

New technology is to spring from old solar modules

MORE KNOWLEDGE

Industry gets fit for quantum computing

MORE ENERGY

Fields to provide plants and electricity

MORE CONTROL

Reducing nitrate pollution with the aid of simulations





It could be a landscape in a futuristic comic. In fact, however, the picture shows a fatal process in the brains of people who suffer from Parkinson's disease: defective alpha-synuclein proteins (green) intertwine into coiled, fibre-like strings. When these fibres – also called fibrils – agglutinate, they probably damage nerve cells. The team of Jülich biophysicist Prof. Gunnar Schröder was able to show for the first time how lipids (grey/red) bind to the fibrils, influencing their arrangement. The findings could open up new approaches to diagnosing and treating Parkinson's.

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Getting a hold on the recycling flood

Solar modules, wind turbines, hydrogen electrolyzers – even renewable energy plants will eventually reach the end of their useful life. Time to build a circular economy for renewables.



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New ideas for old waste

Make yourself comfortable on a lounger made of wind power rotor blades, or build a mini solar system for the balcony from old modules – there are quite a few charming ideas on how to recycle used components

of "renewables". However, solutions like these are only relevant for a fraction of the scrap that will be generated in the future. In order to avoid mountains of waste and, above all, to recover the precious raw materials, comprehensive recycling solutions are needed for disused PV systems, for example. Jülich researchers are working on this challenge, and they are already thinking about the future: how can tomorrow's power plants – like electrolyzers for hydrogen production – be produced in such a way that they can later be easily recycled? We looked at at their ideas. We also asked how stable our electricity grid is, where we currently stand with quantum computing and how Germany may manage to avoid fines for excessive nitrate levels in the soil.

We hope you enjoy reading – and afterwards, if you have a fine idea for upcycling this issue of *effzett*, i.e. for turning the magazine into something new, email us a picture at <u>effzett@fz-juelich.de</u>

Your effzett editorial team

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Authors: Marcel Bülow, Dr. Janosch Deeg, Dr. Frank Frick, Christian Hohlfeld, Katja Lüers, Dr. Regine Panknin, Dr. Arndt Reuning, Dr. Barbara Schunk, Tobias Schlößer, Erhard Zeiss.

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Contact: Corporate Communications, tel: +49 2461 61-4661, fax: +49 2461 61-4666, email: info@fz-juelich.de

CLIMATE RESEARCH Cooling particles

A trail of dust obscures the view of North Africa and the Canary Islands: coming from the Sahara, strong winds can transport the desert dust all the way to northern Europe. The tiny particles not only obscure the view – they also obscure the influence that greenhouse gases have on global warming by reducing their contribution by up to 8 per cent. This is due to various cooling effects that the particles have on the climate, as researchers from Germany, Norway and the USA have discovered.

- INSTITUTE OF ENERGY AND CLIMATE RESEARCH -

BRAIN RESEARCH

Conspicuous patterns

People with different psychiatric disorders show similar changes in the brain. This is what studies by Jülich researchers have shown. The conspicuous patterns in the cerebral cortex obviously do not occur by chance. The changes rarely occurred in individual brain regions alone. Instead, regions that are similar in structure and function tend to be affected together.

- INSTITUTE OF NEUROSCIENCES AND MEDICINE -





"I've always wanted to make a difference, move things forward, have a positive influence and support people."

With this motivation, **Dr. Ir. Peter Jansens** took office as the new member of Forschungszentrum Jülich's Board of Directors at the beginning of 2023. The 56-year-old chemical engineer is responsible for the Institute of Energy and Climate Research, the Institute for Sustainable Hydrogen Economy and the Central Institute for Engineering, Electronics and Analytics. The Dutchman previously worked in research, manufacturing and management; he also brings experience from European steering committees.

1,000 qubits ...

... is the amount intended for the quantum computer to have, which researchers in the new OpenSuperQPlus project aim to develop within seven years. Forschungszentrum Jülich's expert Prof. Frank Wilhelm-Mauch is coordinating the project, which involves 28 partners from ten countries. It is part of the European quantum flagship.

- PETER GRÜNBERG INSTITUTE -

One hospital pioneers

New ways of supplying electricity and heat: for the Hermann Josef Hospital in Erkelenz in North Rhine-Westphalia, the Multi-SOFC project has combined, for the first time, two hydrogen technologies: a SOFC fuel cell system and a LOHC module which will supply the facility with hydrogen from 2025. In the future, it will cover half of the hospital's base load and significantly reduce CO₂ emissions. It is the first project of its kind in technical use and the first demonstration plant coordinated by the Helmholtz Hydrogen Cluster (HC-H2).

- HELMHOLTZ HYDROGEN CLUSTER -

BATTERY RESEARCH Titanium for power storage

Metal-air batteries are considered a cost-effective alternative to lithium-ion batteries. Zinc-air batteries, for example, are used by default as button cells in hearing aids, control modules and sensors. A German-Israeli team has used a rather unusual metal for its battery: titanium. It is the only metal that has the potential to transfer four electrons during discharge. The energy density of a titanium-air battery is theoretically two to three times higher than that of a zinc-air battery. After the first successful laboratory tests, the researchers intend to further improve the performance of their as yet unique battery.

- INSTITUTE OF ENERGY AND CLIMATE RESEARCH -





Monsoon provides data on CO₂ sources

India is considered one of the largest CO₂ emitters. Like a gigantic lift, Asian summer monsoons transports the greenhouse gas, as well as other substances, high into the atmosphere. Researchers from Wuppertal and Jülich were able to show, in a groundbreaking way, how the gas spreads across the Indian subcontinent in heights of up to 20 kilometres. To this end, they carried out high-resolution measurements using an aircraft and model simulations. Their results help to improve existing transport models, thus enabling a better allocation of possible CO₂ sources in South Asia – a region with very few monitoring stations on the ground.

- INSTITUTE OF ENERGY AND CLIMATE RESEARCH -

Earlier detection of Parkinson's

Slightly trembling hands are often the first sign of Parkinson's disease. In the future, one form of this disease could be detected earlier: with the help of a certain protein aggregate in the stool. Researchers from Düsseldorf, Cologne and Jülich were the first to detect an increased concentration of α-synuclein aggregates – the typical Parkinson's deposits – in stool samples from patients with isolated REM sleep behaviour disorder. This medical condition can herald Parkinson's. In people with "body-origin Parkinson's disease", these aggregates first form in the nervous system of the gut. More research is needed, however, before the method can be used in practice.

- INSTITUTE OF BIOLOGICAL INFORMATION PROCESSING -



Getting a hold on the recycling flood

In the years ahead, many photovoltaic systems and wind turbines around the world will go to the scrap pile due to ageing. The raw materials they contain, however, are much too good for that. They could also be introduced into the circular economy.



he object Ian Marius Peters is holding looks like an exquisite bathroom tile: the surface has a dark blue metallic shimmer. Regular silver stripes run across it. "This is a typical silicon solar cell," explains the physicist. "60 of these tiles make up one standard photovoltaic module."

More than 2.2 million solar systems are installed in Germany – on the roofs of houses and warehouses, as small balcony power plants or in huge solar parks. With a total maximum output of 60 gigawatts, they supply around 10 per cent of the electricity produced in Germany. In the meantime, however, the first modules have reached the end of their economic life. Technically, they could still supply electricity, but modern solar cells offer a much higher electricity yield than the old systems due to improved efficiency. These are now being successively replaced. The boom years of photovoltaics, between 2009 and 2014, will see the number of aged plants skyrocket. "In the next five to ten years, we will be faced with a flood of decommissioned modules. We should already be thinking about how we want to deal with this," says Peters. He is researching how the discarded modules can be recycled at the Helmholtz Institute Erlangen-Nürnberg for Renewable Energy (HI ERN), a branch office of Forschungszentrum Jülich.

RECYCLING BY LAW

"The recycling of PV systems is regulated by law in the European Union," explains the solar expert. "80 per cent of a panel – in terms of weight – must be recycled." The glass cover and the aluminium frame account for the largest share of the total mass of a module. Therefore, it is precisely these two components that are usually recycled, along with the valuable silver from the conductors and contacts. The panel is shredded for this purpose and the broken pieces are then sorted. After the process, the high-quality silicon is too contaminated for it to be used in the manufacturing of new solar cells.



Ian Marius Peters is looking for ways to better recycle decommissioned solar panels.

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"80 per cent of a panel – in terms of weight – must be recycled."

IAN MARIUS PETERS

"This would bring us quite close to the idea of a circular modular concept."

STEFAN HAAS

The fact that the materials cannot be separated cleanly enough during sorting, in turn, is due to the highly integrated design of the modules: "They are built to last, while they should actually be made for an eternal cycle instead," says Peters.

In the C2C-PV project, which the European Research Council ERC is funding with €2 million, he is testing alternative processes for recycling solar systems. He started with a special type of cell consisting of components that can be separated again more easily: perovskite solar cells. With the help of metal-organic compounds, they convert sunlight into electricity particularly efficiently – relative to the thickness of the active layer. In addition, they offer another advantage: they are easy to manufacture. This is because, like a sandwich, they are made of individual layers that can be built up into a cell using common printing processes.

"The choice of solvent is crucial here," says Peters. "If a new layer is applied, the solvent must not affect the layer underneath. In recycling, this process can be reversed, and layer after layer can be removed again one by one."

While this method is not suitable for conventional silicon cells, however, the physicist is also looking for innovative ways to recycle these: "My ideal would be a circular process modelled on nature: in a forest, the leaves fall from the trees, they decompose on the ground and thus provide the material for new plants. If we can do that in photovoltaics, we could advance renewable energy to become a truly sustainable energy."

To achieve this, the design of the solar modules themselves may have to change, Stefan Haas points out. Together with colleagues from the Central Institute for Engineering, Electronics and Analytics (ZEA-1), he is working at the Institute of Energy and Climate Research (IEK-5) on a concept to that end. His approach: solar modules that are designed for recycling from the planning stage onwards and that do not require plastics. Normally, each solar cell tile of a module is sealed with a transparent plastic film, which protects it from moisture. This coating interferes with recycling. In his design, Haas does without a lamination foil and instead encases the bare cells directly between the two glass panes of the module. To shield them from environmental influences, the edges of the glass panels must be hermetically sealed: "To achieve this, we apply a thin aluminium foil between the two glass plates on the very outside. We melt the metal briefly with a powerful laser. This is to ensure that the tiles are firmly joined together after cooling."

REFINING THE DESIGN

Joining glass and aluminium already works in principle. In addition to optimizing the joining process, however, it is now also important to refine the design. This is because the plastic coating previously used also fulfilled a second function: it stabilized the module by damping vibrations and preventing the individual cells from shifting within the module. As an alternative, Stefan Haas wants to test disc-shaped spacers on glass that hold the cells firmly in place: "This would bring us quite close to the idea of a circular modular concept."

Many wind power plants are also gradually becoming outdated and are being replaced by more powerful wind turbines. Whereas the steel of the mighty towers can easily be reintroduced into the raw material cycle, there is still a need for development regarding the rotor blades. They are difficult to recycle because they are made of a complex composite material: glass fibres or carbon fibres are embedded in a synthetic resin.

Both components are subsequently difficult to separate from each other. New material systems that can be more easily recycled at the end of a wind turbine's life cycle are currently being developed. Another example of materials with recycling potential are the concrete foundations of the towers, which extend up to four metres into the ground. The material can be ground up and given a second life in road construction – which,



Recycling should already be considered in the designing stage of solar modules: Stefan Haas is developing a concept for this.



however, takes it out of the circular economy. This is not an optimal solution for the multiple recycling of the material.

A LOOK AHEAD

Jülich researchers are already thinking about recycling in another sector that is expected to play an important role in Germany's energy supply: the production of hydrogen using electrolysis. It allows electricity from wind and sun to be converted into a storable form. The National Hydrogen Strategy envisages installing an electrolysis capacity of at least 10 gigawatts* in Germany by 2030.

"So-called PEM electrolyzers are considered particularly well-suited for this purpose. They adapt flexibly to the current electricity supply," explains Heidi Heinrichs of IEK-3. In the MATERIALIZE research project, which is funded by the European Research Council ERC, she is addressing the question of how material bottlenecks can be avoided in the global energy transition by looking at material and energy systems in an integrated way.

A wafer-thin plastic membrane separates the two electrodes of the PEM electrolyzer, where water is decomposed into oxygen and hydrogen. The membrane is coated with platinum on one side



gigawatts

at least is the electrolysis capacity target to be met in Germany by 2030. This is what the National Hydrogen Strategy envisages.*



Heidi Heinrichs detects material bottlenecks in the global energy transition and develops approaches to circumvent such bottlenecks.



and iridium on the other – both critical, indispensable raw materials. "With ever more electrolyzers, and ever more powerful ones, the demand will eventually be so high, there won't be a way forward without recycling, especially of iridium," says the engineer. "But beyond that, we'll probably also need devices that do not contain these critical materials. Alkaline electrolysis, which is already well established, puts itself forward for this. We should therefore focus on a mix of technologies, also with regard to the diversity of possible supply countries for the materials."

WASHING MACHINE FOR METALS

What such a process for recovering valuable materials from PEM electrolyzers could look like is being tested at IEK-14. There, Martin Müller and his team have constructed a "washing machine" with which the precious metals can be detached from the membrane surface.

"With a mixture of water and alcohol, we can reclaim both the platinum and the iridium almost completely," says the Jülich researcher. He was also able to prove in experiments that new membranes can be coated with the used catalysts. In principle, this brings the circular economy full circle.

"With a

mixture of

water and

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almost

High-temperature electrolysis (SOEC) can decompose water into its components even more efficiently than PEM electrolyzers. SOEC is particularly interesting when waste heat from other industrial processes is used to bring the cell to operating temperature and provide steam. In these cells, the two electrodes are separated by a ceramic solid electrolyte, which usually contains yttrium. It is one of the rare-earth metals.

"However, there are many different types of solid oxide electrolyzers," says Stephan Sarner. "This makes recycling a challenge. Even if these cells don't have a significant market share yet, a recycling-friendly design should be considered now."

As part of ReNaRe, which is a joint project in the hydrogen lead project H2Giga funded by the Federal Ministry of Education and Research, the doctoral researcher from IEK-1 has developed a process to recycle the inner life of a certain type of cell. With the help of an acid bath, he first removes the layer that serves as the air electrode. "After that, around 85 per cent of the cell, with regards to weight, remains. We then recycle it as the starting material for new cells." To do this, the metallic and ceramic components from inside the cell are ground into a fine powder after an acid bath. This can then be added to the suspension from which new ceramic parts for the electrolyzers can be produced again. This means that the high-quality powders do not have to be resynthesized, thus saving resources, time, energy and costs.

So far, all of this is still done manually, but in principle, the process can also be automated. It could then serve as an important contribution to ensuring that renewable energies are not only fed from regenerative sources – but that the renewables themselves are renewed in line with the circular economy.

ARNDT REUNING



T Already planning the future: Martin Müller is working on recycling processes for PEM electrolyzers.



With Stephan Sarner's process, a large part of the inner workings of an electrolysis cell can be recycled.

MARTIN MÜLLER

completely."

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"The legal regulations concerning the electricity market are a major problem for frequency stability in the power grid."

DIRK WITTHAUT

Dirk Witthaut heads the "Network Science Group" at the Institute of Energy and Climate Research, Energy Systems Engineering (IEK-10) and is a professor in this field at the Institute for Theoretical Physics at the University of Cologne.



Grid expert Prof. Dirk Witthaut from the Institute of Energy and Climate Research calls for a faster expansion of the power grid. In the interview, he also explains why legal regulations are sometimes a much bigger problem for grid stability than renewable energies.

Mr Witthaut, we are increasingly using renewable energies. What is changing as a result?

Instead of a few large generators, we will have many small ones that, in addition, feed fluctuating amounts of electricity into the grid. Plus, production and consumption diverge geographically. Wind power, for example, can be generated more cheaply and reliably in northern Germany.

What does this mean for the power grid?

The main thing is: we urgently need more power lines in order to bring electricity to industrial consumers in the south. However, grid expansion is bogged down. This is one of the biggest obstacles to energy transition. We must not continue to dawdle over this expansion. We also need greater flexibility regarding storage facilities, back-up generators and consumers for balancing out the fluctuations of the generators.

Will this make the grid unstable?

No, altough the effort to keep it stable increases. For this, electricity generation and consumption must always be at the same level. You can think of it as a scale being kept in balance by the grid operators – for example, by generators reducing or increasing their output at short notice. This is already being done today. Nevertheless, we lack empirical values on how to optimally build and operate a renewable energy grid.

Your working group is collecting important information for this. What exactly are you doing?

We analyze data from power grids mathematically and statistically to see what we can learn from it about the systems and their stability. In particular, we investigate line failures and their possible consequences, also in order to find weak points in the network. We also do research into the control systems that balance generation and consumption. Among other things, we looked at frequency data of the current. They not only reflect many of the characteristics of the networks, they also show that the power grid is not only to be considered from a technical point of view.

Why is that?

Laws, regulations and markets also influence the stability and reliability of the grid. In the frequency data, we clearly see the fingerprints of legal regulations concerning the European electricity market. That is to say, energy is traded in blocks of time – typically 1-hour and in 15-minute blocks. This means that during this period, the supplier must deliver a certain amount of electricity. So the power is ramped up at the beginning of the block to reach the agreed quantity, and it might be abruptly ramped down at the end.

What does that mean?

This creates many erratic ramps in the generator network, while the load from the 300 million consumers in the European power grid changes only slowly and steadily. As a result, there is always a brief imbalance between generation and consumption, which has a negative effect on frequency stability. The legal regulations concerning the electricity market are a major problem for frequency stability in the power grid; problems caused by renewable energies are often overestimated.

THE INTERVIEW WAS CONDUCTED BY JANOSCH DEEG.



The interview in full: <u>fz-juelich.de/en/news/the_</u> <u>blackout_fairy_tale</u>



The blackout fairy tale

In winter, in view of the threat of supply bottlenecks, there was repeated talk of possible blackouts in Germany – in other words, nationwide power cuts. But that did not end up happening. "The risk of such a blackout has been and will remain very low," clarifies Prof. Dirk Witthaut. He is critical of the fact that some media and politicians have equated blackouts with controlled power cuts (brownouts). Here, we explain the differences.



BLACKOUT

An unplanned, uncontrolled, large-scale power failure

BROWNOUT

on 🦲

An emergency measure in case of power shortage

How can this happen?

A line unexpectedly fails. As in a domino effect, more and more lines are affected by overloading and emergency shut-downs. The trigger is usually a damaged or overloaded line.

Not enough electricity is generated to meet demand. Grid operators switch off power in a controlled and locally limited manner. This happens repeatedly in France, for example, but initially it only affects industry.

Who is affected?

A blackout affects everyone. There are emergency power generators for critical infrastructure, which secure the power supply for a short time. First the electricity is switched off for some industries, then individual districts take turns and are briefly switched off.

How likely is such an event today?

Negligible, as the European power grid is quite robust and there are quite a few measures in place for emergencies. Higher than before the attack on Ukraine, given the increased uncertainties in energy supply. However, network operators use computer forecasts and then have a variety of possibilities to intervene.

Sleep deprivation makes the brain look old

One night without sleep is all it takes for the human brain to appear older. However, the changes can be reversed.

n international team of researchers deprived 134 healthy young people of sleep. Afterwards, the brains of the subjects - who had stayed awake for more than 24 hours - showed significant changes. "These typically only appear in people one to two years older. Until now, the direct influence sleep deprivation has on the biological age of the brain had been unknown," says Prof. David Elmenhorst from the Jülich Institute of Neurosciences and Medicine (INM-2), who led the study involving scientists from Denmark, Switzerland, the USA, China and Germany.

Biological age designates the actual physical aging condition. "For example, dementia can prematurely age the brain. So the brain of a 60-yearold can look like that of a 70-year-old," explains the Jülich sleep researcher. Things are not that bleak, however: "After one refreshing night of sleep, the brain age of our subjects between 19 and 39 years of age returned to its initial value. In a sense, the brain 'rejuvenated' again." The researchers were also able to show that partial sleep deprivation - even over several days - does not cause a significant change in brain age.

ALGORITHM ESTIMATES AGE

For the study, the team first determined the biological age of the brains. For this purpose, brain images were taken using a magnetic resonance imaging (MRI) and the biological age was estimated with the help of machine learning. In the ":envihab" sleep laboratory of the German Aerospace Centre in Cologne, the researchers then studied different conditions: complete sleep deprivation, partial sleep deprivation and chronic partial sleep deprivation. Subsequently, MRI scans were again taken and compared with the original images.

ERHARD ZEISS



T. David Elmenhorst is researching the effects of sleep deprivation.



Three tips for better sleep (in German): go.fzj.de/effzetttipps-fuerbesseren-schlaf





What are you researching right now, Ms Kuckertz?

Anika Kuckertz, doctoral researcher at the Institute of Neurosciences and Medicine (INM-1)

"I cut the brain of a rat into about 1,400 of these fingernail-sized, wafer-thin slices and scan them. From this, we create a digital 3-D brain model, which will visualize individual nerve cells and also neurotransmitter receptors on the cell surface. We want to use it to better understand how structural differences influence the communication between individual nerve cells and brain regions and compare this with the human brain. So hopefully, we will also learn more about neurodegenerative diseases in humans."

Double yield

In the future, arable land will not only provide food, but also electricity. For this purpose, it is equipped with photovoltaic (PV) systems. The concept is called Agri-PV. It is a component in energy transition and an opportunity for structural change in the Rhineland region. Jülich researchers, together with partners, are driving development forward.

SOUTH-ORIENTED UNIT

Permanently installed PV modules facing south. Rain-sensitive or shade crops can be grown below.

Demonstration system, can be realized with commercially available components



More information (in German): go.fzj.de/dossieragri-pv

Stand-alone power supply for irrigation, measurement and control electronics

Plant growth – research objectives

- Developing software that calculates how much light and shade reaches the plants in order to optimize the gap between the modules
- Using self-developed mobile probes to record plant growth under PV systems and on reference fields
- Identifying suitable crops for different Agri-PV systems
- Controlling the movable PV modules to protect plants in extreme weather conditions
- Developing rainwater catchment systems and smart irrigation strategies

Mobile probe with optical sensors for plant observation

> Rainwater tank system (planned)

2.5 m Rearance height

(planned)

7

Photovoltaic system - research objectives

- Collecting data on the performance of the different PV systems
- Recording the influence of wind and weather on the systems, which are up to 4 metres high
- Developing PV modules that allow part of the sunlight spectrum to pass through for optimal plant growth*



Renewable energy as a contribution to

energy transition

Protecting plants from extreme weather and too much sun Optimizing irrigation and sunlight with additional technology

turnable

4.5 m

clearance height

TRACKING UNIT

Movable PV modules in rows (east-west orientation) follow the position of the sun and are located between and partly above the plants. Depending on the construction, tractors or even combine harvesters fit underneath.

Research unit – custom-made with variable adjustment options



per cent

of German agricultural land equipped with high-mounted Agri-PV would be sufficient to cover Germany's future electricity demand on a balance sheet basis, according to Fraunhofer ISE.



Projects for acceptance

Special crops

and blueberries

such as raspberries

- Involving potential users in the research projects
- Information, advice, support for citizens and farmers

Trial areas

Research unit in Morschenich-Alt, see graphic (running since 2022)

- Area: about 2 hectares
- Capacity: ca. 300 kilowatts (corresponds to the electricity demand of ca. 100 households)
- Partners: Fraunhofer Institute for Solar Energy Systems (ISE); at Jülich: Institute of Bio- and Geosciences (IBG-2), Institute of Energy and Climate Research (IEK-5)
- Structural change project AgriFEe, innovation cluster BioeconomyREVIER, funded by the BMBF in the immediate action programme PLUS

RWE AG pilot plant in Bedburg-Garzweiler (construction to start in mid-2023)

Comparison of three Agri-PV concepts: high-mounted horizontal system, ground-level tracking system, ground-level system with vertical module arrangement

- Area: around 7 hectares
- · Capacity: up to 3 megawatts
- Partners: RWE AG, IBG-2
- Funded by the state of North Rhine-Westphalia through the progres.nrw programme

Modelling saves a lot of time

For many years, Germany failed to apply the EU Nitrate Directive and was threatened with severe fines. These are now off the table thanks to the amended German fertilizer rules. A nationwide monitoring program is assessing the effects of these rules, and Jülich simulation models are part of this. Frank Wendland is an expert in hydrological modelling – calculating, for example, where nitrate seeps into the soil and how much, where it flows to and how this affects the groundwater.

> ach year, starting in February, the big tractors with their long tank trailers are back on the road. It is the visible and smellable start of the manure season. In Germany, however, fields are often fertilized more than is actually necessary. This is not without consequences: excess nitrate seeps into the soil and can pollute groundwater (see box). The EU limit of 50 milligrams of nitrate per litre is exceeded in several regions of Germany (see map).

> For years, the EU accused Germany of not doing enough against nitrate pollution. A decision by the European Court of Justice in 2018 indicated that the country could face multi-billion euro fines because of that. After Germany revised its fertilizer regulations several times, the EU finally terminated the infringement procedure in June 2023.

> A key element of the new rules is a long-term monitoring, control and analysis system. This impact monitoring will record nitrogen emissions from agriculture and nitrate concentrations in groundwater. In this framework, Germany-wide modelling will be used to estimate how measures, such as less fertilization in agriculture, affect the nitrate contamination of groundwater and surface waters in Germany.

> The model for analyzing nitrate fluxes is currently being developed by scientists in the RELAS project. AGRUM-DE, a model network for the analysis of nutrient fluxes at the level of federal states initiated in 2005, is used as the basis for this. "In the RELAS project, we are further developing AGRUM-DE into a nationwide standard for impact monitoring," says Prof. Frank Wendland from the Jülich Institute of Bio- and Geosciences (IBG-3). His working group has contributed two models for analyzing nitrate fluxes to the network: "With mGROWA, we model the runoff components and the input pathways for nitrate, and with DENUZ-WEKU the nitrate turnover and the transport in soil and groundwater. In this



way, we can simulate how much nitrate finds its way into surface waters and groundwater," Wendland explains.

REGIONAL DIFFERENCES

Moreover, the simulations with the Jülich models can spatially resolve the expected nitrate pollution quite precisely. According to Wendland, "That's important because nitrate concentrations within an individual river catchment or groundwater system sometimes varies considerably."

To this end, the researchers feed their models not only with data from the more than 10,000 groundwater monitoring stations in Germany, but also with a great number of input parameters such as climate data, land use and soil properties. The results of another AGRUM-DE model are also included: RAUMIS, developed by researchers at the Thünen Institute in Braunschweig. Based on various parameters such as fertilizer use, nutrient removal by plants and regional site characteristics, this model calculates how much excess nitrogen is produced by farming. "In the AGRUM-DE model network, we simulate how much nitrogen is in the system, so to speak. From that, we can draw conclusions about the nitrate concentra-



Simulation of the nitrate concentration in the leachate: green signifies low nitrate concentrations and red/purple very high ones. For comparison: the EU limit for groundwater is 50 milligrams of nitrate per litre (mg NO3/L). The map shows the result of a simulation from a previous project. In RELAS, such simulations are repeated with significantly improved input data data for modelling and monitoring.

RELAS

stands for the mapping of regional agricultural nitrogen flows (REgionale LAndwirtschaftliche Stickstoffflüsse) as a basis for developing and optimizing agricultural policy measures to achieve climate protection targets. The project is funded by the Federal Office for Agriculture and Food (BLE). "Our models can simulate how much nitrate-based fertilizer farmers can apply in a given area without exceeding the EU limit there."

FRANK WENDLAND

tions as well as the amount of nitrate that reaches groundwater via leachate. With the help of the simulations, we can then also assess whether a planned measure will reduce the nitrate pollution of groundwater as desired," Wendland explains.

The FZJ models, however, provide even more information: they determine how, via different input pathways, nitrate finds its way into surface waters. The related FZJ model results flow into another AGRUM-DE sub-model, MONERIS, developed by researchers at the Leibniz Institute of Freshwater Ecology and Inland Fisheries (IGB). MONERIS analyzes how certain nutrients, including nitrate, are distributed in rivers and eventually reach the sea.

TARGETED MEASURES

"In this way, the AGRUM-DE-model network is able to identify the cause of high nitrate loads in surface waters including coastal areas," says Wendland. This can be the excessive use of fertilizers, but also wastewater from sewage treatment plants or artificial drainage systems. "Based on this knowledge, we can identify starting points for additional targeted measures – for example, how much nitrate-based fertilizer farmers can use in a certain area without exceeding the EU limit there," says the Jülich researcher.

"With the AGRUM-DE simulation tool, it will be possible to consistently predict how the amended fertilizer ordinance will affect the nitrate pollution of groundwater and surface waters – years before the effects are measurable. This will make it possible to readjust inadequate measures much earlier. The first nationwide modelling should be available by the end of 2025. In the end, the concept of impact monitoring helped to convince the EU Commission to drop the legal action against Germany. However, the discontinuation of the legal action is only a milestone, there is still a long way to go before the protection targets for water resources are achieved," says Wendland.

JANOSCH DEEG

How harmful is nitrate?

Nitrate is a nitrogen-oxygen compound that plants need for their growth. They absorb the substance through their roots and, through photosynthesis, convert it into energy-rich protein compounds. This is why farmers apply nitrates to their fields by way of slurry or mineral fertilizers in order to increase yields. Often, however, much more of the substance ends up on the fields than plants and soils can process and store. Rain flushes the remainder into surface waters and groundwater. In rivers, lakes and coastal areas of the North and Baltic Seas, high nitrate concentrations can unbalance the delicate ecosystems, for example by promoting the growth of algae. As a result, the natural plant life dies – and with it the water body. Too much nitrate in groundwater can also impair the quality of the drinking water obtained from it. According to the German Environment Agency, however, drinking water quality is well monitored and consistently good to very good. Nitrate is actually harmless to humans anyway. In the body, however, it can at times be converted to nitrite, which is harmful in excessive amounts, particularly for babies.





Bernhard Schmid (left) and Maximilian Quentmeier with their stack, which converts climate-damaging CO₂ into carbon monoxide.

CO₂ electrolysis instead of coal

Coal is being phased out – this is the only way to achieve Germany's climate targets. However, the fossil fuel is also the basis for important basic chemicals. New solutions are needed. CO₂ electrolysis is one of them.

ignite from the Rhineland region is not only used to generate electricity, it is also used to produce important basic chemicals such as carbon monoxide (CO), with which the chemical industry produces synthetic materials and acetic acid. Since lignite will soon be phased out, new, climate-friendly sources of this gas must be developed. Researchers at Jülich's Institute of Energy and Climate Research (IEK-9) have cleared an important hurdle to help a promising technology reach a breakthrough: CO₂ electrolysis.

It converts climate-damaging CO₂ directly into pure carbon monoxide. "Without further processing, the carbon monoxide can then be used for many applications," explains Maximilian Quentmeier, doctoral researcher at IEK-9. To-

30

per cent

efficiency is achieved by the current cell stack of the Jülich researchers. gether with his supervisor Bernhard Schmid and other colleagues, he developed a design for a CO₂ electrolysis plant in which the individual cells are arranged in a so-called cell stack. It is known from other electrolysis technologies that such a design can be scaled up well for industrial use.

The stack achieves an efficiency of 30 per cent in laboratory tests – which are not yet tuned for efficiency. "For this type of process, which even takes place at below 100 degrees Celsius, this is already a very promising value," says the institute's director, Prof. Rüdiger-A. Eichel. Plus: if such a system is operated with electricity from renewable energies, it operates in a climate-neutral manner. "If you withdraw the carbon dioxide from the atmosphere, for example using direct air capture, or from biogas plants, the technology is even potentially climate-negative," explains Bernhard Schmid.

The work is part of the structural change project iNEW, which aims to advance the creation and safeguarding of jobs in the Rhineland region. With the help of CO_2 electrolysis, industrial companies in the region could provide carbon monoxide as a basic chemical on a decentralized basis without having to transport the toxic and highly flammable gas at great expense. Until then, the researchers aim to further improve, among other things, the efficiency of their cell stack.

The vibrant diversity of a quantum physicist

Father of three, quantum physicist, ornithologist and committed open science advocate: there are many sides to Dr. Vincent Mourik's life.

ust recently, Vincent Mourik had another interesting conversation about quantum physics - with a dancer. Granted, it was less about the interaction of tiny particles and more about the abstractness of the concepts: "That's exactly what connected the artist, who specializes in modern dance, and me, the physicist: abstractness as a common ground," explains Dutchman Mourik, whom the North Rhine-Westphalian Academy of Sciences and Arts accepted to its Junges Kolleg as a scholarship holder last December. Since the end of 2021, the 36-year-old has worked at the JARA Institute for Quantum Information at Forschungszentrum Jülich and has been setting up a young investigator group as well as his Solid State Quantum Devices Laboratory (SQUAD), which is located on the RWTH Aachen University campus.

Open science as a matter of the heart

Scientific transparency is close to Vincent Mourik's heart. Against this background, he is committed to open science and comprehensive data exchange. He advocates open online publishing including open peer review without rejections of submissions. "Publication platforms should be non-profit and commercial scientific journals abolished," Mourik states. He is also concerned with how to deal with criticism. "It should be perfectly normal to discuss scientific problems publicly – for example, if there are inconsistencies in a paper that has already been published," says the Dutchman. He knows from his own experience that someone who criticizes such a case is quickly considered a whistleblower by the community. "That's why young researchers fear for their careers if they point out possible mistakes. That has to change," says Mourik.

AUSTRALIA AND BIRDS

Today, however, the man with the distinctive, full red beard can be found neither in Jülich nor in Aachen – but in his little house in the Dutch province of Limburg, where he lives with his wife and three children. A few budgies are chattering in the background. "They help against our homesickness," the researcher tells us and laughs: he had been doing postdoctoral research in Sydney at the University of New South Wales from 2016 to 2021. "While there were really many good reasons to return to Germany and Europe, the weather's definitely not one of them. In Australia, we never had to worry about the children's clothes," Mourik says with a twinkle.

What he actually sorely misses: nature and the wilderness. "It was only in Australia that I realized how much pressure bears down on this planet, what role biodiversity plays and how much humans are destroying nature," says Mourik. It was then that he decided – in addition to his work as a physicist – to collaborate on monitoring studies on birds. Even as a child, Mourik had used every free minute to watch birds, though he did not want to become an ornithologist. "That would've been kind of uncool when I was 18," says the broadly interested researcher. So he studied physics at Delft University of Technology.

"Even as a student, I was fascinated by how our macroscopic world emerges from a microscopic world, which in turn is described by quantum mechanics," he says with enthusiasm. The then 19-year-old was fascinated by the contrast between, on the one hand, a theory that has the potential to revolutionize our technologies and thus our society and, on the other, a practice that is difficult for laypeople to access – a fascination that continues to this day.



So far, the physicist has mainly used his time at Jülich to set up his laboratory. This is where Mourik would like to realize his GeBaseQ (Germanium Based Qubits) project, for which he raised €4.8 million in 2022 through the Quantum Futur competition for young researchers offered by the Federal Ministry of Education and Research. His motivation: "Within three to five years, I want to establish experiments with my group that will help to better understand quantum physics and contribute to being able to build quantum computers."

Quantum computers are, as it were, the icing on the cake of quantum physics. The problem: in order to build a quantum computer that calculates things relevant for true use, millions of computing units, the qubits, must be created and controlled. This has not been achieved so far, and it is open which types of qubits will prevail. Qubits can, for example, be generated with the help of superconductors, ion traps or semiconductors.

Mourik counts on semiconductors. This material, which is mostly made of silicon, can already be found today in almost every laptop, smartphone or television in the form of microchips.

CLOSING A GAP

"We want to find out whether a special semiconductor made of a combination of silicon and germanium is suitable for quantum bits," explains Mourik. There is comparatively little research on this combination in Germany. Mourik intends to close this gap.

So he dives deep into his quantum concepts again and again. "And from time to time, I go out into nature: I see, smell, taste and hear life there. It's tangible – and not abstract."

KATJA LÜERS

4.8 million euros

is the sum Vincent Mourik raised in 2022 for his GeBaseQ project through the "Quantum Futur" competition for young researchers.

Getting fit for quantum computers

Experts estimate that it will take at least another ten years before a quantum computer solves everyday problems. However, large companies are already preparing for the use of the new computers. Forschungszentrum Jülich supports them in this.

QUANTUM COMPUTING



Sitting at their fireplace, over which a stew is simmering, they are already working on a cookbook for their electric cooker – which still needs to be designed and built. The situation is similar in quantum computing at the moment. While the hardware is still being developed, researchers are already working on the operations that a quantum computer is to run, step by step, when solving certain tasks: the quantum algorithms. Prof. Frank Wilhelm-Mauch, director of the Peter Grünberg Institute for Quantum Computing Analytics (PGI-12), believes that the simultaneous development of hardware and software is sensible and important: "If you only started working on algorithms when

mature quantum computers already exist, you would have lost a lot of valuable time."

THE MARKET DOES NOT WAIT

The industry also sees it that way. "There are no competitive advantages in waiting until quantum technologies are a completely established technology. Essential new markets would then already be occupied," warns the German information and telecommunications industry association, Bitkom, in its guide on quantum technologies in business. As a consequence, large corporations have long since begun to build up competencies. The challenge today is to find out for which problems a quantum computer would





per cent

of all companies with more than 500 employees are already considering or discussing the future use of quantum computers, according to a study by the industry association Bitkom.



Tobias Stollenwerk develops and tests quantum algorithms.

actually be of practical use and what suitable algorithms might look like.

Science and industry are working closely together to achieve this. "This way, we learn to understand the problems that are significant for the companies. This helps us basic researchers to develop quantum algorithms – not only out of scientific curiosity, but very specifically to advance society this way," says group leader Dr. Tobias Stollenwerk from PGI-12. In the Q(AI)2 project, together with BMW, Mercedes-Benz, Volkswagen and Bosch, Stollenwerk, his team and researchers at the Jülich Supercomputing Centre (JSC) are working on solutions for the automotive industry.

The focus is on tasks for which the companies use artificial intelligence (AI) – so far, just relying on conventional computers. For example, an AI is supposed to recognize workers and their body parts in pictures. This is often a prerequisite so that robots and humans may work together directly and safely during the production of a car part. The computer can then, for example, control the robot arm so that it does not collide with a worker. Dr. Dmytro Nabok from the JSC is exploring quantum algorithms that are to improve this AI application in such a way that it always identifies body parts correctly and within milliseconds.

Nabok uses, among other things, the quantum annealer from the company D-Wave Systems at Forschungszentrum Jülich, called JUPSI, to test these algorithms. Unlike other quantum computers, a quantum annealer is not universally programmable, so it is only suitable for special tasks. JUPSI is part of the "Jülich UNified Infrastructure for Quantum computing" (JUNIQ). Through



T Kristel Michielsen heads the Jülich UNified Infrastructure for Quantum computing (JUNIQ).

JUNIQ, research teams from industry and academia have access to experimental systems, prototypes and commercial quantum computers, as well as the necessary support, for example, in developing algorithms. Prof. Kristel Michielsen from the JSC and head of JUNIQ illustrates how important it is to test and run quantum algorithms on the already existing quantum systems at an early stage. "This generates expertise and contributes to the co-design feedback loop," she says. "In this process, which is known from supercomputing, users, software and hardware developers work together to improve and design future computing environments."

OPTIMIZING THE VARNISH

Volkswagen AG is dealing with another, exemplary problem in the car industry. The starting situation: new cars are to be painted in two separate coating layers. When a car arrives at the coating line, however, the robots there do not apply the two layers directly one after the other. If they did, the robots would have to constantly change the paints, which is time-consuming. This is why a conveyor belt transports each car out of the line after the first painting process and then back in again for the second painting process. This process is to be optimized, that is, the time of a paint change for a certain number of cars must be determined in such a way that the paint needs to be changed as rarely as possible. Tobias Stollenwerk's team is investigating whether quantum computers can solve such problems faster than conventional computers.

"The computational burden of this problem increases enormously fast relative to the number of paints and the number of cars. In addition, we have to take other influencing factors into

What are small companies doing?



Dr. Daniel Zeuch from the Peter Grünberg Institute (PGI-12) has spoken to over 100 representatives of small and medium-sized enterprises (SMEs) about quantum computing over the last two years. Why, Mr Zeuch?

We wanted to find out whether SMEs can be increasingly involved in the development of components or software for quantum computers in the future and, if necessary, help them to invest in this field of development in the near term. We also wanted to know to what extent smaller companies had already familiarized themselves with the topic.

What were the results?

There are marked differences. Some suppliers who produce special power sources or microwave analyzers, for example, are already in the business, others could enter quickly. Users, on the other hand, are still holding back. They lack robust forecasts of computational benefits from quantum computing. Nevertheless, some of them expressed great interest in dealing with the topic, for example in conversations with us.

What do you offer these companies?

Information, advice and support. They are welcome to contact me at any time. Forschungszentrum Jülich is also pursuing various approaches to strengthen contact with industry, including SMEs, for example as a partner in the state-wide network "EIN Quantum NRW", or with the Aachen Fraunhofer Institute for Laser Technology ILT in the planned Center for Quantum Systems and Engineering, or CQSE for short, which aims to promote quantum technologies in the Rhineland region.



More information: <u>https://go.fzj.de/effzett</u> -quantum-ready-kmu-EN



account in practice," explains Stollenwerk. "Sometimes, optimization problems like these cannot at all be solved accurately in realistic time spans, not even with supercomputers." Unlike Nabok, Stollenwerk's team tests the algorithms on conventional computers that mimic the behaviour of quantum computers. "This allows us to specifically co-simulate different types of errors that quantum computers of different maturity levels make. This includes checking the effects of the quantum hardware, for example. This helps us to better understand the influence of these errors on the result," says Stollenwerk.

"Conventional computers are not only useful for testing quantum software. They can also benefit from it."

NILS KÜCHLER

JUNIQ project manager Dr. Nils Küchler tells about a pleasant side effect: "Conventional computers are not only useful for testing quantum software. They can also benefit from it, because with them, the quantum-inspired software sometimes delivers new solutions." Stollenwerk has observed another phenomenon during his collaboration with industry: "Companies are shedding new light on problems by considering how quantum computers could calculate these. In the process, they sometimes discover far better classical algorithms than those they had previously known."

FRANK FRICK

Artificial intelligence for all!

The Al revolution is largely taking place behind closed doors. This is supposed to change now.



Paradise Garden of the Future – generated with the open-source image generator Stable Diffusion, which was trained with the LAION data sets.

rtificial intelligence of the latest generation such as the chatbot ChatGPT is making quite a splash. An image AI like DALL-E 2 or Imagen creates virtual worlds of amazing quality on command. However, such AI models require enormous computing resources, you need to collect enough data, and you need people who are specialized in training the AI. Previously, only large companies like Google, Meta or OpenAI had been able to do this.

The development in these companies, however, takes place behind closed doors. "This makes verification more difficult and leads to security problems, as no one can independently check how the model was created and what data was used for training," says Dr. Jenia Jitsev from the Jülich Supercomputing Centre (JSC). He and his colleague Dr. Mehdi Cherti want to make AI accessible to everyone. To this end, together with German and international partners, they founded the non-profit research network LAION and recently created the largest, freely accessible text-image dataset to date in the network: LAION 5B. It consists of 5.8 billion text-image pairs. For the computationally intensive training, the partners used Germany's most powerful platform for deep learning and AI: the Jülich supercomputer JUWELS.

LAION-5B can be used to train openly accessible, large-scale AI models. It had previously been used by the open-source image generator Stable Diffusion, which generates impressive images on command, or by the openCLIP project, in which pre-trained models are used for open research and for image recognition and analysis. However, current text-image AI can do much more. "The list of possible applications is almost endless. They range from medicine and materials science to the development of new battery components and the prediction of solar activity from satellite images," says Mehdi Cherti. Thanks to LAION-5B, a door has opened up wide for AI developers.

TOBIAS SCHLÖSSER



The full interview with Jenia Jitsev and Mehdi Cherti and more images generated by Al: <u>https://go.fzj.de/</u> effzett-Al-for-all-EN





CERAMICS

Originally, ceramics referred to everyday objects made of clay. Today, ceramics is the generic term for inorganic, non-metallic materials that are characterized by a nide range of properties.



PROPERTIES

Cerannics can be very hard and resistant to heat or corrosion. Some of them conduct electricity, others are insulating. The properties depend on chemical composition and production.



PRODUCTION

Very fine powders are pressed, sprayed or, after being wixed with liquids, poured into shope, then dried and heated. Heating, also called sintering, and powder control the properties.



APPLICATION

The spectrum ranges from tableware or prostheses, electronic components and cutting tools for mechanical engeneering to heat protection in air and space travel.

ANCIENT BEAUTY

Ceramics are considered to be the first material created by humans. At no less than 25,000 years of age, the "Venus of Dolní Věstonice" is the oldest known ceramic figure.





WHAT IS JÜLICH DOING?

Julich develops, characterizes and tests ceramic materials and components for use in batteries and fuel cells, as filter membranes or heat protection in turbines, for example.



THUMBS UP

ALTERNATIVE TO TWITTER Mastodon relies on decentralization

Twitter is popular with Jülich scientists. After the takeover by Elon Musk, however, the network has changed. Users are confronted with questionable updates and the company boss is annoying them with push messages in their timelines. No wonder many are looking for alternatives. Mastodon relies on open source software and a network of decentralized servers. What is more, the "toots" do not have to compete against sponsored links or hold their own against tweets that the algorithm whips to the front. Mastodon shows what users are subscribed to.

- @FZJ@MASTODON.SOCIAL -



Magazine receives awards

We won the race – three races, to be precise! This is the number of awards that our research magazine effzett, which you are currently reading, received at the International Creative Media Award. The jury's recognition included the print and online issue entitled "Icy Machines", from which the illustration shown here is taken. The issue is concerned with Jülich's research into quantum computing – and with an entirely open race.

- EFFZETT.FZ-JUELICH.DE/EN/1-22 -

IMAGE GENERATOR STABLE DIFFUSION

Al creates pictures

Artificial intelligences are currently making quite a splash. What the chatbot ChatGPT can do with words, however, also works with pictures. On the basis of keywords, so-called image generators create virtual worlds – and they are amazingly real. In addition to commercial offers, there are also freely accessible generators, such as the Stable Diffusion project. With LAION-5B, this open-source image generator draws on the largest freely accessible textimage dataset to date and, thus, on Jülich know-how (see p. 29). You can provide the AI with terms or even sentences on the website and see what it creates from them.

- STABLEDIFFUSIONWEB.COM -

RESEARCH IN A TWEET

Heads up, young scientists: gain insights into quantum computing, big data and neuromorphic computing with the #JulichSummerAcademy.



Until September 2023, Forschungszentrum Jülich offers interesting workshops, lectures, summer schools and much more as part of the Jülich Summer Academy. The focus is on "Future Computing Technologies: Hardware, Software and Algorithms for Scalable Simulation and Data Science". The events are aimed primarily at young scientists, and the programme is constantly being expanded – so it pays to check it regularly.

fz-juelich.de/en/jsa/julich-summer-academy

