalytic processes. TUM has always prioritized catalysis research, particularly within its Department of Chemistry. The TUM Catalysis Research Center is now taking this commitment to the next level. The new research building will provide an overarching framework for a coherent research concept, building on basic research to develop catalytic innovations but also turn these results into technical concepts in collaboration with industry partners.

Catalysis I

Small in Size, Big in Impact

Prof. Ulrich Heiz builds nanocatalysts atom by atom. His objective is to produce customized catalysts for the widest range of applications.

Catalysis II

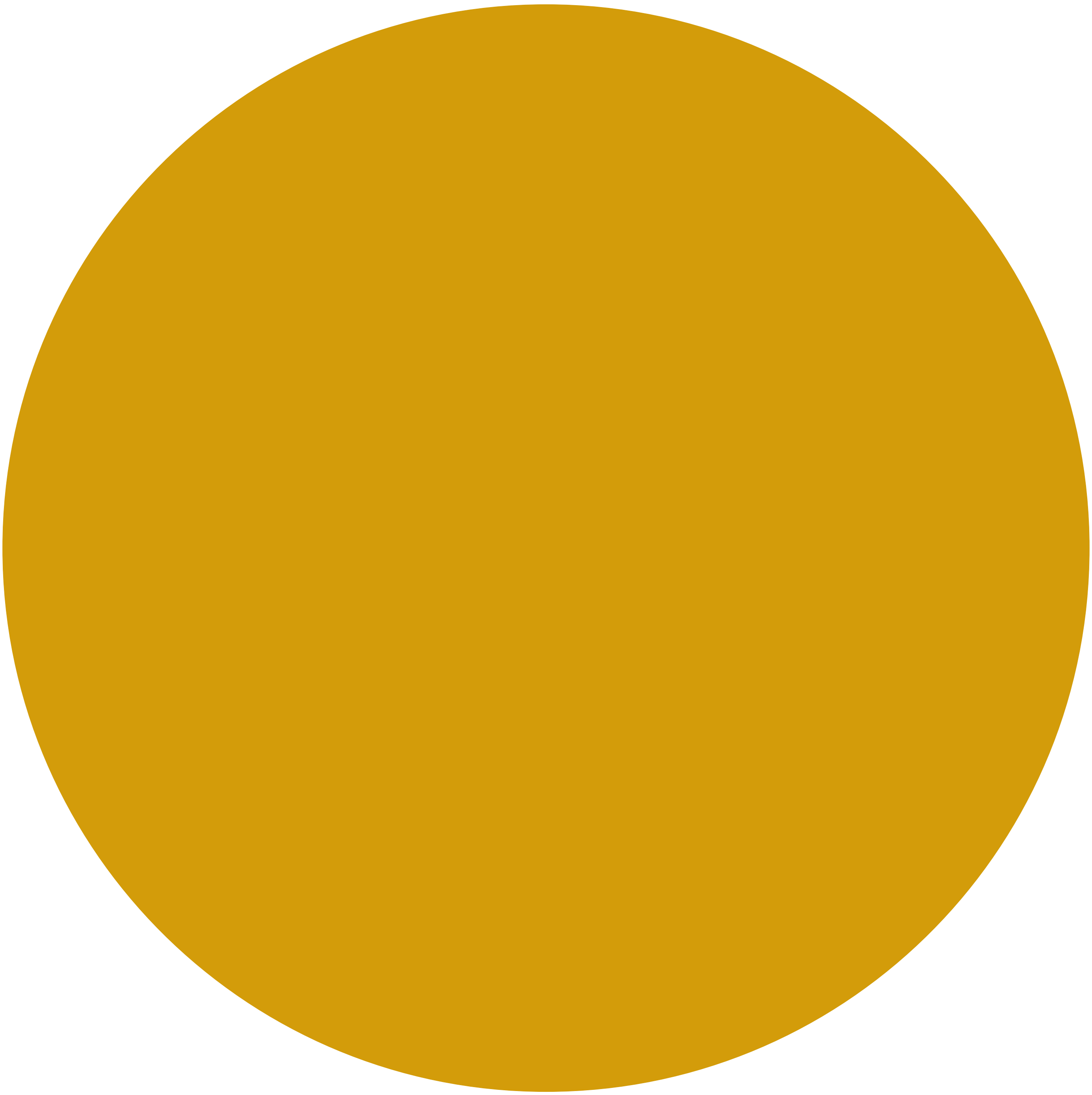
Millions at my Beck and Call!

Prof. Thorsten Bach combines photochemistry and catalysis. His aim: Using light as a natural energy source and suitable catalysts for the efficient and selective production of certain substances.

Picture credits: Jooss, Graphics: ediundsepp

Small in Size, **Big in Impact**

If you take a well-known material – gold for example – and reduce it to the size of just a few atoms, it suddenly becomes something quite different. This inert precious metal is now a catalyst which reacts with other molecules, thus accelerating chemical reactions. Prof. Ulrich Heiz builds nanocatalysts like this atom by atom. His objective is to produce customized catalysts for the widest range of applications.



Graphics: ediundsepp

Gold has long been considered totally unsuitable for catalytic reactions because it is chemically inert in the solid state and therefore highly inactive.

Birgit Fenzel

Winzlinge mit Potential

Auf den zweiten Blick sehen Dinge gelegentlich ganz anders aus. Der Chemiker Ulrich Heiz, Lehrstuhlinhaber für Physikalische Chemie der TUM, ist so einer, der genauer hinsieht. Sein Forschungsgebiet liegt im Nano- und Subnanobereich. Mit eigens dafür entwickelten Techniken und Messmethoden zerlegt er dazu mit seinen Mitarbeitern ausgewählte Elemente in ihre Einzelbausteine, um sie dann wieder Atom für Atom zusammenzusetzen und zu untersuchen. Sein Ziel ist es, maßgeschneiderte Katalysatoren für chemische Reaktionen zu entwickeln, um diese schneller, günstiger oder überhaupt erst möglich zu machen.
Von seinen Expeditionen ins Reich der Zwerge verspricht er sich, an alten Bekannten neue Materialeigenschaften zu entdecken. Denn wie er inzwischen vielfach beobachtet hat, halten sich die Zwerge nicht unbedingt an die Regeln der Makrowelt. Zum Beispiel gilt das Paradigma der Größenunabhängigkeit bestimmter Reaktionen dort nur bis zu einem gewissen Punkt. Je kleiner die Oberfläche, desto geringer ist chemische Reaktivität – dieser eigentlich logische Lehrsatz der Chemie wird ab einer Anzahl von Clustern unter 100 Atomen zu Makulatur. Darunter beginnt der nicht skalierbare Bereich, in dem sich Eigenschaften eines Materials und Größe nicht mehr in einer linearen Funktion befinden und auch nicht mehr vom Festkörper abzuleiten sind. Zum Beispiel zeigt Gold, das lange Zeit wegen seiner chemisch inerten Materialeigenschaften als denkbar ungeeigneter Katalysator-Kandidat galt, in diesem Bereich plötzlich glänzende Katalysatoreigenschaften.
Inzwischen hat Heiz mit seinem Team verschiedene Verfahren entwickelt, um die kleinen Cluster auf unterschiedlichen Trägermaterialien fixieren und untersuchen zu können. Denn wie sie bei ihren Experimenten auch herausgefunden haben, gibt es elektronische Wechselwirkungen zwischen Trägermaterial und Cluster, die die Katalyse beeinflussen können. Zusammen mit der Größe haben sie damit ein weiteres Instrument für das Design ihrer maßgeschneiderten Clusterkatalysatoren gefunden, an dessen Verfeinerung sie derzeit arbeiten.
Ab Mai dieses Jahres wird Heiz seine Arbeit in dem neuen Katalysezentrum am TUM-Campus in Garching fortsetzen, dessen akademischer Direktor er auch ist. „Zentrales Ziel ist dabei die Entwicklung von Clusterkatalysatoren, mit denen wir Kohlendioxid reduzieren oder idealerweise in etwas Sinnvolles umwandeln können“, beschreibt er den Fokus seiner künftigen Forschung, von deren Erfolg für ihn viel abhängt. „Da müssen wir in den nächsten Jahren den Durchbruch schaffen, sonst wird es kritisch.“ □

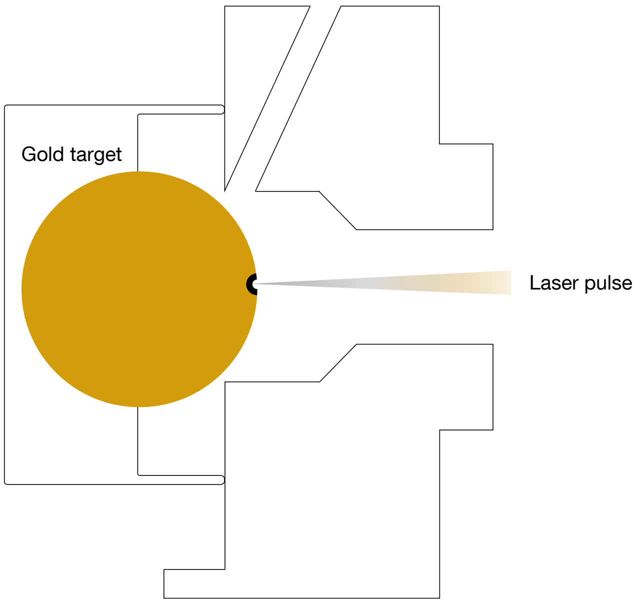
„Wir wollen die neuen Eigenschaften der Materie, die im Nano- und Subnanobereich auftreten, aufzeigen und neue Katalysatoren finden.“

Ulrich Heiz

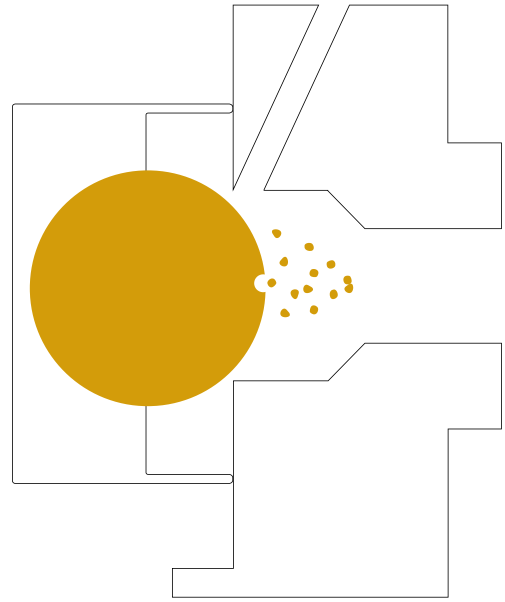
Link
www.pc.ch.tum.de

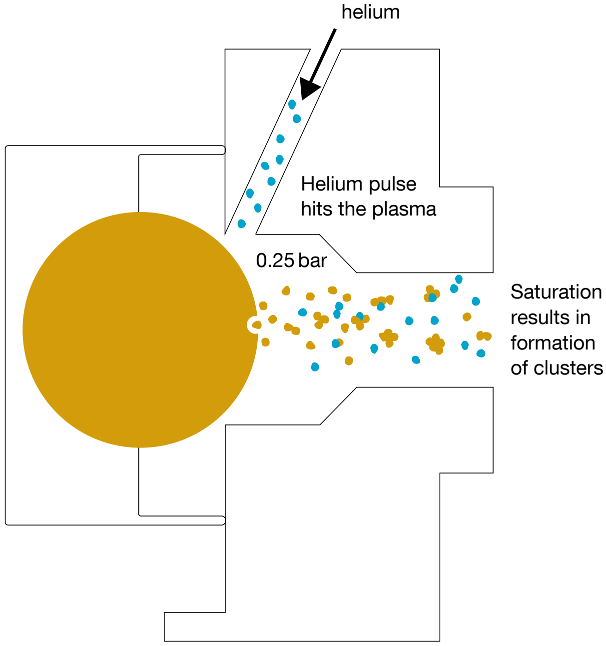
In a size range of
eight to 20 atoms,
gold exhibits excellent
catalytic properties.

Graphics: ediundsepp

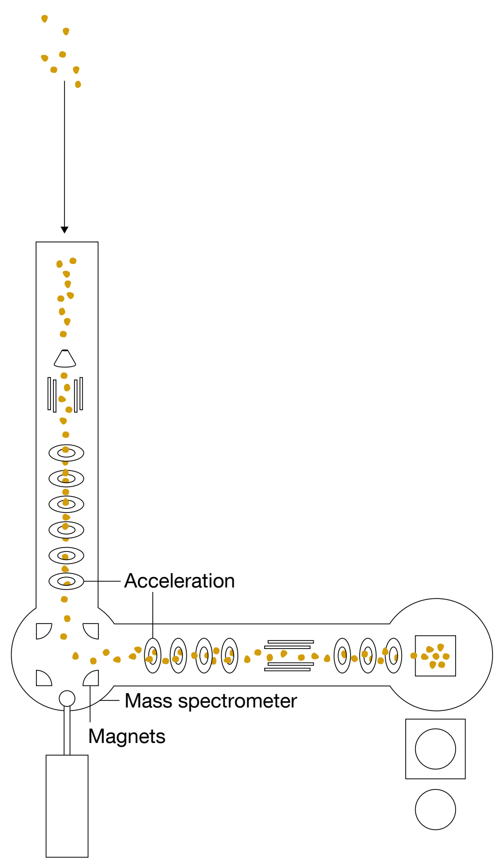


Laser pulse heats target


Plasma exits heated target



Plasma cools due to helium
and expansion into vacuum



How to produce nanoclusters: A laser pulse heats a target and vaporizes some nanograms of material. The resulting plasma is cooled through both a helium gas pulse and expansion into the vacuum of a thermolization chamber. The atoms aggregate into clusters; the size distribution can be varied by setting different parameters. A mass spectrometer is used to select a cluster of a precise number of atoms from the distribution generated by the cluster source.

In times past, alchemists attempted to turn base metals like lead or mercury into gold and other precious metals. Today, scientists at TUM are taking a different approach. For over two decades, Ulrich Heiz and his staff at the Chair of Physical Chemistry have been experimenting with metal clusters. Unlike the earlier alchemists, however, they are not looking to transmutate matter, but rather to nanostructure metals so that their physical and chemical properties can be controlled. So instead of transforming one chemical element into another by changing its atoms, Heiz controls the material properties of his clusters specifically by changing their size. Unreactive metals can suddenly become catalysts and trigger specific chemical transformation processes.

Heiz specializes in heterogeneous catalysis, in other words, catalysis in different chemical phases, on the nano and sub-nano scale. That is where he sees the “philosopher’s stone”. When asked what inspires and drives his work, he says: “Our aim is to demonstrate the new material properties that emerge on this scale and use those insights to discover new catalysts”. It’s a bit like putting Lego bricks together.

Through his basic research, the chemical scientist is thus shedding light on an area that was previously more or less in the dark due to the lack of suitable methods. When it comes to applications, too, his research into the nano universe holds huge potential. Catalytic processes are of major importance in nearly all branches of industry. “More than 90 percent of all industrially manufactured compounds undergo at least one, and sometimes several, catalytic reactions during their synthesis,” he explains. His work may also help provide much-needed answers to the main challenges facing modern society – the need to conserve resources and use them efficiently, protect our climate and store energy.

Size matters

Heiz and his colleagues focus on just one element at a time when they venture into the nano and sub-nano realm. “Basically, you get a big cluster of a precious metal and make it smaller and smaller,” is how he describes his method. This increases the ratio between the number of atoms on the surface and the atoms within the metal. “This is important, because the surface atoms are the ones that catalyze the reactions,” he explains. “The smaller we make the clusters, the more precious metal atoms we have to trigger the catalysis. Initially, however, no new effects can be observed relative to the large cluster. Activity initially scales with size. But this no longer necessarily applies once you get to very small clusters with fewer than a hundred atoms. And it is this non-scalable dimension in matter that interests us. We build clusters using a specific number of atoms – 2, 4, 6, anything up to 100 in fact – and see what happens.”

The atoms which the team under Ulrich Heiz in Garching uses to build their clusters are around 300 picometers in diameter – one picometer equals one trillionth of a meter. By comparison, nanotechnology is like playing with large Duplo building blocks. In other words, they are more than one order of magnitude larger. “We are doing pioneering work in this field,” declares Heiz. The controlled creation of nanocatalysts with a precisely defined number of atoms required new methods and techniques, and the further development and understanding of these techniques also form part of his research. “It’s not like you can hop out to the DIY store to pick up the equipment you need to make clusters,” comments his colleague Florian Schweinberger, research coordinator at the TUM Catalysis Research Center.

How do you build a cluster with just a few atoms?

A self-built cluster machine is positioned just a few steps from Heiz’s office. It includes a pulsed laser vaporization source, a system of electrostatically and radio frequency-driven ion optics, an analysis chamber for examining the properties of the clusters, various controls and sliders for changing the parameters, as well as a tangle of connecting cables and hoses. “With this machine, we can create clusters of a precise size and deposit them on a surface from the gas phase or else store them in a trap in the gas phase. We can then look at the properties of these size-specific clusters and measure them,” he explains. “That is what we specialize in.”

With each pulse of the laser, a few nanograms of the material are vaporized. This creates a plasma, a mixture of atoms, ions and electrons, which is cooled in the thermalization chamber through a helium gas pulse on the one hand and through expansion into the vacuum on the other. The atoms aggregate into clusters, the size distribution of which can be varied by changing the nozzle size, for example, or the pressure in the vacuum. Finally, the scientists use a mass spectrometer to select a cluster of a precise number of atoms from the distribution formed in the cluster source. ▷

Graphics: ediundsepp (source: TUM)

"Our aim is to demonstrate the new material properties that emerge on the nano and sub-nano scale and use those insights to discover new catalysts."

Ulrich Heiz

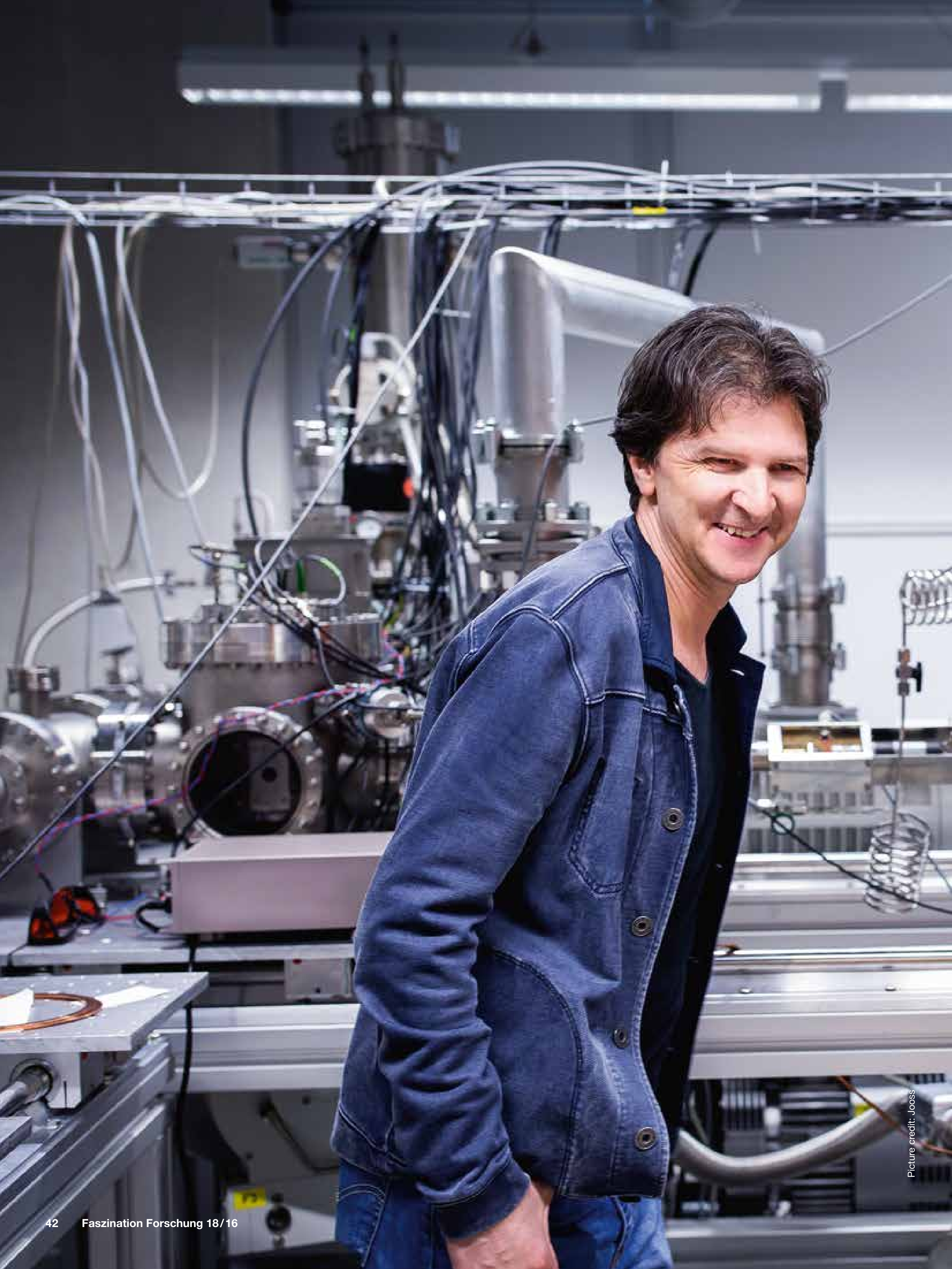
These experiments have shown that different rules apply in the nano realm than in the macro world of solids. Because of its specific properties, gold has long been considered totally unsuitable for catalytic reactions because it is chemically inert in the solid state and therefore highly inactive. In a size range of eight to 20 atoms, however, the normally highly inert precious metal suddenly revealed excellent catalytic properties. With this discovery, the Munich-based chemical scientists had found the smallest known active gold cluster comprising just eight atoms.

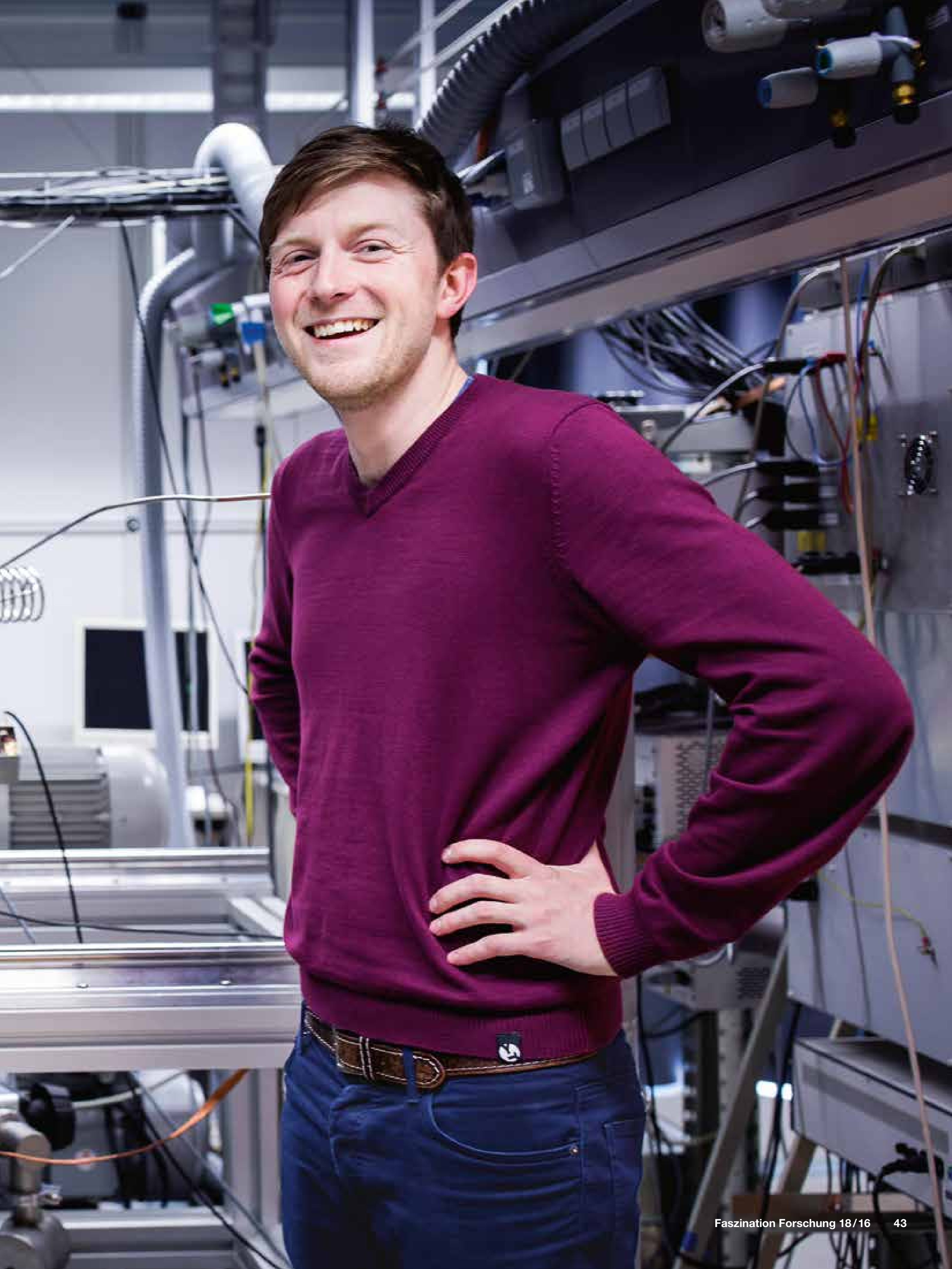
Platinum clusters challenge long-established assumptions

Experiments with platinum have recently shaken up long-established assumptions among scientists working in this field. "For a century or so, there has been an accepted differentiation between reactions that are influenced by the structure and size of the catalyst, and reactions where these two parameters play no role," relates Heiz. "We suspected, however, that this differentiation does not apply to catalyst particles at sub-nanometer scale." In order to find out for sure, he and his team have spent the past two years carrying out further experiments with ethene. This hydrocarbon was chosen because of its ability to react with hydrogen, known as hydrogenation; this reaction is regarded as a typical example of a size-independent reaction. For their experiments, the researchers used platinum catalysts with sizes ranging from one to 80 atoms. Their suspicions were confirmed when they allowed these particles to react with ethene and hydrogen. Clusters with fewer than ten atoms were barely active. Catalytic activity then increased in the presence of more than ten atoms, with maximum activity reached in clusters of 13 atoms. "We have thus provided further clear proof that decade-old theories claiming that size does not matter in this reaction are simply unfounded," maintains Heiz. His assumption now is that all kinds of materials have a turning point somewhere in the nano or sub-nano range from which a linear relationship no longer applies between size and physico-chemical properties. Because quantum size effects then come into play, the properties can no longer be predicted at this scale. "This shift from the scalable to the non-scalable range brings many new opportunities for basic research, but also for applied research," Heiz is convinced.

Theoretical proof of the experimental observations from the recent platinum studies has been provided by the team under physicist Uzi Landman at Georgia Institute of Technology in Atlanta. Landman is one of the world's foremost theorists in the field of nanoscience and a long-time collaborator of Ulrich Heiz in the search for new ways to control chemical reactions. "The fact that our systems are so precisely defined and transparent means that the theorists can accurately calculate and model our results," he comments. In their calculations and computer simulations, they were able to precisely demonstrate which atom is responsible for which activity and why. ▷

Picture credit: Jooss


Picture credit: Jooss



For the hydrogenation reaction of ethene in the presence of platinum, all of the negative charge from the oxide surface is stored in a single atom. All the other atoms keep their original charge. “It is clear that the arrangement of the atoms in the structure of the cluster also plays a role,” concludes Heiz. This is a highly interesting finding for the development of customized catalysts. “It means that we can change a property by adding an atom.”

Stabilizing the nanoclusters

However, the development of catalysts based on nanoclusters reveals a fundamental challenge, explain the Munich-based chemical scientists; it is specific to the process of nano-scaling itself. Tiny particles are unstable because the atoms on their surface are weaker bonded. And because they are only bonded to the substrate over a small area, they are prone to wander off and bond with the next-biggest particle. This phenomenon can be noticed in the corners of many a room. The dust bunnies that gather there are simply conglomerations of tiny dust particles that keep on gathering more dust. It’s the same idea at the nano scale, says chemical scientist Friedrich Esch, one of whose tasks as part of Heiz’s team is to find out how the particles can be stabilized. “It’s not just cluster migration that leads to a change in size distribution: the small clusters can also disintegrate through exchange processes. The smaller they are, the greater the likelihood of atoms vaporizing and exchanging between the clusters. This leads to ever bigger particles,” he explains. This process is known as Ostwald ripening, which was discovered at the beginning of the 20th century by the polymath and winner of the Nobel Prize in Chemistry Wilhelm Ostwald. “So for us, the big question was how can we prevent this process and keep our nanoparticles stable for longer,” Esch explains.

Along with Swedish colleagues from Chalmers University of Technology in Gothenburg, the scientists studied various methods to get their tiny particles under control. “This effect can be pretty well suppressed in clusters with exactly the same number of atoms even at high temperatures,” says Esch. So the scientists overcame the Ostwald ripening challenge by ensuring same-size clusters.

Meanwhile, the Munich team has developed various processes for attaching the small clusters to substrate materials so that they remain stable at high temperatures, are kept at a distance from each other and in each case have the same bonding location with specific properties. The choice of substrate ▷

Prof. Ulrich Heiz

Academic Director of the TUM Catalysis Research Center

Ulrich Heiz, born in 1960, studies the physical and chemical properties of matter at the nano and sub-nano scales. In this size range, the properties of particles are determined by the exact number of atoms they contain and are no longer scaled from the solid state. He considers his work to be a combination of basic and applied research. His discoveries so far lead him to believe that tiny particles hold the key to solving major challenges in the areas of environmental protection and clean sources of energy.

Chemistry did not figure at all in Heiz’s early career plans. In fact, the choice was between physics or medicine. He would most likely have made a good doctor – and even started down that road. After completing his school-leaving exam at Gymnasium Bern Neufeld, he stayed in his home city in Switzerland to study medicine at the University of Bern. After just a few semesters, however, Heiz realized that he was more attracted to the natural sciences. “It so happened that the medicinal chemistry lectures were the ones I enjoyed most,” he recalls. He quickly took up his new calling. In 1987, he completed his chemistry degree at the University of Bern and his doctorate in physical chemistry four years later. He quickly discovered his interest in the nano world of atoms. Even his Ph. D. supervisor Ernst Schumacher had previously conducted experiments with small clusters in the gas phase.

After his doctorate, Heiz spent time as a researcher at the laboratory of the Exxon Research and Engineering Company and at the University of Pittsburgh. In 1998, he completed his postdoctoral lecturing qualification at the University of Lausanne. After taking up various posts in Japan, Berlin and Ulm, he accepted the position of Chair of Physical Chemistry I at TUM in 2004. Ulrich Heiz is also Academic Director of the newly opened TUM Catalysis Research Center. He is married to a French teacher and the couple have one daughter. He likes to listen to jazz in his free time.

Picture credit: Jooss

material plays a decisive role here. It must have a suitable, highly ordered surface structure offering neither overly strong nor overly weak bonding. “Fine, corrugated carbon films – graphene sheets in Moiré patterns – fit the bill. They provide traps for the clusters at precise distances while largely preventing the exchange of atoms between these traps,” is how Esch described the method they used to inhibit the Oswald ripening effect.

The influence of the substrate material

As part of their search for new nanocatalysts, the TUM chemistry researchers experimented with different substrate materials. Stability was not their only concern, either. “Similar to the cluster size, substrate material is a vehicle that we can use to customize the properties for a specific reaction,” declares Heiz. As they also discovered in their series of experiments, these substrates are themselves capable of influencing the catalytic reaction. They had already made use of this effect in a project funded to the tune of EUR 2.3 million by the European Research Council, the objective of which was to create chiral gold clusters. Chiral substances consist of two compounds called enantiomers, which while having the same structure are actually mirror images of each other, like our left and right hands. The researchers wanted to use chiral catalysts to selectively create only one of the two enantiomers. “For this, we created a surface onto which we vaporized single-chirality molecules,” explains Heiz. “When we then deposited gold clusters on the surface, they followed the same pattern. If the substrate is of one chirality, so too will the deposited molecules be.” They observed similar interactions with the substrate material atoms when hydrogenating ethene with platinum as the catalyst.

“These asymmetric catalysts are an important discovery for the pharmaceutical industry in particular,” according to Heiz. In the manufacture of pharmaceutical active ingredients, only one of the two enantiomers can be used as a rule. “The other one can actually be dangerous in some cases,” he points out, referring to the drug penicillamine by way of example. Its active agent is a chiral compound. One enantiomer, D-penicillamine, acts as an antibiotic, whereas its mirror enantiomer, L-penicillamine, is toxic. If both products are created, the undesirable enantiomer has to be detached. This complex process is performed millions of times in industry. In the future, the gold clusters created by the Munich team could save costs and reduce waste in that only one enantiomer would selectively be created.

The next step is to replace the expensive precious metals with cheaper materials. Metals like iron or nickel have not come into the equation until now because they are either too reactive or not reactive enough in solid state. “But when we reduce them to nanoscale, there is a possibility that we can transform them into very useful catalysts – also by tuning the substrate materials.”

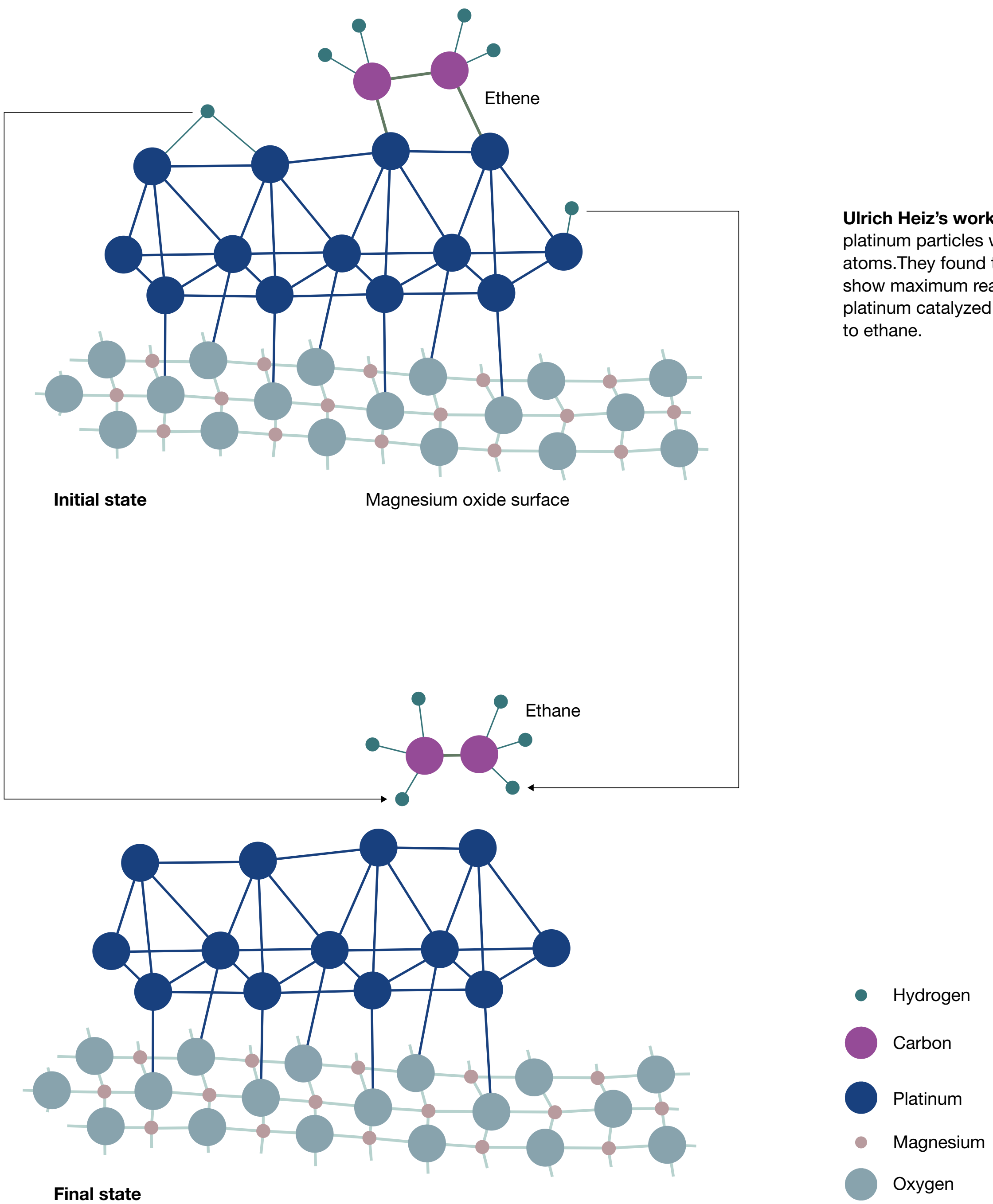
Research alliance with industry

The study and application of innovative catalyst systems is also the focus of the research alliance in place since November 2010 between TUM and chemicals manufacturer Clariant. TUM scientists have been focusing on chemical catalysis with Clariant researchers at the new TUM Catalysis Research Center on the Garching campus since November last year. Clariant is providing funding of up to EUR 2 million per year to support this basic and applied research work. Heiz is the Center’s Academic Director.

One of the research center’s core objectives is to develop catalysts for the efficient transformation of carbon dioxide. “We aim to develop clusters that mitigate carbon dioxide and ideally transform it into something useful,” says Heiz of his plans for upcoming collaborations with colleagues at the research center. Carbon dioxide is after all more than just ▷

“In the new TUM Catalysis Research Center, we aim to develop clusters that mitigate carbon dioxide and ideally transform it into something useful.”

Ulrich Heiz



Graphics: ediundsepp (source: TUM)

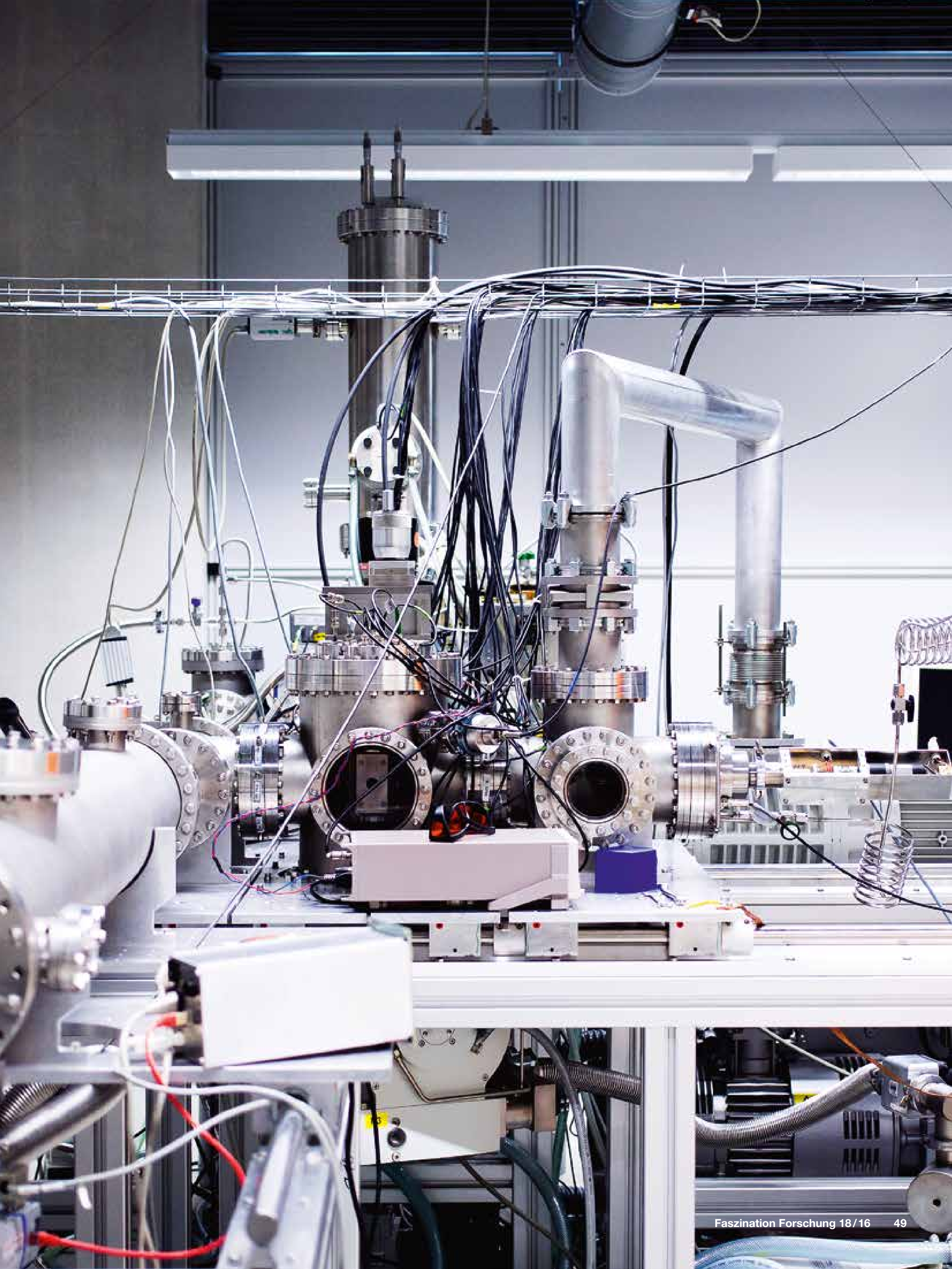
Ulrich Heiz's working group produced platinum particles with only a small number of atoms.They found that clusters with 13 atoms show maximum reactivity. Shown here is the platinum catalyzed reaction converting ethene to ethane.

Sample holder with three single crystals on which the catalyst particles are deposited.

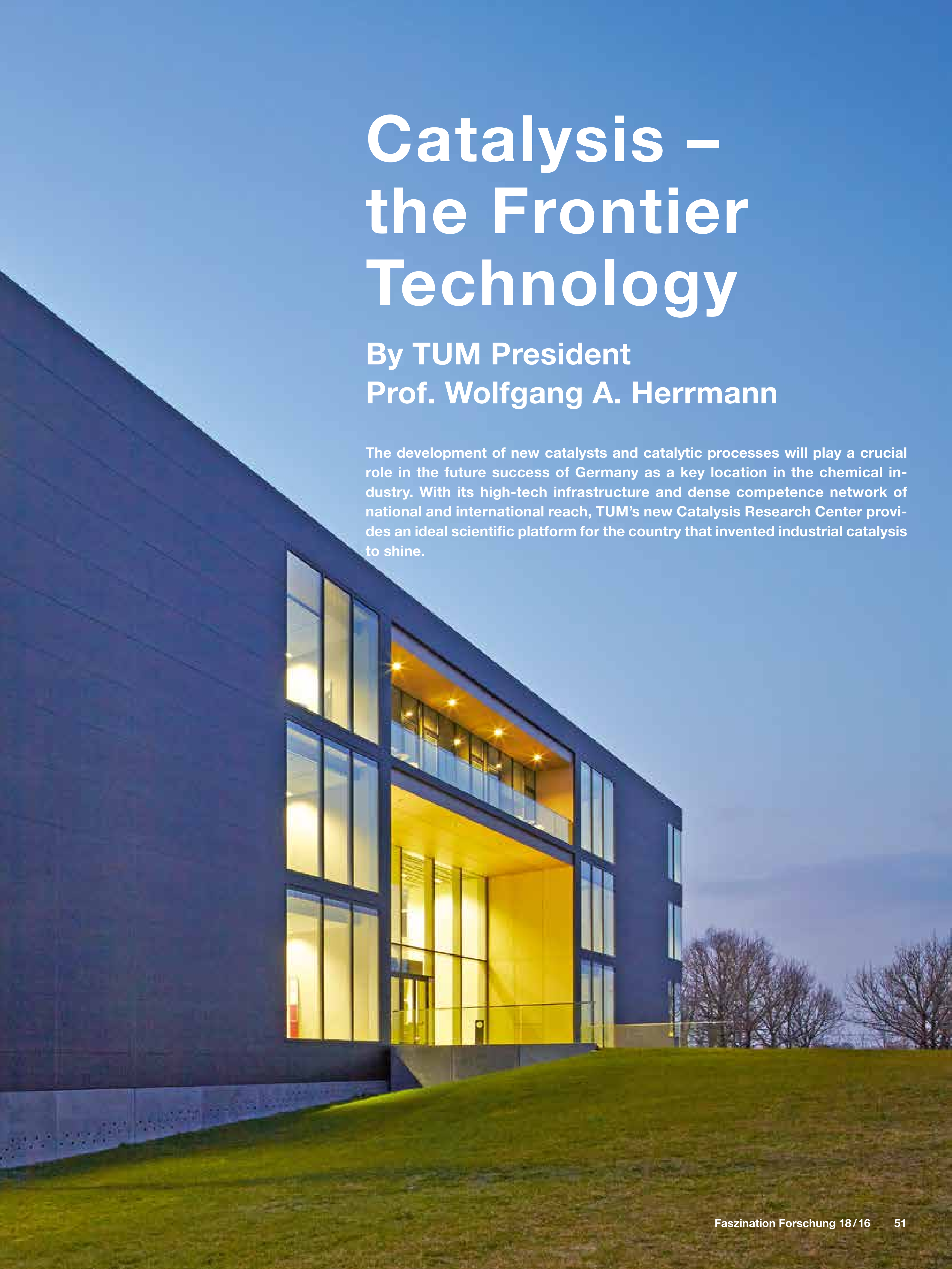
an exhaust gas and a contributor to global warming. It is also a raw material that can be profitably used by industry to make many products. This greenhouse gas may even play an important role in the transition to cleaner forms of energy. When transformed into methane or methanol, it could in the future store surplus electricity from wind and solar farms. Up to now, the awkward properties of this actually quite simple compound have impeded these visions. “We have to make the breakthrough in the next few years, otherwise the need will become critical,” asserts Heiz, who in his roles as scientist and academic director of the new facility has chosen a hard nut to crack. Carbon dioxide is an essentially inert gas with very tightly bonded carbon and oxygen molecules. But it is totally conceivably that a solution will again be found in the nanoscale world. After all, countless experiments with different materials have proven that interesting surprises await on the non-scalable nano level. Not least the transformation of an inert metal like gold into a shining example of a promising catalyst. *Birgit Fenzel*

Heiz is currently moving his laboratory into the newly opened TUM Catalysis Research Center. Here the vacuum chamber, in which the group grows its ultra-small catalysts, is being installed.

Picture credits: Heddergott, Jooss



Picture credit: Hoeglmeier

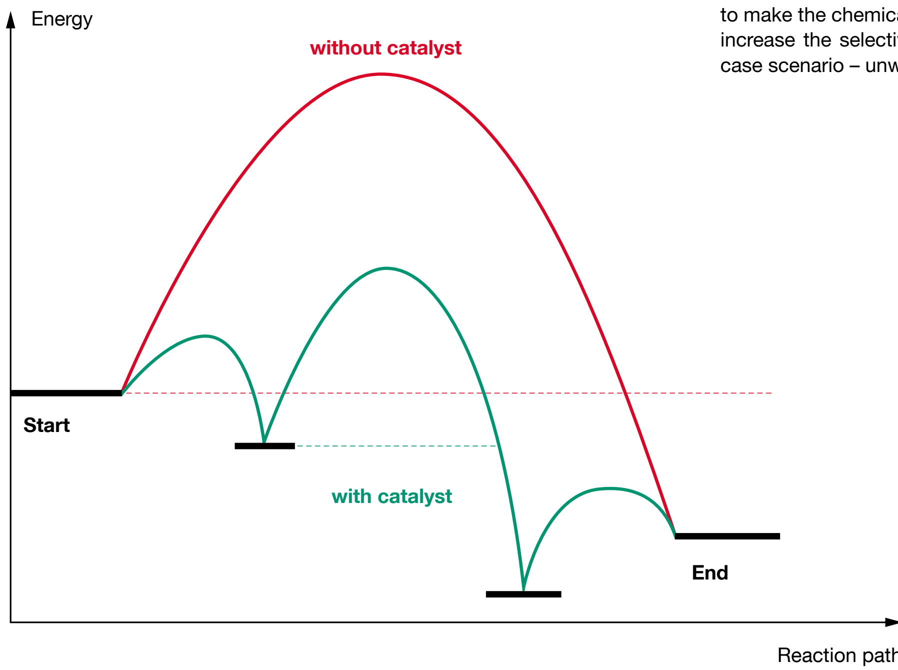


Catalysis – the Frontier Technology

By TUM President Prof. Wolfgang A. Herrmann

The development of new catalysts and catalytic processes will play a crucial role in the future success of Germany as a key location in the chemical industry. With its high-tech infrastructure and dense competence network of national and international reach, TUM's new Catalysis Research Center provides an ideal scientific platform for the country that invented industrial catalysis to shine.

Picture credit: Hoeglmeier



Catalysts lower the energy barriers which chemical reactions normally have to overcome in order to create a target product, and therefore help to make the chemical industry more energy efficient. At the same time they increase the selectivity of chemical reactions and eliminate – in the best case scenario – unwanted by-products.

Of all technology principles, catalysis is unique in its ability to add value by closely aligning both economic and ecological interests. In future, the wide variety of chemical products required by high-tech societies will only be technically and economically feasible if we can harness specific catalysts to create valuable materials, reduce waste and avoid hazardous substances. Examples include the manufacture of stereochemically pure pharmaceuticals, the development of polymer substances with specific properties from simple precursors, the breakdown of end-of-life plastics, as well as the elimination of harmful emissions from manufacturing plants and combustion engines such as cars or power plants. The production, storage and conversion of energy – one of the biggest challenges of our time – also depends on advances in catalysis research – exemplified by electrochemistry and fuel cells.

Catalysis is a way to manipulate chemical reactions and achieve a specific outcome with a minimal energy and resource bill. Considering the massive volume of potential substance conversions – which is what chemistry is essentially all about – and the raw material, energy and waste problems which these generate, catalysis is at the top of today's scientific, economic, environmental and policy-making agenda. Growing resource scarcity is shining the spotlight even more on this key technology. Seriously neglected during the oil age, the future use of biogenic raw materials will heavily depend on advances in catalysis research, as will the chemical

“The catalytic force is reflected in the capacity that some substances have, by their mere presence and not by their own reactivity, to awaken activities that are slumbering in molecules at a given temperature.”

Jöns Jakob Berzelius (1779–1848), who discovered the principle of catalysis

In the chemical industry, over 80 percent of value is added through catalytic processes even today. The international catalyst market is already worth more than USD 18 billion, and the trend is upward. Ultimately, catalysts are the key to an efficient and environmentally friendly chemical industry.

use of natural gas – methane in particular. Previously combusted without a second thought, this gas belongs in catalyst-filled chemical reactors – and not in industrial turbines! The omnipresent gas carbon dioxide should also prove to be a valuable chemical raw material as soon as catalysts to activate this inert gas can be found.

This applies in particular to the Federal Republic of Germany which, with few natural resources, will only remain at the vanguard of the world economy if it keeps on developing technological innovations to renew, expand and improve industrial production. In the chemical industry, catalysis is dominating the scientific discussion around technology leadership. Given the sheer product diversity and production volumes of the chemical, pharmaceutical and biofuel industries, it is obvious that for the foreseeable future, no other field of research has the potential to secure the success of the German chemical industry on the international stage.

The main purpose of applied catalysis is to activate largely inert components and cause a specific reaction. Industrial-scale examples include ammonia (NH_3) synthesis from N_2 and H_2, the conversion of CO and H_2 into fuel using the Fischer-Tropsch process and the conversion of ethylene derived from refining into polyethylene. Several Nobel Prizes have been awarded for breakthroughs in catalytic science since the achievements of Fritz Haber (1918) and Carl Bosch (1931).

To be effective, a catalyst has to be tailored to its specific purpose. This adaptation process ensures that it demonstrates the key characteristics required of a catalyst:

- Selectivity: Only selective products, i.e. the desired ones, are formed.
- Activity: The catalyst function repeats itself as often as possible in the exact same way, i.e. the effect is reproducible.

A catalyst is said to be highly selective if it achieves the target product at a rate of $\geq$99%. It is regarded as highly active – depending on the situation – at turnover frequencies of up to 10^6/h. This means that a catalyst unit activates one million molecular substance conversions per hour up until its deactivation. This level of performance is achieved not only by many enzymes, which are natural biological catalysts, but also by lab-created catalysts (like metallocene) in the technical synthesis of polyolefins from ethylene and propylene.

The search for new catalysts and catalytic processes is driven by three overarching goals: higher activity (smaller reactors, less energy), higher selectivity (smaller separation units, less waste) and greater sustainability (variable and, if possible, renewable raw materials; industrial biotechnology).

Catalysis research at TUM

Between 1964 and 1984, Ernst Otto Fischer achieved international acclaim at our university for his ground-breaking work in organometallic synthesis enabling a host of new substance classes. In 1973, he received the Nobel Prize in Chemistry for his research. Fischer laid the foundations for the application of these families as catalysts in chemical reactions. An early example of the work produced by his students (Hafner and Jira) was the Wacker-Hoechst process for the simple and clean production of the base chemical acetaldehyde (1958). The Munich laboratory where he worked has since become a top-flight center for organometallic catalysis research. Over the years, TUM's Department of Chemistry has prioritized catalysis research, with practically all disciplines now involved following a number of new appointments. Particular mention should go to the systematically expanded field of Biological Chemistry within the Department, which the Shanghai Ranking places among the top ten in the world for the quality of its research. Today, catalysis research at TUM is renowned for the depth and breadth of its coverage, its interdisciplinary approach and close ties with industry.

Now TUM is taking catalysis research to the next level with the *TUM Catalysis Research Center* (CRC). The initial application submitted to the German Council of Science and Humanities (WR) on August 1, 2007 was promptly approved. Representing an investment of over EUR 70 million, the new building, located at Ernst-Otto-Fischer Strasse 1 in Garching, has now been completed. The scientific aims, according to the strategy paper "are specifically focused in the medium-term on the investigation of multifunctional, nanostructured catalysts based on an interdisciplinary approach incor- ▷

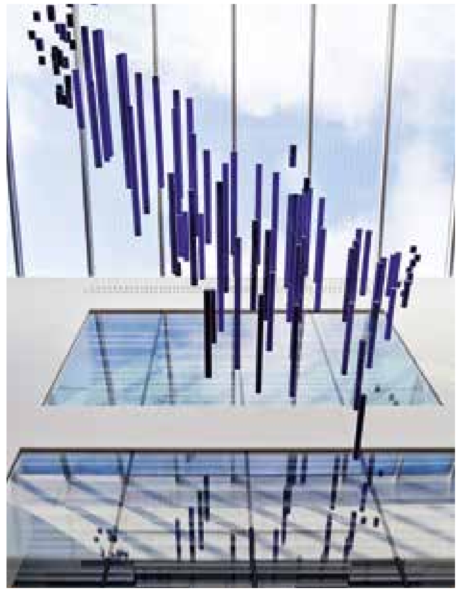
Graphics: ediundsepp (source: TUM)

porating fields of engineering." Even back then, the paper pointed out that "in the chemical industry alone, today over 80 percent of value is already added through catalytic processes." The international catalyst market is already worth more than USD 18 billion, and the trend is upward. Ultimately, catalysts are the key to an efficient and environmentally friendly chemical industry.

The TUM Catalysis Research Center

The CRC steps up to the interdisciplinary challenges of modern catalysis research. It is home to a host of highly varied yet synergized methodological approaches that interact to identify the molecular chemisms of catalytic reactions, for instance, or gain an understanding of fundamental processes with solid state catalysts. This type of research breaks down the boundaries between traditional scientific disciplines. The investigation of new, structurally tailored catalysts will hinge on instrumental analysis of molecule to surface spectroscopy, as well as on reaction kinetics, theoretical models and simulation calculations, as well as technical developments in the area of process control. Parallel screening in miniature reactors in combination with numerical modeling on ▷

Picture credits: Hoeglmeier

The Catalysis Research Center

The CRC is an interdisciplinary research hub at the interface of engineering and natural sciences. The building with a net area of 6,500 m^2 is solely dedicated to laboratory research work. It offers state-of-the-art infrastructure for chemical and physical research including lab-scale pilot plant facilities. Seven large laboratory areas with a total of 75 separate laboratories are complemented by well-equipped analytical core labs and two seminar rooms. □

supercomputers is set to significantly speed up progress in catalyst optimization. The Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities in Garching has the facilities to support this work. On the Garching research campus, scientists have access to a unique combination of methods to determine catalyst structures with great precision. As well as X-ray structure analysis, there is the Bavarian Nuclear Magnetic Resonance Center and the Heinz Maier-Leibnitz neutron source research reactor (FRM II).

The CRC planning and building phase was used to expand the research portfolio and adapt it to the latest scientific and technical challenges. The following institutes have been established at TUM in the meantime:

- The Research Center for Industrial or White Biotechnology – a center of excellence in engineering sciences equipped with a Pilot Plant for White Biotechnology;
- The teaching and research domain Synthetic Biotechnology funded by the Werner Siemens Foundation (EUR 11.5 m);
- New catalysis-relevant Chairs for bioinorganic chemistry, computer-aided biocatalysis, industrial biocatalysis, technical electrochemistry, physical chemistry/catalysis, silicium chemistry, solid-state NMR spectroscopy, biomolecular NMR spectroscopy, selective separation technology, systems biotechnology;
- The Bavarian NMR Center (BNMRZ) with its 1.2 gigahertz spectrometer;
- The TUM International Graduate School of Science & Engineering (IGSSE; under the 2006 Excellence Initiative), which is the scene of numerous catalysis research projects;
- The Institute of Silicon Chemistry in cooperation with Wacker Chemie AG;
- Munich Catalysis Alliance of Clariant and TUM (MuniCat).

The research activities of the Center of Excellence for Renewable Resources in Straubing are associated with the CRC. The development of biochemistry and biophysics research at TUM, likewise supported by the creation of several new professorships, lays the foundation for an expansion of catalysis research into the biopharmaceutical sphere. Our coherent overall concept puts us in a strong position to compete on the international stage in the future.

Picture credits: Hoeglmeier

Graphics: ediundsepp

In photochemistry, light delivers the energy for chemical reactions to happen. Photosynthesis is probably the most well-known example of such processes.

Millions **at my Beck and Call!**

Thorsten Bach is in the unusual business of "taming" tiny molecules, teaching them to do exactly as he commands. His aim is to reduce waste. A visionary Italian pioneer is lighting the way – literally!

Thorsten Bach will eines Tages das Sonnenlicht als kostenlose Energiequelle für bestimmte Katalysereaktionen nutzen.

Claudia Steinert

„Millionen machen, was ich will!“

Licht ist extrem energiereich und kann chemische Reaktionen anstoßen. Dann entstehen neue Stoffe, und was für welche! Lichtenergie ist so stark, dass sie es schafft, Moleküle in herrlich nützliche, aber unglaublich unbequeme Positionen zu zwingen. Deshalb ist die Photochemie oft der einzige Weg, um starre chemische Gerüste herzustellen, wie sie zum Beispiel für Medikamente oder Pflanzenschutzmittel gebraucht werden. Einziger Nachteil: Die Reaktionen sind oft schwer steuerbar. Der Chemiker Prof. Thorsten Bach hat jedoch sehr präzise Vorstellungen davon, was er am Ende einer photochemischen Reaktion in seinem Reagenzglas vorfinden will. Sein Spezialgebiet sind sogenannte chirale Verbindungen.

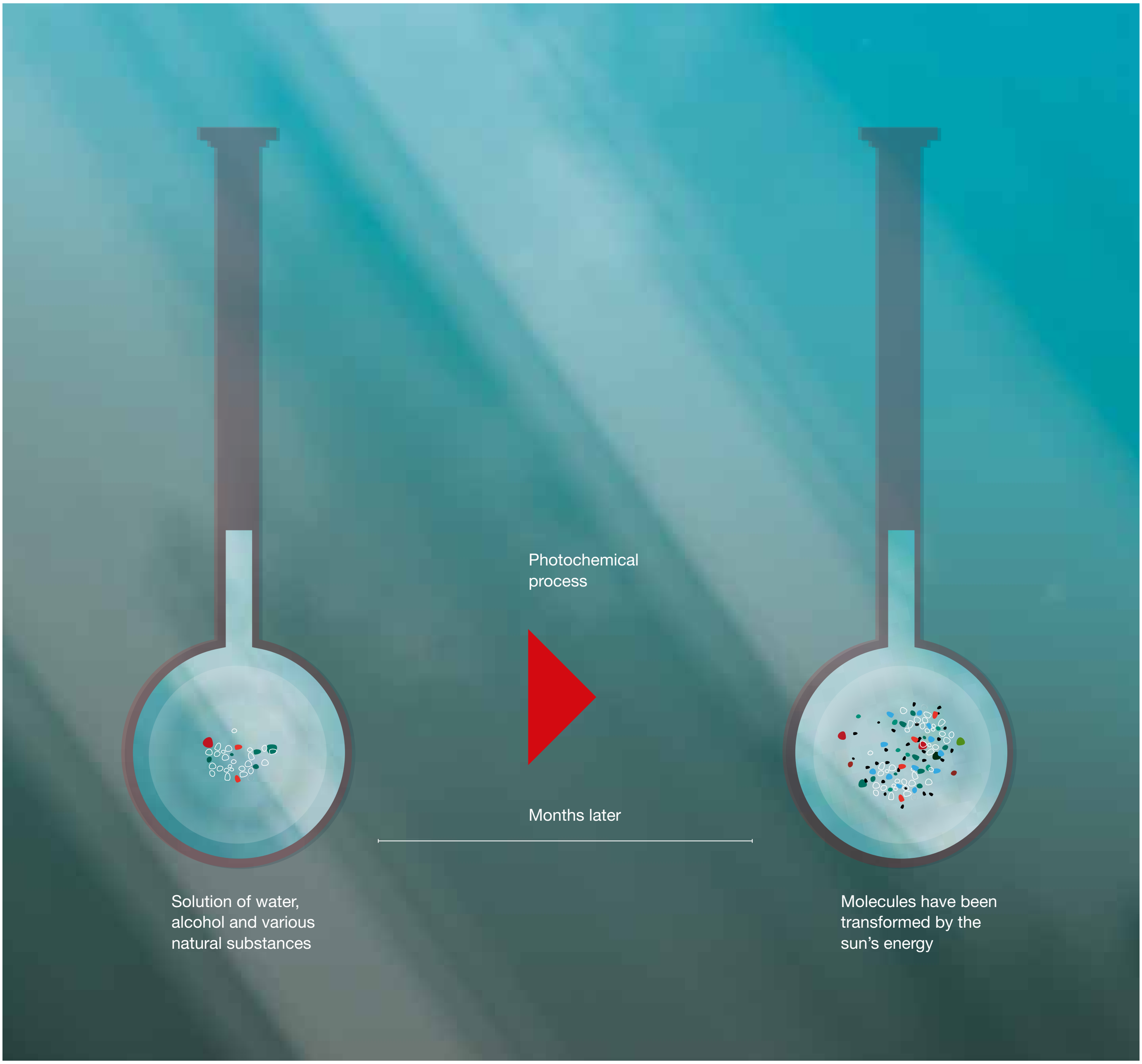
Das Wort Chiralität kommt vom griechischen cheir, die Hand. Denn Hände sind chiral. Sie bestehen aus denselben Teilen und sind spiegelbildlich aufgebaut. Egal wie man sie dreht und wendet, nie wird es so aussehen, als hätte jemand wirklich zwei linke Hände. Chemiker sagen: Die linke und rechte Hand sind Enantiomere.

Die Natur liebt Chiralität. Wer mit Medikamenten an Rezeptoren andocken will, wer Enzyme blockieren oder Bakterien attackieren möchte, der braucht jedoch ein ganz bestimmtes Enantiomer. Das andere ist für den Körper mitunter sogar giftig. Heutzutage werden viele chirale Verbindungen trotzdem als Enantiomerengemisch produziert. Erst hinterher wird aufwändig getrennt. Damit gibt Bach sich nicht zufrieden. Er will von Anfang an so präzise konstruieren, dass er am Ende nichts verschwenden muss. Dafür entwickelt er hochkomplexe Katalysatoren, die ebenfalls chiral sind.

Diese Katalysatoren greifen einen der Ausgangsstoffe und positionieren ihn so, dass nur eine Reaktion stattfinden kann. Nur ein Enantiomer entsteht. Chemiker sprechen von asymmetrischer Katalyse.

Ein Drittel von Bachs Mitarbeitern tüftelt zurzeit an diesem Projekt. Sechs bis acht Wochen dauert allein die Herstellung eines Katalysators. Zurzeit arbeitet Bach viel mit Kunstlicht, die wählerischen Katalysatoren mögen nur bestimmte Wellenlängen. Eines Tages möchte Bach jedoch auf Lampen verzichten können. Er will dann die kostenlose Energiequelle Sonnenlicht nutzen. □

Picture credits: Jooss



More than a hundred years ago, Italian chemist Giacomo Ciamician discovered that light could help transform molecules into new forms. Back then, Ciamician already said that someday we might no longer need fossil fuels.

Link
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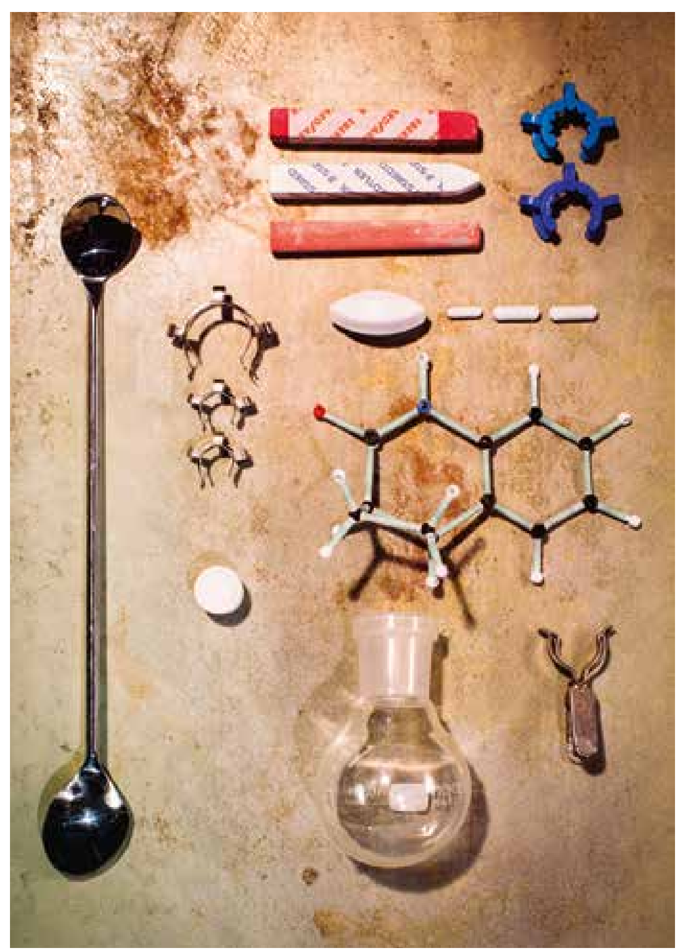
Sometimes it takes more than just a good idea – you also need to be in the right place at the right time. For chemist Giacomo Ciamician, that place was Bologna – around 1910. Summers there are hot and bright, flooding the Italian city with nine or ten hours of blazing sunlight each day. Having already passed the fifty-year mark, Ciamician was considered an old man by the standards of the time – but an active one. Along with his assistant, he hauled numerous flasks onto the balcony of the institute where he was teaching and researching. The two men balanced them on shelves, ledges and balcony railings, filling every available space. Long necks stretched to the sky, the glass bulbs sat and waited. Solutions of water, alcohol and various natural substances lay dormant inside.

The very first photochemical experiment

What happened next took what seemed like an eternity and was utterly unexciting to watch. Hours, days and weeks went by with no sign of anything at all. Nothing that you could see, hear or otherwise perceive in any way. Inside the flasks, though, change was afoot. Very gradually, the sun's glare was transforming the molecules – splitting compounds and forming new ones. Months later, when Ciamician came to analyze the contents of the flasks, he found different substances to the ones he had originally mixed into them. So with this experiment he was able to prove to the world that we can harness energy from sunlight. And that, he said, might someday mean that we would no longer need fossil fuels. At a time well before any talk of crude oil shortages or climate change, Ciamician was already predicting artificial photosynthesis. He was a ▷



Picture credit: Jooss, Graphics: ediundsepp

"It's great when you're heading into entirely new territory and come up with the very first ideas." *Thorsten Bach*

Prof. Thorsten Bach

A pioneer in photochemistry

Thorsten Bach's involvement with photochemistry began more by accident than design. During his doctorate at the University of Marburg, he was working with metal complexes that could only be photochemically generated. "That meant I had the right equipment, so then I gradually built up my knowledge," he explains. At that point, at the start of the 1990s, nobody else was pursuing similar concepts. Was he worried about barking up the wrong tree? On the contrary: "It's great when you're heading into entirely new territory and come up with the very first ideas," counters Bach.

Following a period of research in Harvard, he returned to Germany, qualifying as a lecturer in Münster before taking up his first professorship at the University of Marburg. In 2000, Bach went on to join TUM as Professor of Organic Chemistry. His wife, also a chemist, teaches at the Weihenstephan-Triesdorf University of Applied Sciences. As far as Bach is concerned, the best thing about his job is the level of autonomy he enjoys. "When it comes to research, I'm given free rein," he confirms. At the same time, he sees himself as having a social responsibility, feeling that artificial photosynthesis is something chemists like him are now called upon to develop. Ciamician would have been thrilled.

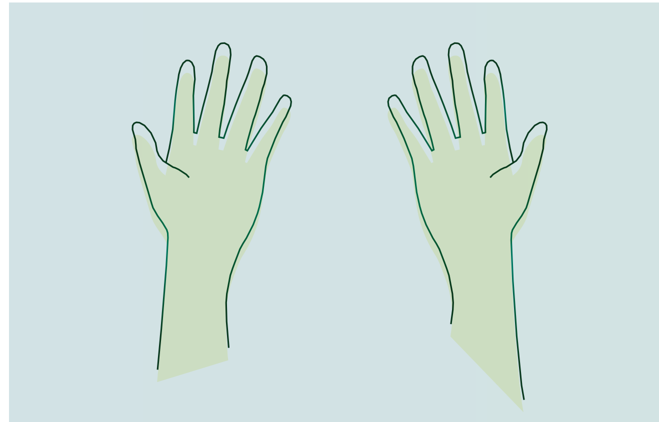
Picture credits: Jooss

visionary in the realm of photochemical research. Around a hundred years later, Prof. Thorsten Bach stands in his office at TUM's Garching campus on a gray winter's day. Looking up at the cloudy sky, he notes: "Ciamician's experiments wouldn't have worked here at all." Way too overcast; nowhere near enough light. Definitely not the right place.

Focus on chiral compounds

Meanwhile, though, things have moved on in this field and today's photochemists are no longer dependent on sunshine. Bach's lab is equipped with lamps that cast rays of all wavelengths within cylindrical mirrors. The spectrum ranges from longwave, low-energy green light through blue beams to shortwave, high-energy ultraviolet – the UV light that is invisible to the human eye but sometimes makes itself felt as sunburn after a day at the beach. Bach needs all these different lamps because molecules are very particular – they only accept light energy at specific wavelengths. So depending on the reaction Bach sets out to test, he switches on different lights.

Light is full of energy, and molecules can absorb this and move into an excited state. However, they do not stay at this elevated energy level for long. They either emit their excess energy in the form of light or store it in one or more chemical bonds. This creates new substances, and that is where things get interesting! The light energy is so strong that it forces the molecules into exceptionally useful but astonishingly awkward positions. Unlike Ciamician, Bach is not just trying to generate any old molecules, however. On the contrary, he has a very precise idea of what he hopes to find in his test tube at the end of a photochemical reaction. His particular focus is on chiral compounds. ▷



Chiral molecules exhibit the same symmetry as our hands: They consist of the same elements and mirror each other. No matter how you rotate them, they can never be converted into each other.

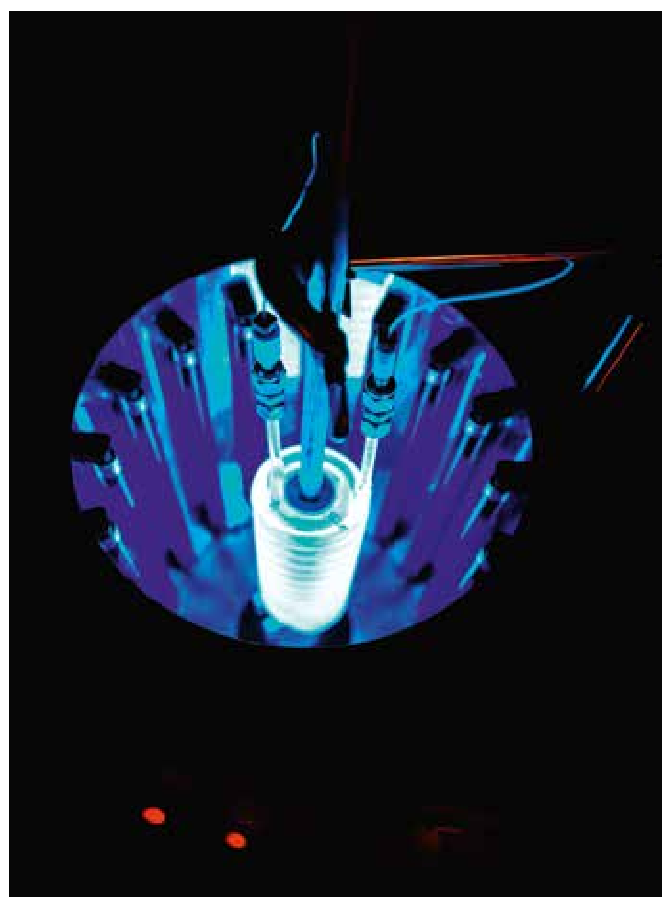
The word chirality is derived from the Greek cheir, or hand. And looking at your own two hands is a good starting point when considering this concept. Our hands themselves are chiral. There are two reasons for this. Firstly, they consist of the same elements and secondly, they mirror each other. No matter how you turn or rotate them, you can never make it appear as though you truly have two left hands. Chemists refer to enantiomers when talking about chiral molecules that mirror each other. A mixture of corresponding enantiomers is known as a racemic mixture or racemate.

But no matter how similar enantiomers may appear, they can work in deceptively different ways. The drug penicillamine is a good example. Its active agent is a chiral compound. One enantiomer, D-penicillamine, is an antibiotic, whereas its mirror enantiomer, L-penicillamine, is toxic. Only one of the two possible enantiomers in this type of compound can be successfully used as medication.

Designing new catalysts for efficient production

Many chiral compounds are still produced as racemic mixtures, which then require effort to separate. “You can separate almost anything, but it is certainly costly,” confirms Bach. It also means throwing away half of what you produce – much to Bach’s discontent. His aim is to increase production precision to such an extent that there is no waste at the end.

When Thorsten Bach is pondering a new reaction, he turns to plastic balls the size of cherry stones and sticks the size of matches, which he crafts into molecular models. He bonds nitrogen and oxygen, forms a ring of black carbon spheres and then adds enough hydrogen atoms to occupy all available ▷



Light with different wavelengths delivers the energy the molecules need to undergo certain photochemical reactions.

Picture credits: Jooss, Graphics: ediundsepp connection points. This handicraft is not strictly necessary, since molecules can now be simulated by computer. But that is just not the same, in Bach's book – he needs something tangible for inspiration. So there he sits, model in hand, and considers how best to produce it. Chemists like Bach are architects that seldom set eyes on their elaborate constructions. A great deal exists only as theory, in formulas and abstract concepts. Or, indeed, as plastic models. Bach, however, does not find this frustrating – on the contrary, it fascinates him. Without even seeing the molecules, he can control them precisely. "Millions of molecules at my beck and call!"

A general difficulty is that many molecules are far more similar to us humans than we might think. They are not actually all that keen on changing themselves and creating something new. They prefer to mooch about lethargically in corners. They could be breaking bonds, forming new ones, combining to form completely different molecules – in theory. But they actually prefer not to.

To get things moving, energy must be applied to the molecules – activation energy, as chemists call it. Heat is very simple and effective in this respect, but light works sometimes too.

Light energy and catalysts in combination

Another possibility is to accelerate the reaction by using catalysts. Catalyst molecules are only added to the reacting solution in tiny amounts, since the catalyst itself is not expended during a reaction. So at the end, when all the starting substances have turned into new products, the catalyst remains unchanged. Bach is using both methods at once: light energy and catalysts. But accelerating reactions is not the primary purpose of his catalysts – they are intended to increase precision. Highly complex, chiral catalysts engage one of the initial substances, position it and thus ensure that new bonds can only occur at precisely defined points. This means that only one of the two possible enantiomers is formed in the reaction. The more selective the reaction, the better. Researchers consider it a positive outcome if at least 95 percent of the desired enantiomer is present at the end.

Like photochemistry, asymmetric catalysis is still a very new research field. It was in the 1970s that scientists were first able to apply this method to large-scale pharmaceutical production, manufacturing L-DOPA for the treatment of Parkinson's disease. And in 2001, the Royal Swedish Academy of Sciences awarded a Nobel Prize for advances in asymmetric catalysis. So Bach is linking the two emerging fields of photochemistry and asymmetric catalysis. Funding from the European Research Council is lending momentum to his project, and he has allocated a third of his team to developing chiral photocatalysts.

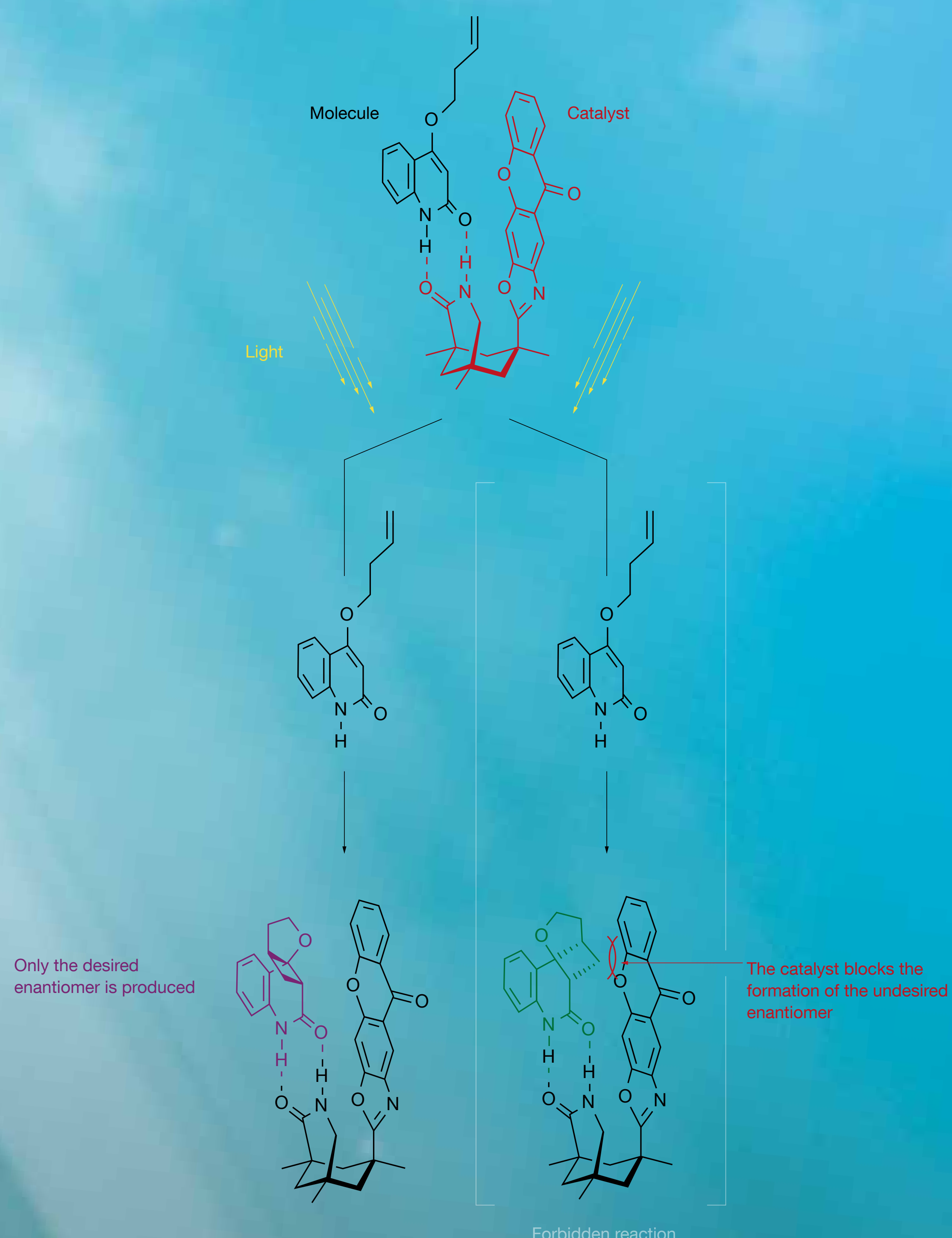
Asymmetric catalysts enable selective production of enantiomers

First, the chemists consider which molecule they intend to produce. From there they can work out what a catalyst would need to look like to force the initial substances into the right geometry. Generating the catalyst alone takes six to eight weeks, and then the scientists place a solution consisting of initial substance, catalyst and solvent into a test tube. This they position inside a circle of lamps and switch on the cooling system – the lower the temperature, the less the molecules move. Light shines through the glass from all sides. But no-one can see what exactly is happening inside. Whether the team's work over the past weeks has paid off only becomes evident when they test the substances in the test tube.

At that point, Bach and his researchers gather around the analyzer – and wait. At some point, a number pops up on the display – a sign from the first enantiomer. Deep breaths and another wait. If no second number appears, the reaction is a success. The light and the catalyst have worked with the precision Bach envisaged.

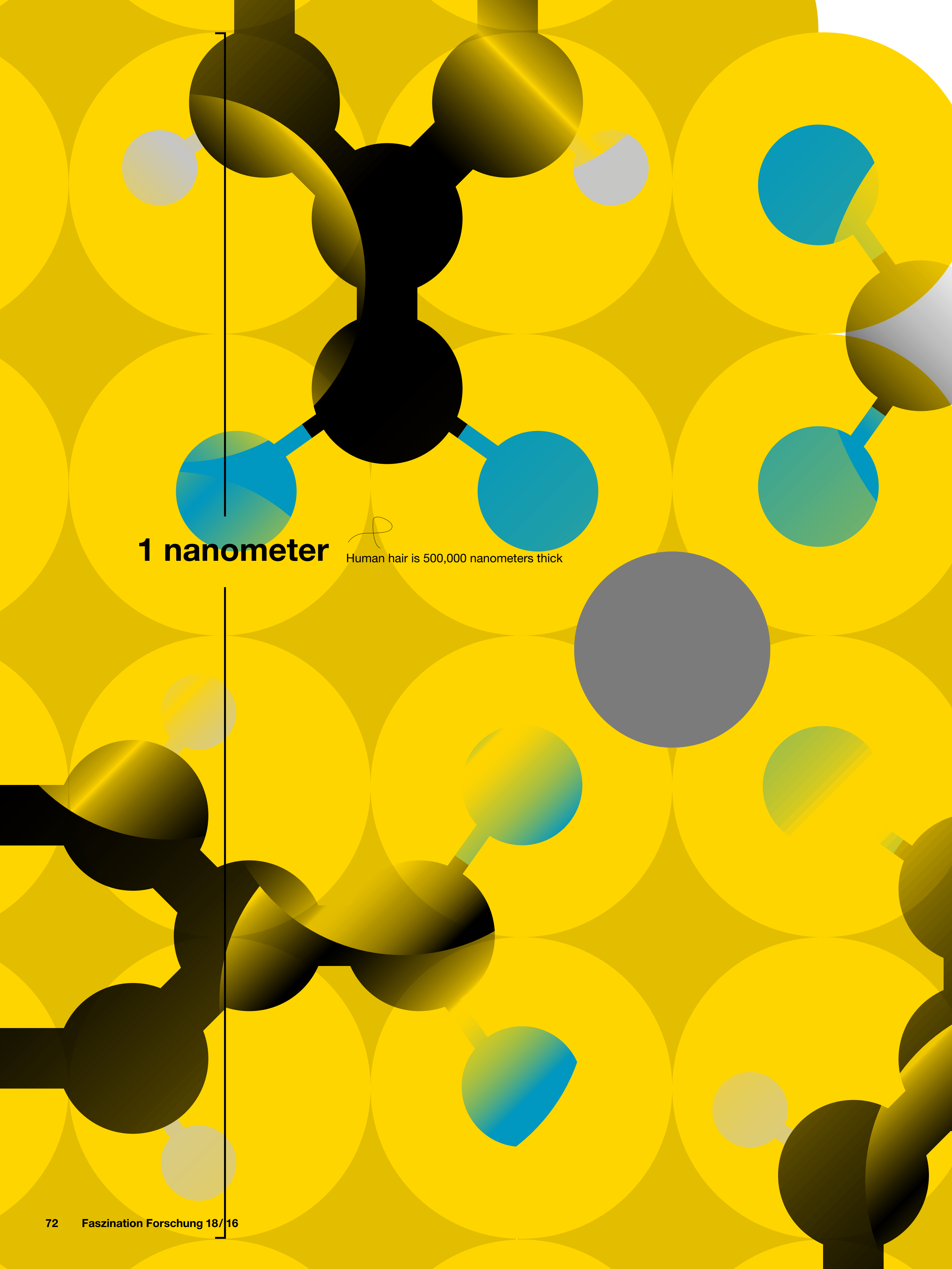
The team is currently focusing on reactions known as [2+2] cycloadditions. Here, two functional groups each consisting of two carbon atoms bond to form a four-membered ring. This scaffold is extremely taut and robust. Chemists can attach all kinds of side groups to its edges to produce substances with widely varying effects. Rigid is good, as far as Bach is concerned. As long as nothing wobbles, the side groups can latch onto the possible receptors in precisely defined positions and the outcome is better than with molecules that move. However, rigid is also chemically challenging. The energy input required to force the atoms into this shape is particularly high, so photochemistry – i.e. light – is essential. Bach's working group has already developed a few promising potential catalysts. The only drawback is that most of them are very fond of artificial light, finding the sun's longer wavelength problematic. Someday, though, Bach hopes to abandon his lamps and get right back to where Ciamician started a good hundred years ago – free energy in the form of sunlight.

Claudia Steinert



Bach's research subject are photochemical reactions that produce chiral molecules, i.e. molecules exhibiting two enantiomers. He designs catalysts that make these reactions more precise by ensuring that only the desired enantiomer is produced.

Graphics: ediundsepp (source: TUM)



1 nanometer

Human hair is 500,000 nanometers thick

Magically Drawn to the Interface

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Johannes Barth likes to research at the edge. He is interested in harnessing the properties of complex single molecules and creating nano-scale architectures with useful functionalities. The research of his team is laying the groundwork for novel kinds of materials and processes in molecular nanoscience and technology.

Graphics: ediundsepp (source: TUM)

Gerlinde Felix

Grenzflächen als magische Spielwiese

Molekulare Nanostrukturen sowie winzige Funktionseinheiten auf Grenzflächen stehen im Mittelpunkt der interdisziplinären Grundlagenforschung des Physikers Prof. Johannes Barth und seiner Mitarbeiter. Barth und sein Team suchen insbesondere innovative Ansätze, um gezielt funktionelle Nanosysteme aufzubauen. Diese ebnen die Grundlagen für innovative Konzepte im Bereich der Nanomaterialien, Nanoelektronik, Photonik und Spintronik – um einige der möglichen Anwendungsbereiche zu nennen. Die Wissenschaftler nutzen für die Herstellung von Nanostrukturen ein Prinzip, das sie sich von der Natur abgeschaut haben: Die Selbstassemblierung, die auf der Erkennung und auf gerichteten Wechselwirkungen zwischen den einzelnen Akteuren beruht. Die Natur erzeugt dadurch biologische Gebilde wie Zellmembranen, Zellfabriken und die DNS. Dafür bedarf es keines Baumeisters, keines Plans und keines Gerüsts, denn die Strukturelemente tragen ihre Bestimmung schon in sich. Ähnliche Vorgänge laufen in Barths Labor ab, wenn sich beispielsweise Metallatome und maßgeschneiderte organische Moleküle auf einem geeigneten Substrat zu metall-organischen Nanostrukturen zusammenfinden. Die Kunst dabei ist, die richtigen Komponenten mit abgestimmten Funktionalitäten auszuwählen, um die Wechselwirkungen, die zur Selbstassemblierung führen, gezielt zu nutzen. Barths Forschung geht aber noch weitere Schritte. So entstehen in den Münchner Labors beispielweise honigwabenförmige Nanonetzwerke mit kleinen Rotoren, Quasikristalle, Nanosolarzellen und molekulare Drähte. Insbesondere die Forschung zu sich selbstassemblierenden Nanostrukturen wurde dank eines European Research Council Grants, den Barth 2009 für sein Projekt MolArt – Surface-Confined Metallosupramolecular Architecture erhielt, möglich. Barth, der seit bald vier Jahren auch Dekan ist, schreibt dem ERC einen Booster-Effekt für seine Forschungsaktivitäten im Bereich der Nanowissenschaften und für die Förderung von Nachwuchswissenschaftlern zu. Dass seine administrative Arbeit mit Wissensgewinn vereinbar ist, sei, so der Physiker, innovativen Ideen, einem guten Stamm an Mitarbeitern und synergetischen Kooperationen, beispielsweise auch mit Partnern am Zentralinstitut für Katalyseforschung und im Exzellenzcluster Munich Center of Advanced Photonics, zu verdanken. □

Prof. Johannes Barth

Always at the interface

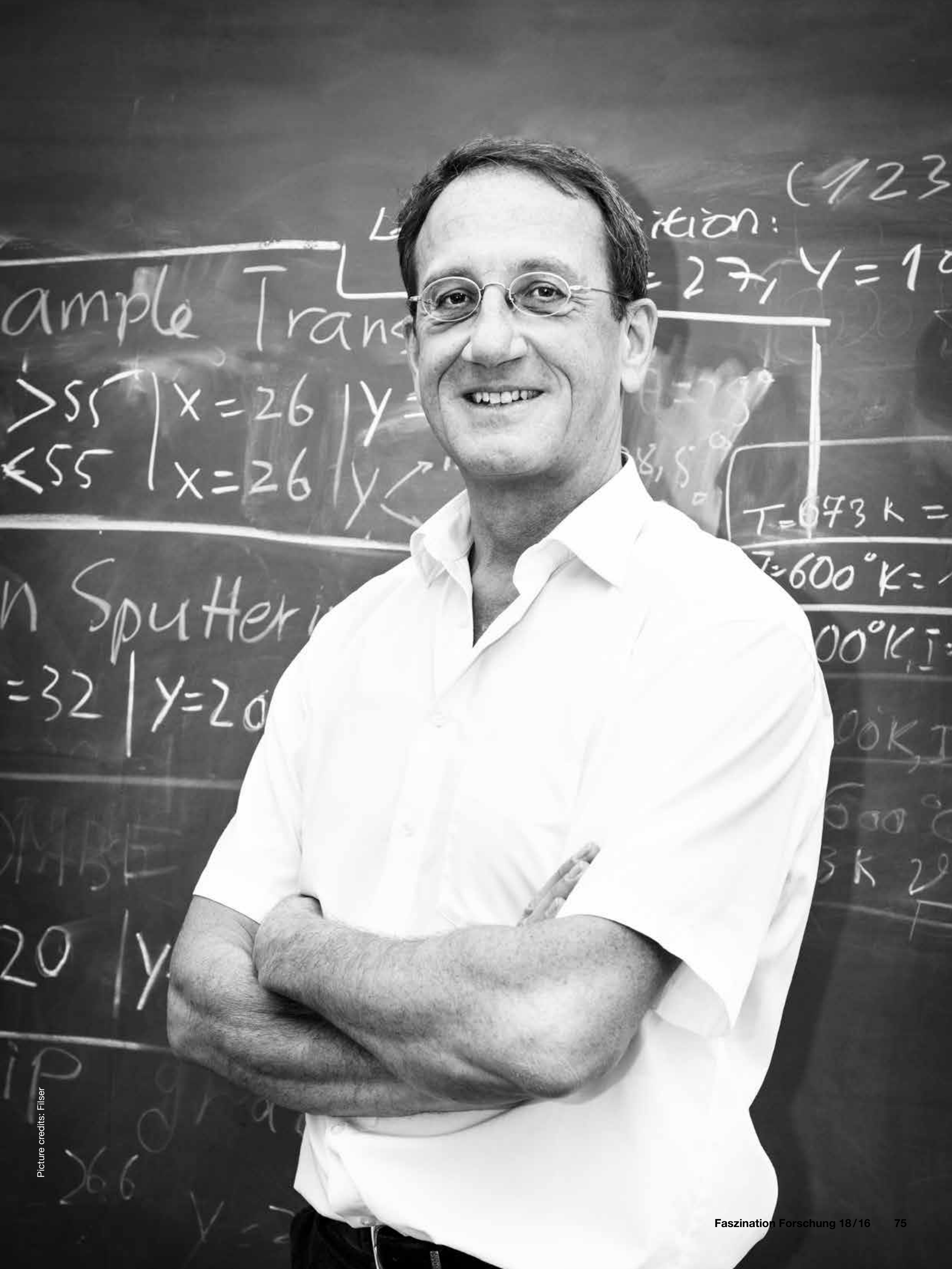
After toying with the idea of studying music or humanities, Johannes Barth eventually decided on physics, guided by his fascination with quantum mechanics. He was tempted by medicine along the way, but neurophysiology simply did not have a strong enough fundamental physics element. In 1988, he focused on his diploma thesis, which was half experimental and half theoretical, in Munich and Berlin at the Fritz Haber Institute of the Max Planck Society. So he experienced the special atmosphere – and all the restrictions – that defined Berlin before the wall came down. In 1989, he nonetheless moved to Berlin and the Fritz Haber Institute. There he received his doctorate in physical chemistry, specializing in surface studies, with Prof. Gerhard Ertl, who went on to win the Nobel Prize in Chemistry. He was in Berlin to witness the historic events surrounding the fall of the wall. "Previously, the S-Bahn only went as far as Friedrichstraße, but suddenly it just kept going. Those were amazing times."

After obtaining his doctorate in 1992, he moved to the IBM Almaden Research Center in San Jose, USA where he spent 18 months as an IBM Postdoctoral Fellow and Humboldt scholar. His research there focused on ultrathin magnetic films for storage technology. IBM went through a financial crisis at the time and had to close several labs, so Barth attended a large number of farewell parties. After that he returned to Berlin before moving on to the École Polytechnique Fédérale de Lausanne in Switzerland. He dedicated all his research efforts there to interface chemistry, transport processes of adsorbates and growth of thin films. He later went on to work with organic molecules and focused his experimental efforts on supramolecular structures and metal-organic architectures. He received his lecturing qualification (venia legendi) in 1999. After spending more than ten years in Lausanne, and having climbed a series of 4,000 m peaks in the Alps, he accepted an offer as Canada Research Chair from the University of British Columbia, Vancouver, in 2003. While rapidly installating a successful lab, he was also able to enjoy sushi, beach barbecues, jogging by the Pacific and powder snow in the nearby ski resort of Whistler.

In 2007, he moved to TUM as a full professor while remaining an adjunct professor at UBC Vancouver for a few more years. Barth has had a large number of papers with high impact published in renowned scientific journals. In 2009, he received the ERC Advanced Investigator Grant for his "MolArt – Surface-Confined Metallosupramolecular Architecture" project. The ERC grant provided the creative headroom and extra manpower needed to bring his research to the next level. Four years ago, Barth was appointed Dean of the Physics Department.

"Our basic research represents a starting point for the development of new materials and concepts. Looking beyond molecular electronic components, spintronics, solar cells and IT building blocks, we are also thinking designer catalysts."

Johannes Barth



Picture credits: Filser

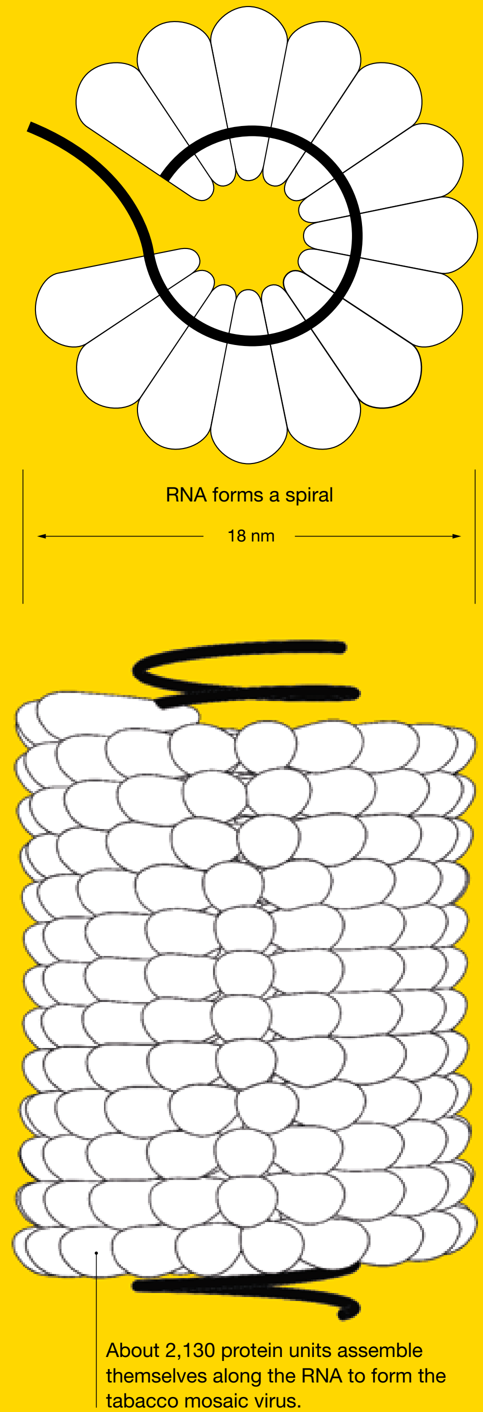
Welcome to the nanocosmos, a world where structures are measured in billionths of a meter. These could be aggregates of atoms, ultra-precise magnetic and semiconductor elements, or likewise a virus, the bacterial ribosome in which the gut bacterium *Escherichia coli* creates its proteins, or even the double helix of a DNA molecule. At first glance, the latter biological structures have very little in common with the research of Prof. Johannes Barth, Chair of Molecular Nanoscience & Chemical Physics of Interfaces. But a closer look shows a different picture. The physicist, who is also Dean of TUM's Physics Department, and his team base their work around a scenario devised by evolution long ago: the principle of self-assembly. Without this principle, there would be no life on earth. It facilitates energy-optimized

Thanks to the ERC project MolArt, Johannes Barth's research group now operates this scanning tunneling microscope combined with an electrospray ionization scanning setup. It is designed to handle complex and thermolabile species for nanoscale investigations.

structures spontaneously evolving from basic constituents that themselves originate from chemical reactions. Their spatial arrangement, that is, the formation of ordered, typically highly organized structures, results from the subtle interplay of "weak" intermolecular forces. "The phenomenon of self-assembly is incredibly fascinating and multi-faceted," enthuses Barth, who has a certain weakness for biophysical chemistry and is now conducting interdisciplinaary research embracing physics, nanoscience and supramolecular chemistry. In 2009, he received a EUR 2.6 million grant from the European Research Council (ERC) for his "MolArt – Surface-Confined Metallosupramolecular Architecture" project. This grant paved the way for a number of basic research projects on self-assembled nanostructures; the success of which – according to Barth – was attributable to excellent working conditions, a wealth of ideas and the high commitment of the researchers. Several projects brought TUM's physicists and chemistry departments together with scientists from Karlsruhe, Linköping, Lyon, Namur, Paris and Zurich. Quite a few endeavors left the realm of self-assembly, including very challenging experiments with individual molecules. It is possible that major technical applications will be found for the molecular functional architectures created by Barth and his team. "Our basic research represents a starting point for the development of new materials and concepts. Looking beyond molecular electronic components, spintronics, solar cells and IT building blocks, we are also thinking designer catalysts," says Barth. This echoes the words spoken many years ago by eminent physicist Richard Feynman, who asserted that the control of matter at atomic level could open up a huge number of new applications: "When we get to the very, very small world we have a lot of new things that represent completely new opportunities for design … We will get an enormously greater range of possible properties that substances can have, and of different things that we can do … We can manufacture in different ways."

Emulating natural processes

So what "recipe" are the researchers following to realize self-assembled functional architectures? The key to their design is a selection of the right building blocks with programmed properties that are brought together under suitable conditions. Self-assembly on the nanoscale makes use of intermolecular interactions – just like nature, where molecular recognition also plays a crucial role. These interactions include hydrogen or van der Waals bonding, the electrostatic forces between charged particles, and metal-ligand interactions (combining metal atoms and molecules). With the help of thermal energy and these "weak" forces, the players "push



Nature employs self-assembly to form stable structures such as viruses. Protein subunits are organized around a single strand of RNA to form a stable structure capable of self-replication.

Picture credits: Filser, Graphics: ediundsepp (source: TUM) and shove" until they arrive at their optimum position. Unlike chemical reactions, atomic bonds are typically not formed. In order to produce surface-confined metal-organic or other hybrid systems, the first step involves selecting a suitable substrate. This can be a regular grid of silver, gold or carbon atoms, for example. Importantly, the geometric and electronic structure of a metal lattice influences the processes that take place thereon and the properties of the evolving structures. Accordingly the surface – acting as a "design platform" – must be atomistically clean and well-defined. Any imperfections could hinder the movement and association of the atoms or molecules. The physicists thus have to lend a "helping hand" and first prepare the surface. "Optimum interfaces are not always easy to achieve. But after extensive practice we have the necessary expertise," says Barth.

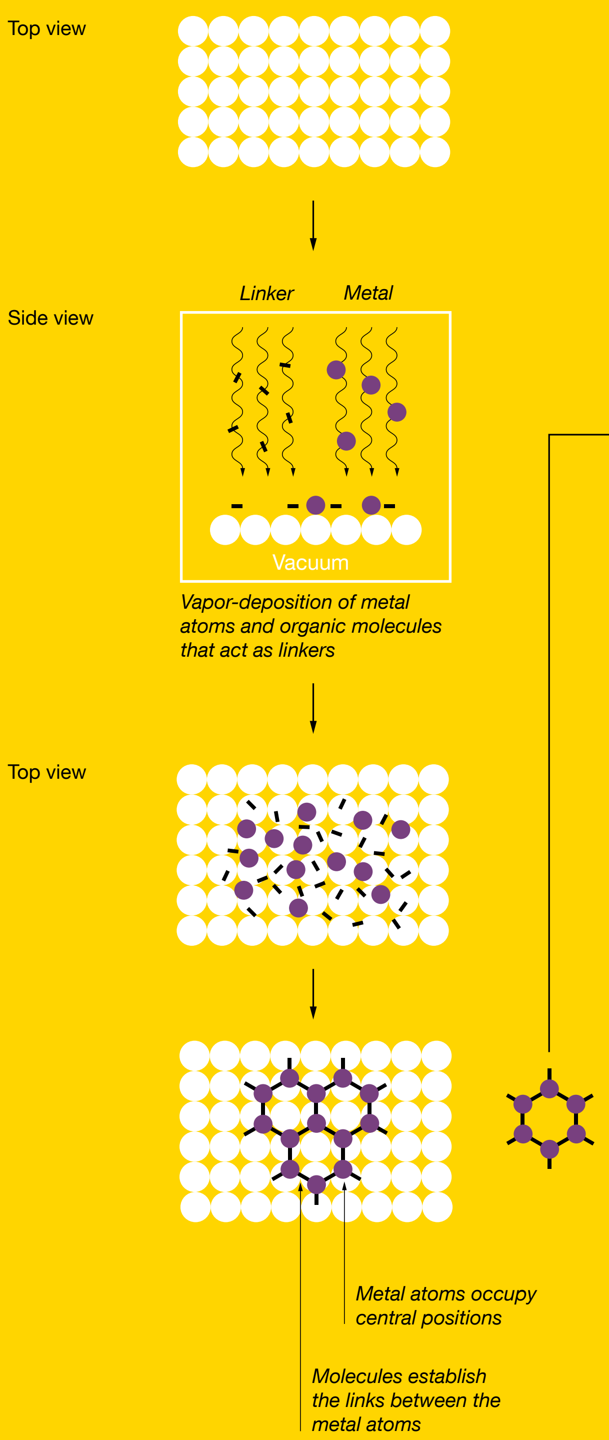
How nanostructures are formed

The substrate is "only" the base layer, however. In order to create metal-organic nanostructures, the researchers vapor-deposit selected organic molecules (so-called linkers) followed by metal atoms (such as iron) under vacuum conditions. Once all the players are in place, they reassemble into new one- or two-dimensional structures as if by magic. During self-assembly, the organic molecules are linked to the metal atoms, which occupy central positions in the resulting structures. In fact, through their properties, they steer the self-assembly process. Suitable metal candidates include iron and cobalt, both magnetic elements, then cerium or europium, which are rare earths (lanthanides), as well as catalytically active transition metals like rhenium, tantalum, tungsten, vanadium and chromium. With these metals, only a small amount of energy is required to detach valence electrons. For reasons related to quantum mechanics, an atomic magnetic moment may additionally arise which could also be important for targeted functionalities and for the interplay between metal atoms, substrate and linkers. Suitable organic molecules include biologically important tetrapyrrole rings, carboxylic acids and de novo synthesized linear polyphenylene-dicarbonitrile molecules. These building blocks may have complicated, tongue-twisting names but – and this is the crucial ingredient – their end groups and backbone have suitable characteristics. Thus a rich variety of structures is produced. These may be individual metal-organic complexes such as a macrocycle with a metal atom at its center. Or they include one-dimensional chains or regular two-dimensional metal-organic coordination networks, which may even act as seed layers for 3D structures. Depending on the properties of a given structure, possible future applications include new nanomaterials, molecular electronics, organic solar cells, molecular magnetism, new catalysts and biosensors.

Importance of scanning probe microscopy

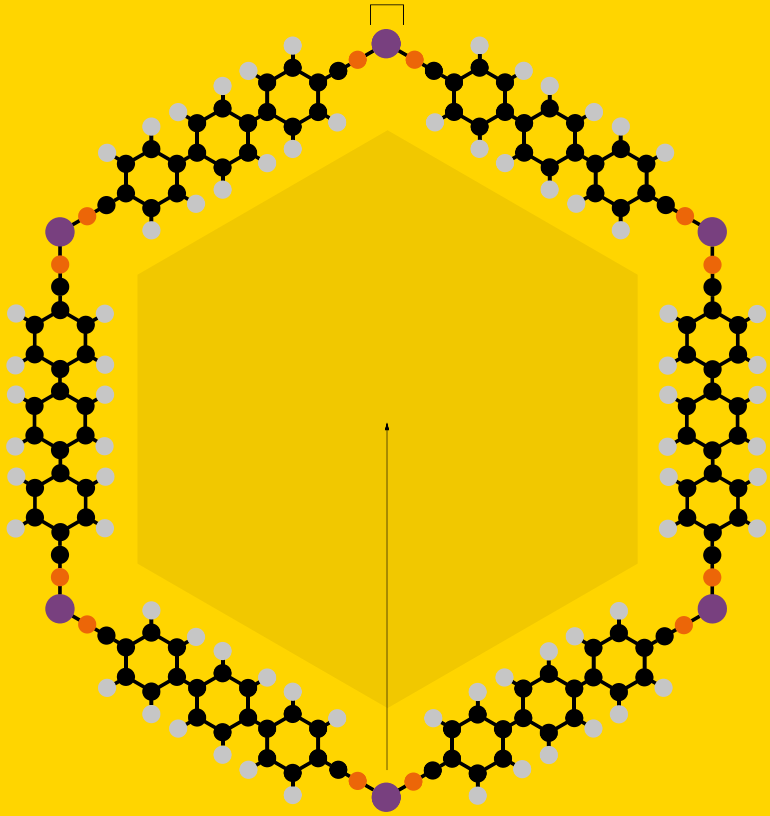
Barth's basic research into interface phenomena and nanostructures would hardly be feasible without a special tool: ▷

How to produce self-assembled functional structures at interfaces



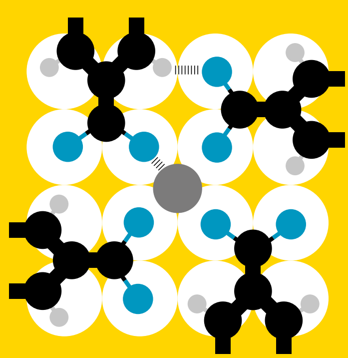
Graphics: ediundsepp (source: TUM)

Correlation between structure and functionality

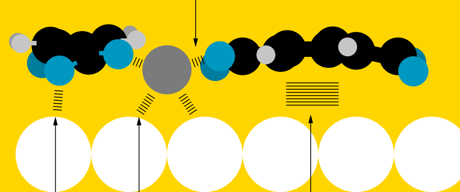


Forces behind self-assembly in 2D

Top view



Side view



Substrate
Hydrogen
Oxygen
Nitrogen
Carbon
Iron
Cobalt
Stabilizing forces

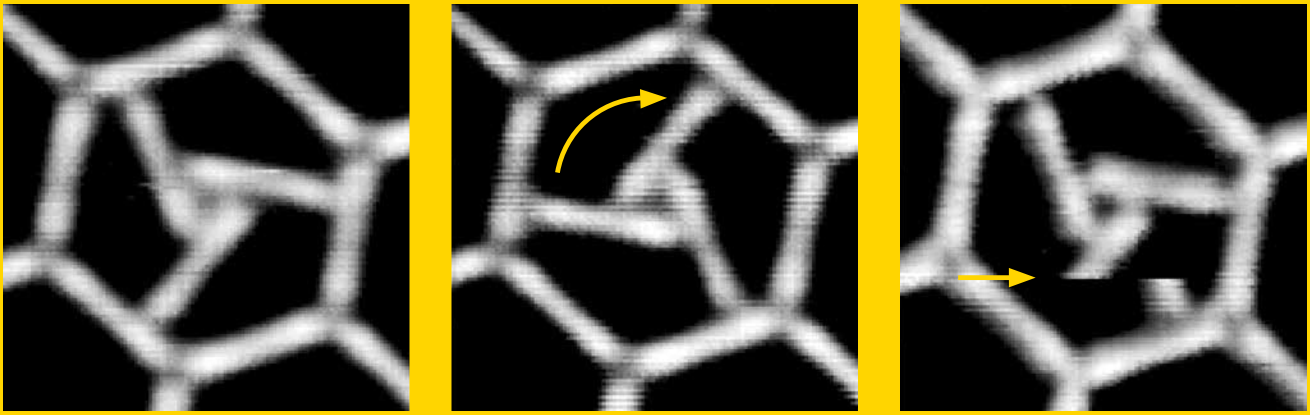
This combined scanning tunneling and scanning force microscope is used by the researchers to investigate molecular features and functionalities in unprecedented detail.

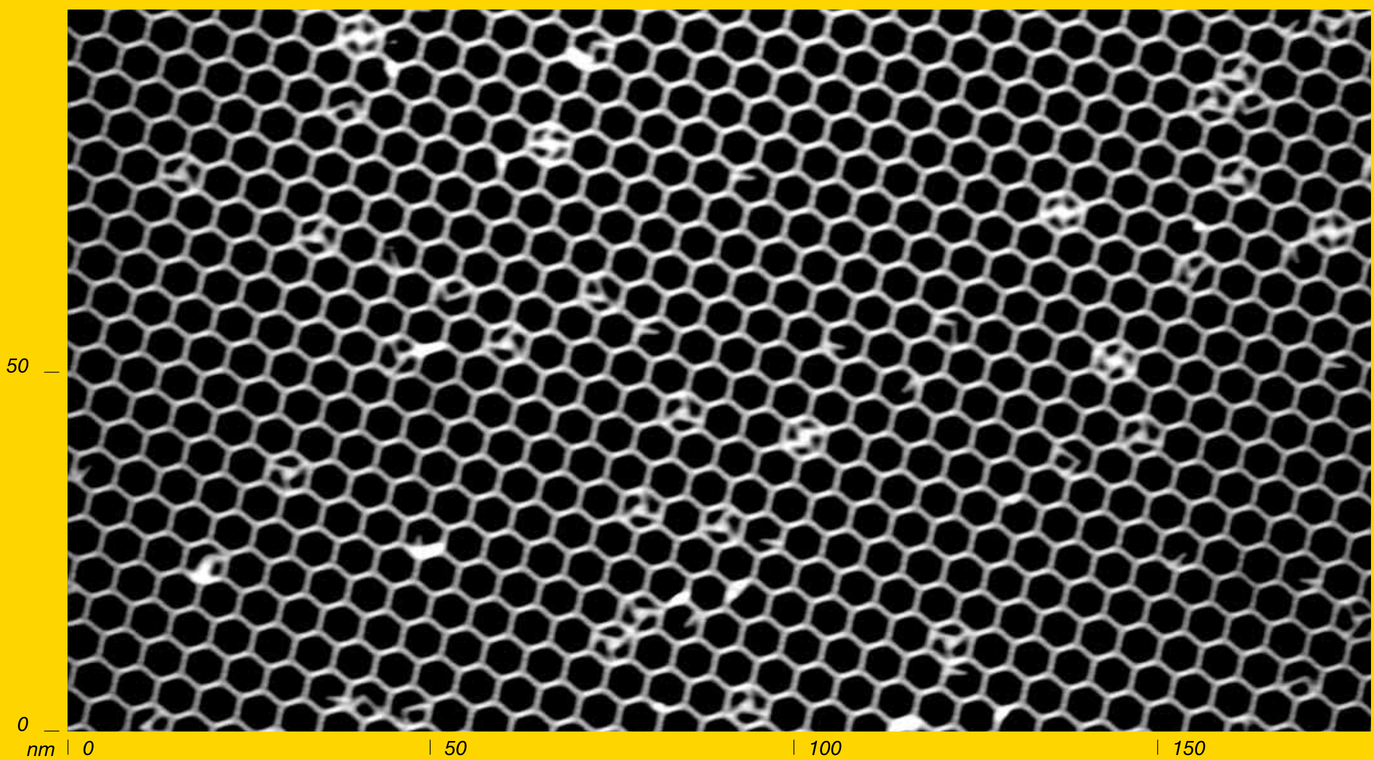
the scanning tunneling microscope (STM). This microscope scans the surface with the overlying structure and measures the local density distribution of the electrons. It allows the researchers to track what happens at the atomic level if one of the players undergoes a change. “In this way, we can follow structure formations and dynamics with molecular- or even atomic-level precision. The scanning tunneling microscope along with other techniques provides a rounded picture,” says Barth. The team can also track the nature of diffusion processes on a surface. Other methods, such as X-ray photoemission spectroscopy or computer-aided (simulation) models, are used to investigate the resulting structures and their properties. X-ray absorption spectroscopy provides complementary information on the chemical composition, geometry or magnetic features. Computer-aided simulation models reveal the bond characteristics and the nature of the underlying processes and driving forces.

The inner workings of a honeycomb

What are two-dimensional, metal-organic coordination networks exactly? Well, they can be created, for example, when cobalt atoms and rod-like organic molecules acting as connectors are vapor-deposited consecutively onto a silver substrate. Then they form a strikingly regular “honeycomb” structure no more than one atomic layer thick. This is a network of many, side-by-side hexagonal cells only a few square nanometers in size. The cobalt atoms define the six corners of the cell and the organic molecules the rims. The fact that a network of hexagonal cells is formed rather than simple chains is down to the fact that the cobalt atoms prefer to “bond” at the corners of the cells in three directions. The researchers varied the length of the linkers and observed what happened. Together with their cooperation partners from the Karlsruhe Institute of Technology, they discovered that the size of the cells or pores (e.g. 24 nm^2) can be systematically adjusted through the length of rod-like organic molecules. The players repair any faults in the network themselves. So what happens when the network is fully developed and additional “rodlets” are vapor-deposited? The answer is something astonishing, which also took the TUM researchers by surprise. Three small rodlets tend to accumulate in certain cells of the honeycomb, while other cells remain empty. It seems that it is more energy-efficient to gather in one cell as a threesome than for each to occupy its own cell. Highly detailed observations with the scanning tunneling microscope reveal why this is so. The three rod-like molecules arrange themselves in this way because they can form a node while their ends simultaneously interact with the edge of the pore. Viewed from ▷

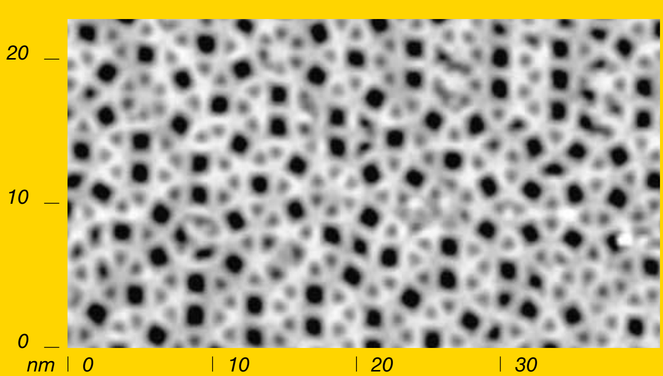
Picture credits: Filser, TUM

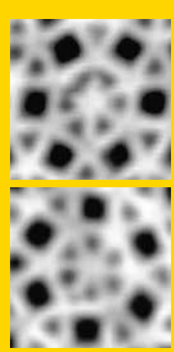


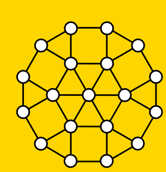



24 nm^2

Cobalt atoms and rod-like organic molecules (see page 79) form a “honeycomb” nanomesh no more than one atomic layer thick when deposited onto a silver substrate. If additional “rodlets” are vapor-deposited onto a fully developed network they assemble in certain cells of the honeycomb, forming a three-blade rotor whose movement the physicists can control by adjusting the temperature. The above images show the rotation at a temperature of 64 kelvin, 204 seconds elapsed between subsequent stages.







The influence of the metal atom on the nanostructure. While cobalt atoms and organic molecules called cyano-linkers yield a “honeycomb” nanomesh (top), replacing cobalt with europium leads to a radically different structure with quasi-crystalline order characteristics.

> *"The phenomenon of self-assembly is incredibly fascinating and multi-faceted."*
>
> *Johannes Barth*

above through the STM, the pattern looks like a three-blade rotor. This arrangement of the molecules is so robust that additional energy in the form of temperature increase does not cause the trio to disintegrate. "This movement is not a rotation in the usual sense, but rather a sequence of transitions between four different states." By turning the temperature knob, the TUM researchers were able to determine the energy threshold at which the dynamics sets in.

Research to advance photoresponsive nanosystems

Besides other functionalities, architectures and units with promise for photoactive device elements are explored. Dr. Carlos-Andres Palma has, for example, developed refined concepts in the study of sunlight as a source of energy. If dye molecules, that is molecules that are able to absorb light of a particular wavelength, are brought with a complementary species to a monolayer sheet of graphene (a form of carbon organized in two-dimensional honeycomb structures), they will self-assemble into a network because of the large number of hydrogen bonds expressed. The dyes absorb light energy at a wavelength of 740 nanometers. As a result, electrons are displaced and induce a photocurrent, that can be detected with the help of a gallium counterelectrode. It is therefore possible to create a photoactive structure at the monolayer scale to convert sunlight into electricity. Dr. Joachim Reichert investigated how even individual large molecules can be used in practice for photovoltaic and photoelectrochemical purposes. The pertaining experiments show that it is possible to specifically control an individual molecular unit as a component of an optoelectronic nanoelement and use its natural functionality for photovoltaic applications. The researchers employed a special biomolecule called Photosystem I (PSI), which plays a key role in photosynthesis. Laser light is used to trigger a series of redox reactions, that is, chemical transformations in which one partner transfers electrons to the other. In the course of this sequence, one electron is transported along a transmission chain from one side of the protein to the other. The resulting photocurrent flow is surprisingly large – approximately 10 picoamperes or 10 trillionths of an ampere.

Heterogeneous catalysis and molecular nanowires

Exploring "true" chemical reactions on the nanoscale is the research focus of Dr. Klappenberger. In this work, the substrate surface, for instance a noble metal lattice, effectively replaces the test-tube. The reaction steps at the interface are vastly different to those that take place in solution environments. Here, the reactions go beyond the concept of self-assembly; proper electron pair bonds or atomic bonds between carbon atoms are formed. So how did the researchers approach the task? Everything revolves around organic molecules consisting mainly of a carbon skeleton with highly reactive carbon-containing end groups. Already at room temperature, bonds are formed between the molecules confined at a silver substrate. The metal surface becomes a catalyst that helps to lower the energy barrier for direct coupling between two terminal carbon atoms of neighboring molecules. What follows is an intricate reaction pathway culminating in atomic carbon-carbon bonds. This results in one- and two-dimensional nanostructures related to the hypothesized materials graphdiyne and graphyne, which are closely connected to the two-dimensional carbon lattice graphene. On account of some of its properties, graphene has limitations as an electronic component, whereas graphdiyne and graphyne are perfectly suitable for such applications. Physicists love to experiment, and in this case they had the idea of polishing the silver substrate surface to give it a step-like structure. Their thinking was that molecular chains would be able to form along the steps from the carbon-based molecules used. And that is exactly what happened. These chains could be described as wires, capable of acting as a medium to transport electricity for high-frequency components in the gigahertz or terahertz range. As for the two-dimensional graphdiyne structures and their nanopores, they could serve as a type of "prison" for guest molecules or as a hydrogen store in the batteries of the future.

The human factor

The basic research on new structures at the interface being undertaken in Barth's Chair goes far beyond the projects described. The physicists are also exploring the know-how needed for application-oriented research. "High-level scientific output relies on innovative ideas and concepts. It can only be achieved by combining a dynamic work environment with excellent equipment mastered by promising doctoral candidates and postdocs," comments Barth. They are encouraged with plenty of freedom to develop their own creativity and potential, but at the same time he is always available and ready to listen to any problems or questions. "His level of awareness is just amazing," praises a young investigator from the research group.

Gerlinde Felix

"High-level scientific output relies on innovative ideas and concepts. It can only be achieved by combining a dynamic work environment with excellent equipment mastered by promising doctoral candidates and postdocs."

Johannes Barth

Head of a scanning tunneling microscope which the group uses to manipulate and analyze the structures they created. The tip of the STM is pointing towards a copper surface mounted on the sample holder.

Authors

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Gerlinde Felix is a freelance journalist for medical and scientific topics. She holds a degree in physics and attended medicine courses at the university. Gerlinde Felix has been working as an author for newspapers, magazines and online publications for many years.

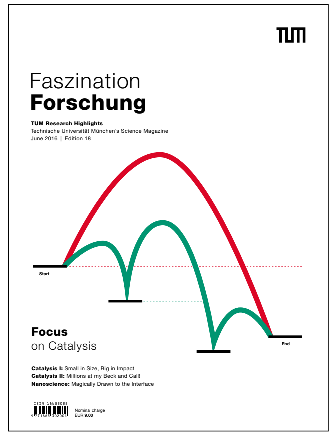
Birgit Fenzel studied German language and literature, philosophy and educational sciences before starting her career in journalism. After finishing university and completing a year of voluntary service, she worked as an editor for a daily newspaper, also completing freelance assignments for other public service broadcasters. She worked on scientific articles for the ddp news agency and was most recently employed as an editor at the Max Planck Society.

Patrick Regan has been a member of the TUM Corporate Communications Center since 2009. He came to TUM from PBS and NPR affiliate New Jersey Public TV and Radio in the US, where he produced 800 news reports on science and technology and hosted two interview series. In prior work at Bellcore and Bell Labs, he served as a science writer, magazine editor, executive speech writer, media relations manager and corporate spokesperson. He is a senior member of the IEEE.

Dr. Brigitte Röthlein has been working for many years as science author for magazines, TV and radio broadcasting and for newspapers. She holds a diploma in physics and a Ph.D. in communication science, education science and history of natural sciences. Her main interest lies in basic research.

Tim Schröder is a freelance science journalist based in Oldenburg, Germany. He works as an editor for the daily "Berliner Zeitung" newspaper, also regularly contributing to the "Frankfurter Allgemeine" (Sunday edition), "Neue Zürcher Zeitung" and "Mare" newspapers. His specialist areas are basic and applied research, energy and the environment.

Claudia Steinert studied biochemistry in Leipzig, Germany. Between 2010 and 2013 she worked in the press office of several institutes of the Max Planck Society. In 2013 she started freelancing as a science journalist. She is currently studying journalism at the Deutsche Journalistenschule (German School of Journalism) in Munich. Her articles focus mainly on ecology and health.



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Getting a Grip

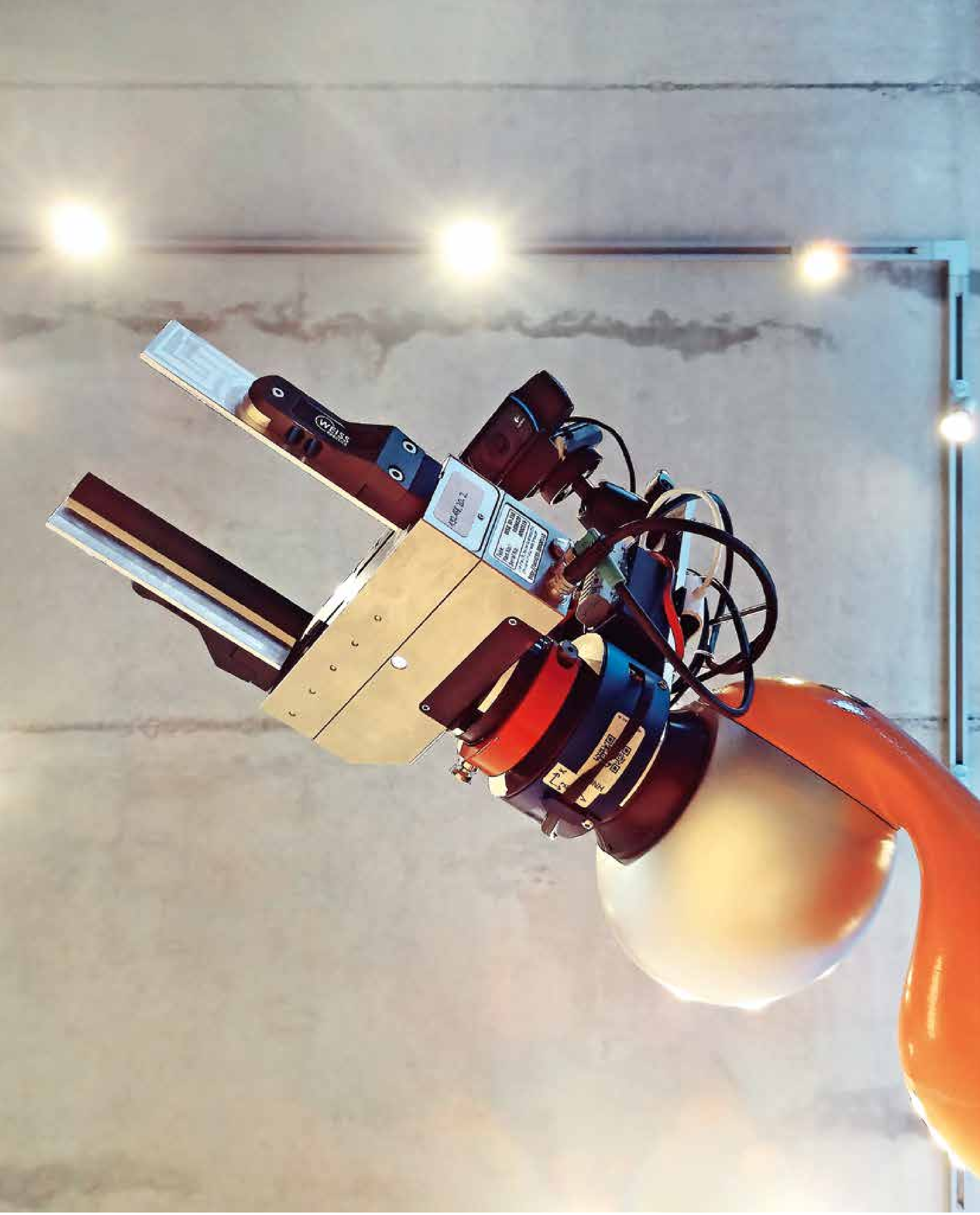
Industrial robots are engineered for extreme levels of precision, using sophisticated sensors to grab and manipulate objects with millimeter accuracy. However, they are also very expensive. That fact prompted Prof. Eckehard Steinbach and his team to develop a light and affordable robot that doesn't need costly sensors thanks to camera-enabled motion control. This machine is particularly suitable for smaller industrial companies that are currently priced out of the robot market.

Tim Schröder

Einfach greifen

Industrieroboter sind Präzisionsmaschinen, die dank ausgeklügelter Sensorik millimetergenau zupacken können. Doch diese Geräte sind teuer. Das Team von Prof. Eckehard Steinbach hat deshalb einen leichten und erschwinglichen Roboter entwickelt, der seine Bewegungen mit einer kleinen Kamera kontrolliert – und ohne teure Sensoren auskommt. Das Gerät eignet sich vor allem für kleinere Industrieunternehmen, die bislang wegen der hohen Kosten auf Roboter verzichten.

Moderne Industrieroboter sind Hightech-Maschinen. In ihren Gelenken sitzen jede Menge Sensoren, die Kräfte oder Drehmomente präzise messen. Solche Roboter können einen Punkt im Raum auf wenige Zehntel Millimeter genau anfahren, ohne dass etwas wackelt. So ein Roboter-Arm für die Industrie kostet mitsamt der Sensorik aber schnell einmal 100.000 Euro oder mehr. Für kleine Unternehmen sind Roboter damit oftmals unerschwinglich. Steinbach, Leiter des Lehrstuhls für Medientechnik der TUM und sein Doktorand Nicolas Alt haben deshalb ein kostengünstiges Robotersystem für kleine und mittelständische Unternehmen entwickelt, das eine Bewegung nicht mithilfe vieler teurer Sensoren überwacht. Stattdessen wird das Greifen ganz einfach mithilfe einer kleinen Kamera beobachtet und gesteuert. Das ROVI (Roboter Vision) genannte System nutzt einen Greifer, dessen Backen aus einem robusten Gummi bestehen. Greift der Roboter, werden die Gummibacken langsam zusammengepresst. Und diese Verformung nimmt die Kamera wahr. Damit kann das System ganz ohne Kraftsensor sehr genau einschätzen, wie stark der Gegenstand gepackt wird. Zugleich beobachtet die Kamera die Verformung des Gegenstands, um zu verhindern, dass dieser zerquetscht wird. Da sich jeder Gummityp bei einer bestimmten Kraft anders verformt, wird dieser vor Beginn der Experimente genau vermessen. Aus der Verformung des Gummis im Kamerabild kann der Computer später die momentan aufgewendete Kraft ermitteln. In ersten Experimenten konnten die Forscher sogar weiche Plastikflaschen greifen; eine Aufgabe, an der herkömmliche Roboter oftmals scheitern. Steinbach geht davon aus, dass ROVI nur den Bruchteil eines herkömmlichen Industrieroboters kosten wird. Das ist entscheidend, um klein- und mittelständische Unternehmen zu erreichen. Derzeit wird ein Prototyp entwickelt, der genau auf industrielle Applikationen zugeschnitten ist. Denkbar ist, dass ROVI beim Sortieren von Kleinteilen oder beim Abpacken von Artikeln für den Versand eingesetzt wird. Eine weitere Anwendung wären Roboter für den Spiele- und Unterhaltungsmarkt, beispielsweise für Roboterbausätze. □



A low cost robot gripper with precision: The ROVI system employs gripper jaws made of rubber. When it grips an object, the rubber is compressed and a camera registers this deformation.

The aim is to develop a robot gripper that operates with precision but costs just a fraction of the price of an established industrial robot.

If you would like to test a robot's grip, just hand it an open detergent bottle or – even better – a Capri Sun juice pouch with a straw. The robot will obediently latch on to what you give it – and then, in most cases, make a huge mess. Today's robots can securely grasp firm objects as often as 10,000 times a day with sub-millimeter precision, but pliable objects such as plastic bottles and drink pouches still pose an insurmountable challenge for many of them.

Robots nowadays obviously feature the most sophisticated of technologies. Their joints contain numerous sensors that precisely measure forces and torques, and they can be positioned with an accuracy of a few tenths of a millimeter without wobbling. They can lift televisions or even entire car parts with ease and set them down with the utmost care. However, complete with sensors, the price of this type of industrial robot arm quickly soars to 100,000 euros or more – which usually proves prohibitive for smaller companies. That is why, some time ago, Eckehard Steinbach from TUM's Chair of Media Technology (LMT) began a new project along with his doctoral student, Nicolas Alt. They set out to develop an alternative robot gripper – a device that would operate with precision and dexterity but cost just a fraction of the price of an established industrial robot.

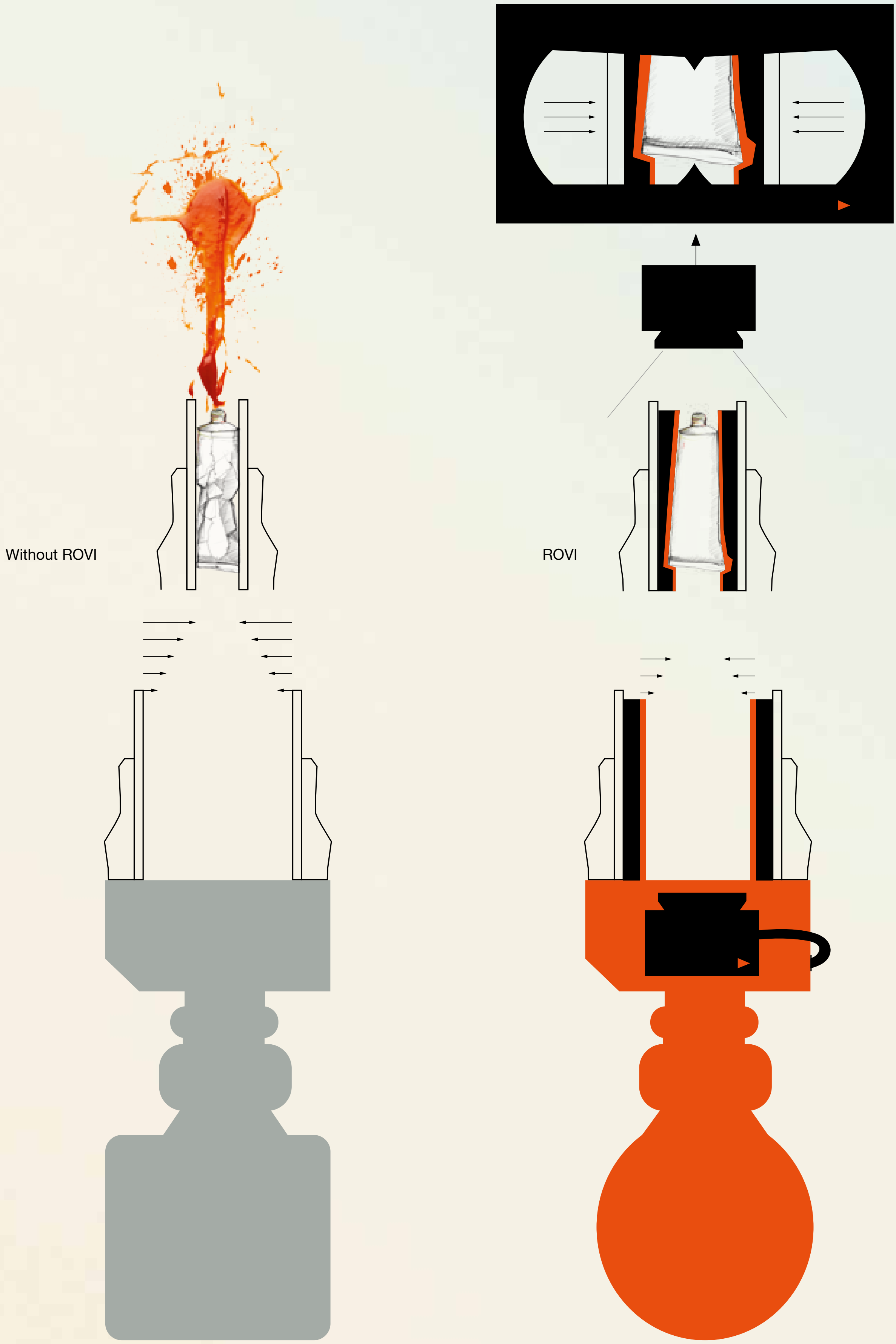
The team defined two clear design criteria at the outset: the new robot should be small and streamlined in order to reduce mass and thus cut manufacturing costs, and it should not involve expensive sensors or complex cabling. "Our aim was to develop a gripper concept that would also enable small and medium enterprises to automate simple and repetitive tasks," confirms Eckehard Steinbach. "A cost-effective robot that could sort small parts or help pack items for shipping, for instance."

Picture credit: Bauer

Gripper in focus

It was only a matter of time before the researchers had their brainwave: why not imitate the way people do it? When a person grasps something, they look at what they are doing. They size up the situation, set their sights on the object in question, put out their hand and then take hold. So the new robot should do the same. Instead of monitoring every motion with several expensive sensors, the device should simply use a small camera to observe and control its grip. The colleagues applied to the European Research Council and received funding in the form of an ERC Proof-of-Concept grant – not least because the focus on small and medium-sized enterprises means the robot has significant commercial potential.

Nicolas Alt focused his doctoral thesis on the development of this robot. And the fruits of his work with Steinbach over the past few years are certainly impressive. Extending beyond a single robot arm that can grip specific objects, the outcome is new concept where robots simply watch ▷



Picture credits: Bauer, iStockphoto; Graphics: ediundsepp

Robots can precisely grasp firm objects but pliable objects still pose a challenge – unless they are equipped with force and pressure sensors. The ROVI system determines the force from the deformation of gripping jaws made of rubber, which is picked up by a camera.

what they are doing. The machines in Steinbach's lab can use a bottle opener to push off crown caps, nimbly move objects to one side and even unscrew pliable plastic bottles – a challenge that continues to elude many more established machines. The duo calls their optical system ROVI – which simply stands for "robot vision".

Defined deformation

At first glance, the ROVI system seems surprisingly simple. The jaws of the gripper are made of robust rubber. When the robot grasps something, the rubber jaws are slowly compressed – and the camera picks up on this deformation. This means the system does not need a force sensor to assess with precision how hard the object is being gripped. At the same time, the camera also monitors distortion of the object, to avoid it being squashed. Since various types of rubber deform differently under any given force, this behavior is precisely measured prior to the experiments. The crucial factor is the extent to which the polymer is deformed by a specific force. "So we generate a characteristic curve that gives a very accurate picture of the plastic," explains Alt. "Based on the deformation of the rubber in the camera image, the computer can later determine the force applied at the time."

The measurements for bottle opening work a little differently. For this experiment, Alt attached the opener to the end of a metal rod. Once the opener was latched onto the crown cap, the robot slowly began to raise the rod, which was thus subject to gradual deformation. To measure this with the camera, Alt stuck a printed pattern to the rod. The further the rod was bent, the more distorted this pattern became in the camera image. In this case, then, ROVI deduced the force applied from the distortion of the photo. "The same principle could be used to measure the deformation of a robot arm when lifting a weight," adds Steinbach. "We could stick image templates to the joints and then monitor their distortion by camera." And the price of this would be negligible, since small cameras are already available for just a few euros.

The ROVI system is even able to guide small assistive robots. Vacuum cleaning robots, for instance, often use infrared beams to scan their surroundings. But infrared does not always work with transparent objects. Put a glass vase in the path of an assistive robot and the vase may well end up smashed. For this reason, Alt equipped his robot with a type of plastic bumper. As with the gripper jaws, a camera was used to monitor deformation of the plastic in this experiment. When the robot encountered an object, the system was well able to determine whether measured force could be applied to move the item out of the way or whether the robot needed to navigate its way around the immobile object.

Assembly line assistance

Needless to say, pushing vases out of the way is not the researchers' main preoccupation here. One of their aims is to advance ROVI to the point where it can perform small tasks for industrial companies with high precision and speed. "Of course, our optical system is not as accurate as a large industrial robot with sub-millimeter precision," concedes Steinbach. ROVI is not always on target with millimeter accuracy – it might be one or even two centimeters off. But that is not an issue, since the ROVI system continually checks itself. If the gripper is a little off the mark, the camera spots this and gives a command to correct the position. The correction process is so fast that ROVI exhibits smooth movement overall and the gripper reaches its target relatively quickly. This capability would be of particular interest if ROVI were to be used to pick and sort components on an assembly line, for instance. Steinbach also envisages applications in laboratories at research institutes and universities, where repetitive tasks such as pipetting fluids are currently still performed by lab technicians and students in many cases. An affordable ROVI would make an ideal assistant here. ▷

"I can only encourage young people to pursue a scientific career. There are now so many more opportunities to convert your own idea from a research project into a commercial product."

Eckehard Steinbach

Prof. Eckehard Steinbach

Fostering young scientists

For Eckehard Steinbach, there are many reasons why he enjoys his work as a researcher – including the desire to discover new things. "But another important reason is definitely that I find working with young people extremely enriching. There are so many talented up-and-coming researchers – and I learn more myself with every doctoral candidate." The ROVI robot gripper is an excellent example of this collaboration at work. Steinbach is an electrical engineer who has long been engaged in teaching machines to see – his focus lies on audiovisual media. And then he had the idea of incorporating touch in the form of gripping. But using a rubber gripper and monitoring its deformation by camera to measure forces was the brainchild of his postgrad.

"I can only encourage young people to pursue a scientific career," Steinbach confirms. "There are now so many more opportunities to convert your own idea from a research project into a commercial product." He feels the prospect of starting their own company can give huge impetus to young people in their research work. And, he observes, they can now take advantage of targeted training in entrepreneurial skills, for instance through events run by UnternehmerTUM (Center for Innovation and Business Creation at TUM), bringing participants up to speed on business plans or patent law.

Steinbach's own fascination with mathematics, physics and technology was evident at an early age. As a teen he was building his own amplifiers – for sound systems with proper power. Another thing that caught his enthusiasm early on was the international dimension of research – the opportunity to share scientific knowledge and tackle topics with people from other cultures and teams. Steinbach himself studied at the University of Essex in England and the ESIEE (Ecole Supérieure des Ingénieurs en Electrotechnique et Electronique) in Paris. He later took a postdoc job in the Information Systems Laboratory at Stanford University in the US. And today, flanking his professorship at TUM's Chair of Media Technology, he is also foreign student advisor for his faculty and coordinator of international research partnerships, reflecting his commitment to sharing his overseas experiences with the next generation.

Picture credit: Bauer

Vacuum cleaning robots normally use infrared beams to scan their surroundings. But that does not always work with transparent objects.This robot is equipped with a type of plastic bumper. A camera monitors deformation of the plastic.

When the robot encounters an object, the ROVI system detemines whether measured force can be applied to move the item out of the way or whether the robot needs to navigate its way around it.

“Our aim is to build the ROVI prototype, so we can show just how well this technology works in real industrial applications.” *Eckehard Steinbach*

As with many other developments that look astoundingly simple at first, the devil is in the detail with ROVI. “We developed an entire toolbox of technologies for ROVI,” confirms Steinbach. The researchers first had to investigate the correlation between force and deformation. To describe this relationship mathematically, they carried out measurement experiments with an industrial robot equipped with force sensors. However, gripping was not the only aspect – they also had to cover image analysis. To interpret distortion on the photographs, for instance, ROVI needed a software system that could recognize templates and track their movements in the camera image. Another aim was dynamic and high-resolution analysis of the material deformation, which meant the researchers writing special algorithms. And both scientists were keen for ROVI to be able to identify transparent objects such as plastic bottles too. Traditional programs for recording surroundings with 3D cameras are not able to accomplish this, so they had to devise new algorithms here as well.

Lightweight and affordable

Steinbach anticipates that ROVI will cost just a fraction of the price of a conventional industrial robot – probably a few hundred euros. This is key to reaching small and medium-sized companies. So it comes as no real surprise that the European Research Council has agreed to fund Steinbach and Alt’s project for another 18 months. “We intend to use this time to develop a prototype that is precisely tailored to industrial applications,” reveals Steinbach. “At the same time, we will be conducting market analysis to ensure our plans remain in line with industry requirements.” To achieve this, Steinbach is currently seeking industry partners who see a need for a small and light ROVI system. Robots for the games and entertainment market would also be a potential application, for instance as part of robot kits.
ROVI’s future development path when ERC funding runs out has not yet been mapped. Steinbach could imagine bringing the robots to market via a start-up company or licensing the technology to larger robot manufacturers. “But for now our aim is to build the ROVI prototype, so we can show just how well this technology works in real industrial applications.”

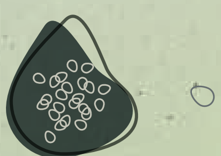
Tim Schröder

Picture credits: Bauer

The Search for Efficient Processes to Generate **Green Crude**

Crude oil

400 dollars
per ton of fossil kerosene



1.4 percent of global CO_2 emissions

The production of “green aviation fuels” from algae is not yet commercially viable because of the extensive costs and amount of space required. Researchers from the Industrial Biocatalysis Group at TUM are looking to change that.

Global aviation industry

1.7

1.7 billion liters
of kerosene per year

1.7 cubic hectometers or volume of water in the Ammersee near Munich

Algae

2,000 dollars
per ton of biokerosene

No additional CO_2 emissions

Estimates of the area needed to produce enough algae to cover the EU's total fuel requirements:
92 km²–580,000 km²

Graphics: ediundsepp

TUM has built a globally unique AlgaeTec Center in cooperation with Airbus Group. This high-tech facility located at the Ludwig Bölkow Campus in Ottobrunn/Taufkirchen is a new innovation hub for the development of sustainable biokerosene production processes based on algae biomass.

Picture credit: Heddergott

Bernhard Epping

Kerosin aus Algen – die Suche nach der Billigproduktion

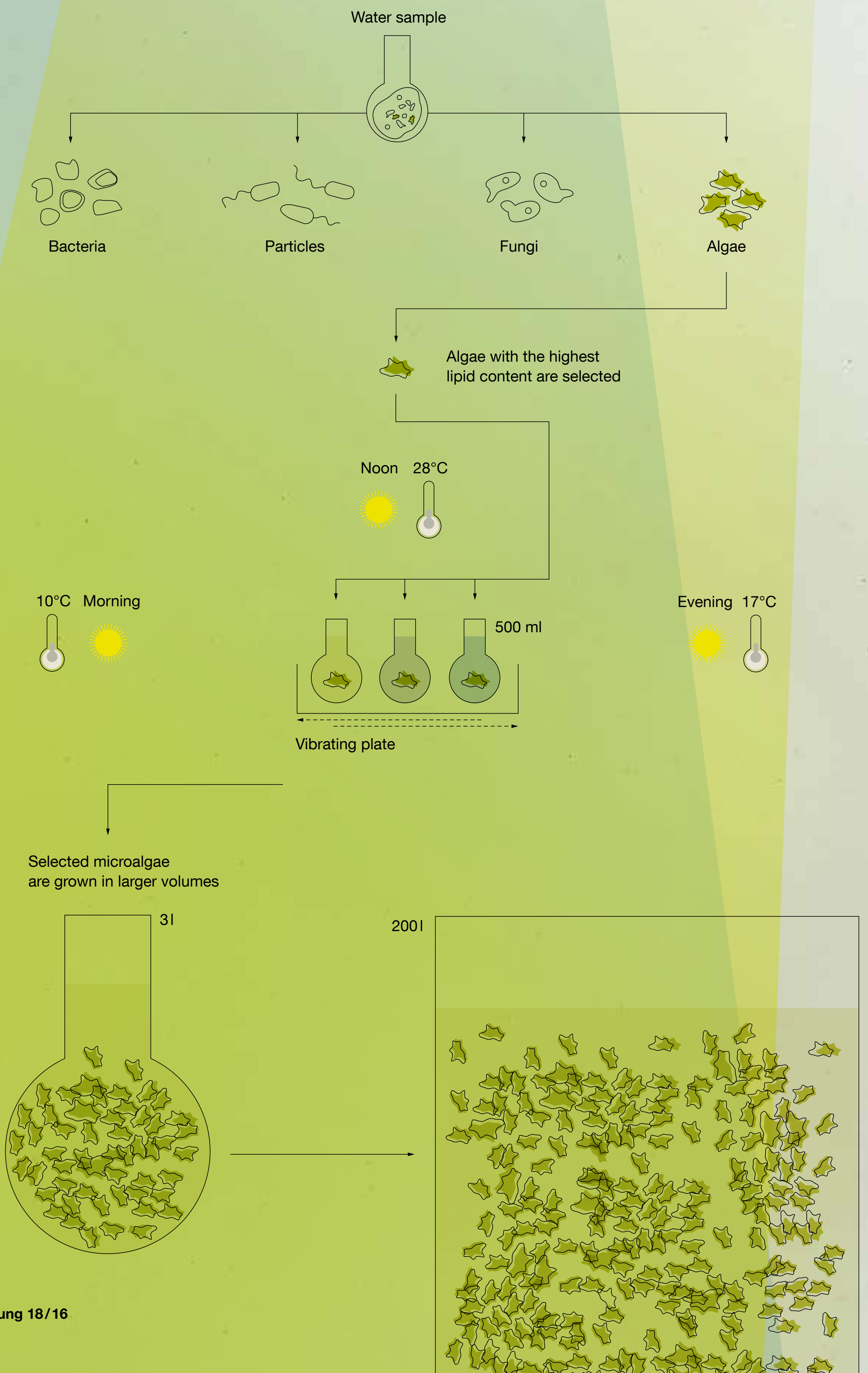
Das Fachgebiet für Industrielle Biokatalyse der TUM in Garching unter der Leitung von Prof. Thomas Brück koordiniert mehrere Großprojekte für die Entwicklung einer neuen Rohstoffbasis für Kerosin aus Algen.

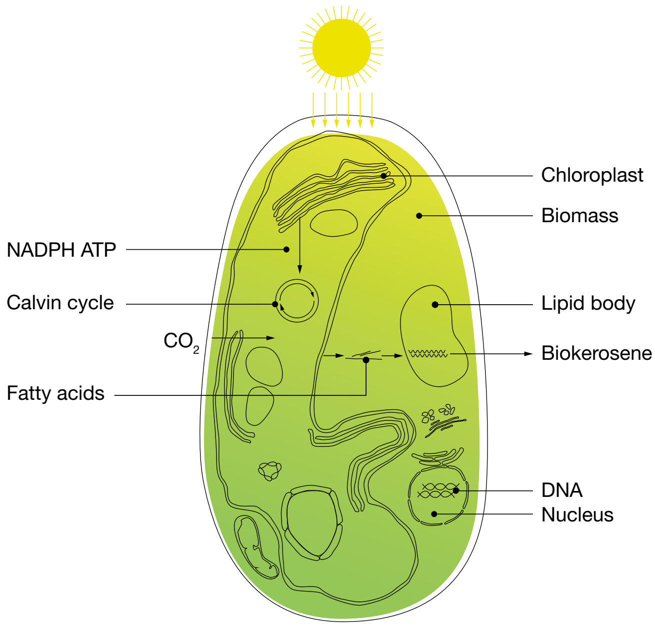
Mikroalgen gelten zwar schon seit einigen Jahren als Kandidaten für die Produktion von Lipiden, die sich danach chemisch-katalytisch zu Kerosin reduzieren lassen. Weltweit fehlt allerdings ein Durchbruch zu einer auch wirtschaftlich konkurrenzfähigen Produktion.

Ein Teil des Problems ist die bislang oft zu unsystematisch betriebene Forschung auf diesem Gebiet. Die TUM-Projekte setzen daher auf eine systematischere Optimierungsarbeit auf allen Ebenen der Prozesskette. Nach drei Jahren erster Forschungsarbeit deuten sich bereits Verbesserungen an.

Ein Screeningprogramm fahndet nach Algenarten, die von Natur aus besonders hohe Mengen an Lipiden synthetisieren. Im Fokus stehen Algen, die von Natur aus im Meerwasser oder noch salzhaltigeren Gewässern vorkommen. Das erlaubt in Sachen Sterilität und CO_2-Sättigung der Nährlösungen eine besonders stabile und damit preiswerte Prozessführung. Gute Lipidproduzenten sind Vertreter aus zwei Gattungen von Grünalgen, genannt *Scenedesmus* und *Picochlorum.* Ein neu entwickeltes Anzuchtprotokoll lässt unter Stickstoffmangel-Bedingungen einige Arten bis zur Hälfte ihrer Biomasse als Lipide synthetisieren, ohne dass die Organismen ihre Teilung, alias ihr Wachstum, einstellen. Bislang hörten Algen unter solchen Nährstoffbedingungen mit dem Wachstum auf. In einem 2015 neu errichteten Algentechnikum in Ottobrunn, Landkreis München, ist auch die Optimierung von Anzuchtbedingungen im bis zu 200-Liter-Maßstab möglich. Es ist die letzte Stufe, der größte Versuchsmaßstab vor dem möglichen Start einer industriellen Produktion. Das Forschungskonsortium um Prof. Brück schätzt den Zeitbedarf für weitere großtechnische Erprobungen auf sechs bis zehn Jahre. Danach könnte eine erste industrielle Produktion in Kooperation mit Firmen starten. Eine Algenproduktion wird es, wenn überhaupt, in tropischen Regionen oder im Mittelmeerraum geben. Die TUM könnte sich aber sehr wohl auf Dauer als Forschungs- und Entwicklungszentrum etablieren. □

Identification of the most process-relevant microalgae from environmental samples. Algae with the capacity to generate a high intracellular lipid content are initially grown in a 500 ml shake flask utilizing specific climate and light conditions.





Algae consume CO_2 for growth and release the same amount when burned as fuel. Algae which produce lipids as energy stores form the basis for biofuels.

Link

www.ibc.ch.tum.de

Green, roundish in shape and not particularly exciting to look at as they float around individually or sometimes in groups. Such is the life of *Scenedesmus* sp. algae. “Oh look, one of them is swimming.” “Not exactly,” says Ph. D. student Johannes Schmidt. “They can’t move by themselves – they are propelled by gentle flows in the nutrient solution.” The tiny algae, each one measuring only a hundredth of a millimeter, are lying on a slide which Schmidt has just positioned under a microscope. They belong to a species known as green algae. Since they contain chlorophyll, they are able to photosynthesize like land plants; in other words, produce all the compounds they need – fats, sugars and proteins – from water, carbon dioxide (CO_2) and the sun’s light energy. “We gathered this *Scenedesmus* strain from the silty shores of the Baltic Sea – from a sort of lagoon known as a bodden,” explains Schmidt. These little unicellular organisms live for just a few weeks, reproduce by division and, sad but true, often end up being devoured by small crustaceans or fish.

High volume production is the key

The exact species is strictly classified information. Understandably so – in just a few years, this microalgae could produce large volumes of crude for biokerosene, a sustainable fuel for jet engines. First though, the process chain has to be developed, in complete secrecy, although a number of patent applications are in the pipeline. “Progress in this field will require an interdisciplinary approach and cooperation with industry,” maintains Prof. Thomas Brück, head of the Industrial Biocatalysis Group at TUM. For the time being, the researchers are keeping their cards close to their chest.
Biokerosene is yet another biofuel with the potential to help relieve rising climate mitigation pressures. The global aviation industry currently consumes 1.7 billion liters of kerosene per annum, thereby contributing 1.4 percent to global CO_2 emissions. So far, the industry has escaped regulations to cap emissions. In 2013, however, the International Air Transport Association (IATA) set its members the target of halving CO_2 emissions by 2050 – with 2005 as the base year. More efficient jet engines are already being produced, but that measure by itself will not be enough in the face of rising passenger numbers. “A sustainable raw material will be needed as well,” explains Brück. ▷

Picture credit: Bauer, Graphics: ediundsepp (source: TUM)

Certain microalgae are able to synthesize oils and fats naturally, using these lipids as energy stores. Scientists have the technology to isolate these lipids and reduce them to kerosene by means of a chemical reaction called hydrodeoxygenation. The end product is just as effective as the crude oil equivalent. Kerosene, composed of straight-chain alkanes and hydrocarbons with 10 to 16 carbon atoms per molecule, has the highest energy density of all fuels.

So the process is viable in principle. The problem is that it is much too expensive. The current price for a ton of biokerosene is USD 2,000, whereas the conventional fossil version was selling at less than USD 400 at the start of the year. Added to this, with the current state of the technology, the EU alone would need to cover an area at least the size of Portugal with algae tanks in order to meet its total fuel requirements. This calculation was undertaken by Maria Barbosa and René Wijffels from Wageningen University and Research Center. “That is optimistic, under current process conditions. It would more likely be the whole Iberian peninsula,” comments Brück. The reason for this huge footprint is that since they require light, algae live on the surface of the water, descending only a few millimeters or maybe a few centimeters at most.

Of the 27 staff employed at IBC, eight work in the field of algae biotechnology together with half a dozen project partners, including Airbus Group. With this powerhouse of knowledge, Brück plans to accelerate the momentum in this particular research field. “What we need is a more systematic approach to the research in order to identify improvements all along the process chain. This is the only way to bring the cost down.” The IBC has been working on two major projects to this end since 2013. The first is “AlgenFlugKraft” (AFK; Algae Powered Aviation), financed by the Bavarian Ministries of Economic Affairs and Science. The goal is to produce lower-cost biokerosene jet fuel from algae. Then there is the Advanced Biomass Value (ABV) project, which is being funded by Germany’s Federal Ministry of Education and Research. Here, the researchers will be working on an intermediate step – certain algae will initially be used to produce special greases and oils as industrial lubricants. The biomass remaining after extraction of the lipids will then be transformed into kerosene with the help of special yeasts and novel chemical processes.

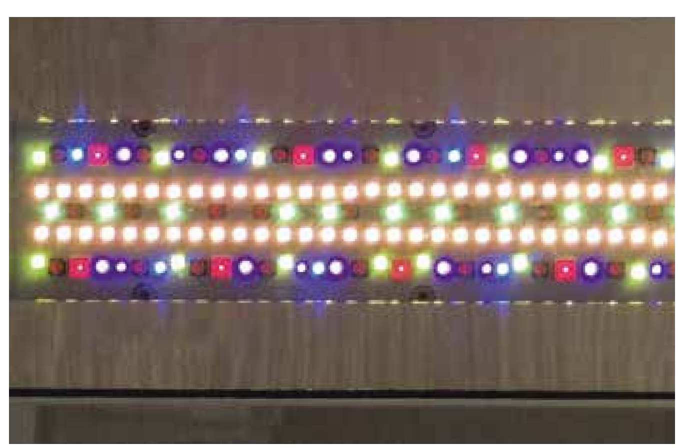
Finding suitable algae candidates

This first step involves painstaking and systematic screening of suitable varieties of algae capable of producing lipids. There are between 40,000 and 150,000 species of microalgae, microscopic single-cell organisms like *Scenedesmus*. The huge span of this estimate shows just how little scientists actually know about these organisms. A mere dozen species have been exploited commercially to date as food supplements as they have been found to be good sources of protein, starch and pigments. When it comes to “lipid specialists”, however, science seems to have drawn a complete blank thus far.

And so the search is on. Researchers at IBC are even on the lookout while on vacation – bringing water and soil samples back from selected locations so that algae can be isolated from them. A FACS (fluorescent activated cell sorter) then gets to work, automatically separating the green-glowing microalgae from the other particles, bacteria and fungi in the samples. “In a second step, we add a pigment which specifically binds to lipids. Our FACS device selects the microalgae with the highest lipid content for us,” says AFK project leader Dr. Daniel Garbe as he pats the large gray box in a corner of the lab. “Then we carry on from this vantage point.”

The IBC has already collected more than 50 proprietary strains of algae. Safely stowed in metal cabinets under lighting and kept in small sterile flasks and test-tubes – all of the painstakingly acquired species are subject to contracts concluded in accordance with the Nagoya Protocol to the Convention on Biological Diversity. This protocol guarantees the country of origin a share of the benefits if a species from their territory proves to be commercially successful.

Iteratively, test after test establishes whether and how these algae can be optimized for lipid synthesis. In practice, this means growing them at different temperatures and light conditions, and using different concentrations of salt, nitrogen and phosphorus in the nutrient solution. In stage 1, the same amount of starter culture is automatically pipetted into the 96 wells of a plastic tray. In accordance with the different protocols developed, widely varying concentrations of sodium chloride and nutrients, primarily nitrogen and phosphorus, are also added. Then it is off to the bioreactor, where the light levels and temperatures change as the day progresses. A few days later, the researchers test the optical density with a photometer, checking how well the algae have grown in each of the experimental conditions – and how much lipid content they are storing. ▷



Proprietary LED based lighting simulates the different radiation intensities and spectral characteristics found in latitudes from the Baltic to the tropics.

The AlgaeTec Center allows simulation of the climate and illumination of any potential production site. The Brück-led research consortium developed an optimized "cascade" cultivation system, which encompasses two small steps that have been incorporated into the 200 liter tanks. Gravity causes the algae cultures to flow down into the next-lowest tank. In the collecting basin at the bottom, the entire solution is re-saturated with CO_2 and then pumped back up to the highest level.

Picture credits: Bauer

A focus on saltwater species

This project has already managed to establish a number of new basic strategies. The future lipid-producing algae will be at home in briny water. Seawater has a salt content of 3 percent, but some ponds and lakes in tropical regions in particular have salt levels of 10 percent and higher. “We love species from biotopes like these,” underlines Brück. Any organism that is able to survive in such harsh, even hostile, conditions, will be particularly adaptable to large-scale cultivation. There will be little need for disinfection, as the high salt content will take care of most potential competitors like bacteria and fungi. Another advantage from the researchers’ perspective is the fact that CO_2 dissolves particularly well in alkali salt water in the form of bicarbonate ions ($(HCO_3)^-$). This is the form in which algae are able to utilize CO_2. In fresh water, the gas does not dissolve as readily. “The use of saltwater species therefore makes the overall process much more efficient,” explains Brück.

Thanks to the new nutrient solution protocols developed by the Brück group, the algae are for the first time able to form lipids and still keep on growing. Previously, it was not always possible to combine the two. Garden pond owners will know that high levels of nitrogen in the water promote algal growth. In order to yield the maximum amount of lipids, the algae must be deprived of nitrogen. In this particular metabolic state, they can no longer create their favorite product, nitrogenous proteins, so they switch to oils instead. Frustratingly, they usually also stop growing at that stage, too. Until now: *Scenedesmus*, which in its natural form has a lipid content of around 10 percent, has been plumped up to 40 percent lipids thanks to a new cultivation medium devised by the lab researchers in Garching. Interestingly, despite being deprived of nitrogen, the algae are happy to keep on growing. Even more surprisingly, this impressive feature has been outperformed by a microalga of the genus *Picochlorum* which was originally collected from a hypersaline lake in the Bahamas: “*Picochlorum* is our champion. It grows extremely quickly, 15 times faster than *Scenedesmus*, and is currently already forming oil stores of up to 30 percent in each cell,” enthuses Brück. Ramping up the oil production to 50 percent and above is only a question of finding the right media, and the team are already on the case.

Scaling up

The next stage involves scaling up – there is no guarantee that an alga that performs well in the test-tube will also thrive in large tanks. As part of phase two in the lab, the candidates will first be cultivated in 500-milliliter flasks, and after that in three-liter photo-bioreactors. This will reveal whether *Scenedesmus* and *Picochlorum* are on track.

Technical enhancements in the lab will help. It is important for climate conditions to be simulated as realistically as possible; otherwise the entire screening process will produce nothing more than artifacts. Lighting is the key factor. ▷

Prof. Thomas Brück

Exploring marine algae for industrial applications

For Thomas Brück, successful research revolves around interdisciplinary cooperation, ideally also engaging with relevant industry partners.

Born in Cologne in 1972, Brück decided to move to the UK to conduct interdisciplinary studies in natural and social sciences for his undergraduate degrees. After receiving double Bachelor degrees in chemistry and biochemistry with a subsidiary in management science, he went on to complete his Master of Philosophy in molecular medicine at Keele University in Stoke-on-Trent, England. In 2002, he was awarded the title of Doctor of Philosophy at the University of Greenwich (London), for his studies in biochemical reaction mechanisms of the peroxidase enzyme family. Subsequently, Brück moved to Florida Atlantic University, Boca Raton, USA, where he developed an interest in marine algae. For the next few years the biochemist focused on isolating and exploring the structure of pharmacologically relevant compounds derived from marine coral, which are produced in conjunction with symbiotic algae.

In 2006, Brück returned to Germany to take up a position in industry. He started as research manager at Süd-Chemie AG (acquired by Clariant in 2011) before taking up the position of Technology and Patent Portfolio Manager two years later. In 2010, he returned to the world of academia, becoming head of the research group for Industrial Biocatalysis (IBC) at TUM, where he and his team managed to acquire significant funding for projects focusing on biochemical process development for biomass valorization in order to generate sustainable biofuels, platform chemicals, polymeric materials and new pharmaceutical compounds. He is very matter-of-fact about his research. Although he does maintain that research into algae has been grossly neglected around the world. He is convinced that there is a very high chance that algae will provide a sustainable source of biokerosene and also form the basis for new drugs.

Brück is married, with two children aged seven and three. His family is truly international, speaking both German and English at home, since Brück’s wife Diane is British.

Picture credit: Bauer

"Being able to simulate all kinds of climate conditions in this one place gives us a huge advantage when it comes to selecting the most suitable candidates for biokerosene production." Thomas Brück

In many labs, the light fed to algae for photosynthesis in previous tests was much gloomier than the daylight they were used to in their natural environment. Brück reveals that microalgae often had to make do with light in wavelengths between 500 and 600 nanometers in past studies. But visible light alone has a wavelength range between 380 and 780 nanometers, and on top of that a certain amount of UV light also seems to play a major role in effective lipid synthesis. Together with the Berlin-based SME FutureLED, the Munich-based researchers have developed proprietary LED-based illumination solutions that mimic a large portion of the sunlight spectrum. With these lights, they can simulate the different radiation intensities found in latitudes from the Baltic to the tropics.

Without the LED lights, *Scenedesmus* would probably have never made it past the screening. Which would have been a mistake. As this species is native to the Baltic Sea, conventional biology theory would contend that it should be optimally adapted to the test location. It should in fact perform best under Baltic conditions. On the contrary, the algae reached lipid values of 40 percent during the preliminary experiments only when the scientists ramped up the light intensity and temperatures to Mediterranean levels. “The species clearly felt more at home in the climate of Almeria in southern Spain,” notes Brück. Which sets the scene for the third and final phase of the experiments at TUM. For this, the 1,500 m^2 glass-roofed AlgaeTec Center has been purpose-built on the Ludwig Bölkow Campus in Ottobrunn, south of Munich. The 10 million euros funding for the new facility has been provided by the state of Bavaria and the Airbus Group. Inaugurated in October 2015, it is at the very heart of the AFK project. Every kind of climate from tropical humidity to desert dryness can be simulated in the building, and Brück is keen to point out that no other facility in the world has these climate and light variation capabilities. All that can be heard within is a faint hum, while the eye is drawn to the bright green glow of *Scenedesmus* growing in the large open tanks, each currently with a

“Progress in developing high-volume production chains for algae will require an interdisciplinary approach and cooperation with industry.”

Thomas Brück

The final laboratory-stage algae process scale-up is realized in custom-built bubble column reactors holding 30 liters.

Picture credit: Bauer, Graphics: ediundsepp (source: TUM)

Brück and his team are testing algae from all over the globe with respect to growth efficiency. The new AlgaeTec Center allows them to simulate production conditions at any location. The most promising sites are expected to be situated in the Mediterranean or in the southern hemisphere.

capacity of 200 liters. The next scale-up level focuses on reaction volumes of 1,000–2,000 liters, which would provide data for industrial process realization. The design and planning for relevant algae cultivation systems is currently ongoing.
Another innovation is the optimized "cascade" cultivation system, which encompasses two small steps that have been incorporated into the tanks. Gravity causes the algae cultures to flow down into the next-lowest tank. In the collecting basin at the bottom, the entire solution is re-saturated with CO_2 and then pumped back up to the highest level. It is important to note that all of this happens at the gentlest pace. Algae cultivation experiments around the world still mostly rely on raceway ponds – large tanks in which the algae solution is vigorously pumped along long rather deep oval ponds. A certain amount of mixing is important to ensure that the cultures receive sufficient light penetration, which is reduced within just a few centimeters of the water column. "We have recently discovered, however, that many species do not cope at all well with mechanical stress," says Brück. Less agitation in the tanks therefore saves energy and reduces the facility's operating costs.

Identifying the best production locations
Brück hopes that his team will be able to offer industry customers the first algae strains for large-scale production of biokerosene in six to ten years. The Ottobrunn based AlgaeTec Center is well set to become a leading international facility for the screening of algae species. "Being able to simulate all kinds of climate conditions in this one place gives us a huge advantage when it comes to selecting the most suitable candidates for biokerosene production," underlines Brück.
After that though, it will be adios to Bavaria! The sunlight levels at this northerly latitude will not be strong enough for future biokerosene production. Brück is planning on moving his algae to more helpful southerly climates, perhaps the Mediterranean, California, Mexico, the coast of Chile or Africa. He has already reached out to potential cooperation partners in various locations. So, how much will the price of biokerosene come down? "It will become cheaper – but everything in its own time," assures Brück. After all, it took 150 years for oil refining to reach its current state of development. "We have a good few years of research and development to go yet," claims Brück. The algae researchers are only just getting into their stride. *Bernhard Epping*

The AlgaeTec Center in a Nutshell

1,500 **m²** area

2 **climate zones** can be tested independently

2–6 **weeks** is the duration of an algae production test

up to 4 **species** can be tested in parallel in two different climate zones

4 **cascade reactors** are currently in place (2 of 200 liters, 2 of 80 liters)

In the future, up to 7 **species** can be tested in parallel; additional cascades are being built for that purpose

Picture credit: Heddergott, Graphics: ediundsepp

Joe Kaeser

Joe Kaeser is President and Chief Executive Officer of Siemens AG, a global powerhouse in electronics and electrical engineering. He has over 30 years of experience at Siemens, where he has held a variety of leading management positions in finance and strategy both in and outside Germany.

Joe Kaeser began his career at Siemens in 1980 in the field of components and semiconductors, where he also worked in Malaysia and the U.S. In 1999, he joined the Corporate Finance department. In 2001, he was appointed Chief Financial Officer of the Information and Communication Mobile Group. From 2004 to 2006, he served as Siemens' Chief Strategy Officer. Immediately prior to his appointment as CEO in August 2013, Joe Kaeser had served as Siemens' Chief Financial Officer for seven years.

A new Chapter **in the History of Innovation**

Siemens to blaze new trails in research

A leading technology company like Siemens has to do everything possible to identify paradigm shifts in time and adapt to new realities. Today, digitalization is triggering paradigm shifts that impact all of our company's businesses – whether in the area of manufacturing, energy systems, infrastructure or medical engineering.

And digitalization has radically changed research and development in the last few years. The solitary inventor has been replaced by the creative team, silo thinking has given way to networking, flexible approaches have taken the place of strict regulation. All this is impacting the way we manage innovation. As a large company, Siemens has extensive capabilities and global reach. It's process-oriented. But its sheer size sometimes slows things down. Startups, on the other hand, are creative, often disruptive, fast and solution-oriented. The ideal is a combination of both worlds. That's why we've set up Innovation AG – a separate unit that will provide consulting and promote business and project ideas independently of our core businesses and that will offer entrepreneurs eager to blaze new trails a dynamic working environment.

At their summit in Elmau last June, the heads of the G7 countries agreed to "decarbonize" the world by 2100. At Siemens, we see this as a mandate to utilize our innovation power to free the world of CO_2 emissions. And it's in precisely this area that we've set up our first project: a venture to develop hybrid electric propulsion systems for airplanes. Together with Airbus, we're going to employ automation and digitalization technology – that is, 3D simulation, computer aided engineering, computer aided design and product lifecycle management software – to advance the electrification of air travel. And to make this happen, we're going to invest a substantial amount of money and set up a team of around 200 experts from both companies.

I'm convinced that Innovation AG will provide answers to many of the future's most pressing questions: Where is artificial intelligence taking us? What role will autonomous systems play in the manufacturing industry of the future? How will we distribute energy intelligently? How will we travel from point A to B? In a word: How do we want to live in the future?

But Innovation AG is just one of the things we're doing to move our company forward. Our experts are also working at universities and research institutes worldwide to link our research activities more closely to those of the scientific community. For example, in the next few years, around 300 Siemens employees will be relocating to the Garching campus of TUM, where they'll work side by side with scientists on topics like IT security and autonomous systems. Collaboration with TUM – one of our nine key strategic partner universities worldwide – will provide us with ideal conditions for strengthening our global R&D network.

All this represents a new chapter in our history of innovation – a history that began with Werner von Siemens' invention of the pointer telegraph in 1847. This year's celebration of his 200th birthday are an added incentive for us to be inspired by his example and to lead our company into a successful future. □

Picture credit: Siemens AG