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Advanced Materials

WINTER 2021

SPREAD KNOWLEDGE

Editorial

Spread knowledge

A very special year has passed. Covid-19 gave the framework for our professional and private life. This was not always easy, it was not always nice, but it was no stop sign to research. Research has actually gained a lot of visibility. European leaders decided to tackle Covid-19 by listening to scientific advisors, use evidence-based scenario's, see hypothesis been proven wrong or right and reacting to it. The teams working on Covid-vaccines have made enormous leaps in a short time to provide new, safe vaccines that may help to recover society.
This new focus on scientific advice and research solving a problem, may be an enormous opportunity to build on for all scientific disciplines. Science is not a hobby; it is not just an opinion. Science is ideally balancing existing knowledge, new results, interpretation and critical discussion to a sound consensus. It provides solutions to complex problems, some of which overseen by the public, some of which at the center of interest. Wherever in this spectrum research on Advanced Materials is, investing in it may be essential already in the near future.
And spreading the knowledge on what is going on in our labs may create ground for the next good to happen. Therefore: stay safe, stay curious, enjoy our stories here, and keep telling your story.

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In this issue

AI reduces computational time required to study fate of molecules exposed to light

by Rene Fransen (ScienceLinX)

Light-induced processes are critical in transformative technologies such as solar energy harvesting, as well as in photomedicine and photoresponsive materials. Theoretical studies of the dynamics of photoinduced processes require numerous electronic structure calculations, which are computationally expensive. Scientists from the University of Groningen developed machine learning-based algorithms, which reduce these computations significantly. The Open Source software package that they developed, PySurf, was presented in a paper in the Journal of Chemical Theory and Computation on 24 November.

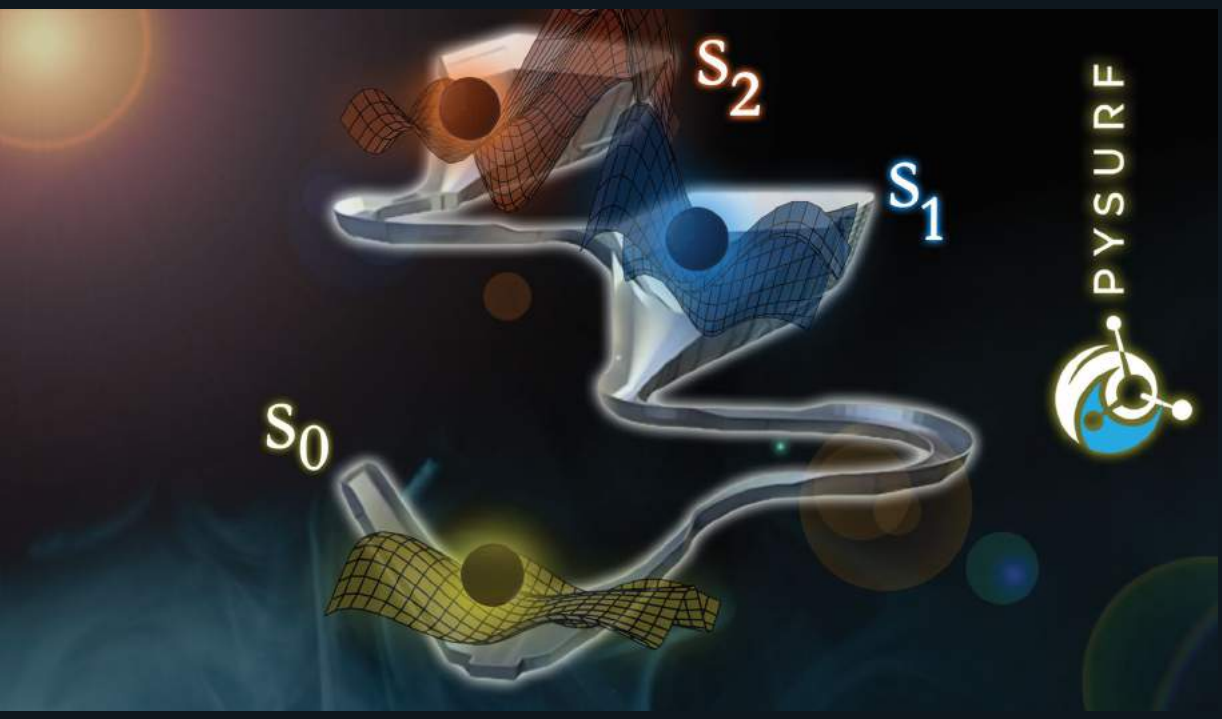
How do molecules behave when they are exposed to light? Knowledge of this process is not only central to crucial processes in nature, such as photosynthesis and vitamin D production, but it is also critical for the rational design of new molecules with specific photoresponsive properties.

Machine learning

Yet, despite great advances in hardware and computational methods, calculations of the interaction between light and molecules is still a challenge, explains Shirin Faraji, Associate Professor in Theoretical Chemistry, the lead author of the paper. 'The high-level electronic structure calculations are already very costly for medium-sized molecules, typical chromophores have around thirty heavy atoms.' Including the influence of the environment at quantum mechanical level on such a system is practically impossible.

> "Our software, therefore, requires several orders of magnitude less computational time than existing direct dynamics software"

'Current software searches the entire conformational space, but we use machine learning to exclude parts of this conformational space search, making it a very smart search,' Faraji explains. 'Our software, therefore, requires several orders of magnitude less computational time than existing direct dynamics software.' In the paper, the developers report the photodynamics of two benchmark molecules, SO_2



Representation of machine learning electronic-structure based excited states of a molecule responding to light
Illustration: Faraji Lab.

and pyrazine, and show that their results are comparable to those obtained using simulations that are based entirely on quantum dynamics.

Algorithm

Furthermore, the software package was developed from scratch and is easy to adapt for specific purposes, for example by using plug-in and workflow engines. Faraji: 'A PhD student could easily dig into the code and develop a specific algorithm, for example a new neural network-based algorithm.'

Faraji contributed code to several software packages, most notably Q-Chem, one of the world's leading quantum chemistry software programs, and is currently a member of the Q-Chem Board of Directors. The new PySurf package will interface with Q-Chem, but also with other electronic structure software. PySurf is Open Source, which means that it is available as a free download together with the manual, and Faraji's team will provide support for users.

First release

The PySurf software is the result of a project funded by a personal grant to Faraji from the Dutch Research Council (NWO) Vidi programme. Faraji: 'We are only a year and a half into this five-year project. So, the current version is just the first release. We continue to work on the program to optimize it and to create a user-friendly interface.'

Reference: Maximilian F. S. J. Menger, Johannes Ehrmaier, and Shirin Faraji: PySurf: A Framework for Database Accelerated Direct Dynamics. J. Chem. Theory Comput. online 24 November 2020.

This work is part of the Innovational Research Incentives Scheme Vidi 2017 with project number 016.Vidi.189.044, which is (partly) financed by the Dutch Research Council (NWO).

> "A PhD student could easily dig into the code and develop a specific algorithm, for example a new neural network-based algorithm."

Combining incipient ferroelectrics and graphene leads to new insights into memristive devices

by Rene Fransen (ScienceLinX)

Transistors can have just two values: 0 or 1. Our brains process information via neurons, which are more complicated: they can have any intermediate value, based on the memory of the input they received in the long-term or short-term past. Scientists are trying to build transistors with a similar type memory, called memristors. One interesting material for creating memristive devices is strontium titanium oxide. Scientists from the University of Groningen discovered how this material can change its resistance based on changes in the number of electrons or the accumulation of defects created by the absence of oxygen atoms in the crystal structure. These insights, derived by combining strontium titanium oxide with the 2D material graphene, could lead to the creation of memristors responding at different timescales, corresponding to short-term and long-term memory.

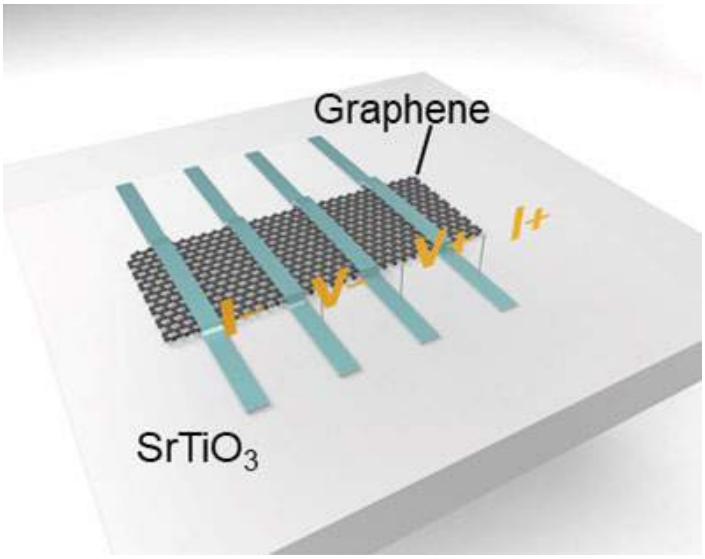
Scientists are working on new materials to create neuromorphic computers, with a design based on the human brain. A crucial component is a memristive device, the resistance of which depends on the history of the device – just like the response of our neurons depends on previous input. Materials scientists from the University of Groningen analysed the behaviour of strontium titanium oxide, a platform material for memristor research and used the 2D material graphene to probe it. On 11 November 2020, the results were published in the journal ACS Applied Materials and Interfaces.

Computers are giant calculators, full of switches that have a value of either 0 or 1. Using a great many of these binary systems, computers can perform calculations very rapidly. However, in other respects, computers are not very efficient. Our brain uses less energy for recognizing faces or performing other complex tasks than a standard microprocessor. That is because our brain is made up of neurons that can have many values other than 0 and 1 and because the neurons' output depends on previous input.

Oxygen vacancies

To create memristors, switches with a memory of past events, strontium titanium oxide (STO) is often used. This material is a perovskite, whose crystal structure depends on temperature, and can become an incipient ferroelectric at low temperatures.

> "... the combination with graphene opens up a new path to memristive heterostructures combining ferroelectric materials and 2D materials."



The combination with graphene opens up a new path to memristive heterostructures combining ferroelectric materials and 2D materials. Illustration: Banerjee lab

The ferroelectric behaviour is lost above 105 Kelvin. The domains and domain walls that accompany these phase transitions are the subject of active research. Yet, it is still not entirely clear why the material behaves the way it does. 'It is in a league of its own,' says Tamalika Banerjee, Professor of Spintronics of Functional Materials at the Zernike Institute for Advanced Materials, University of Groningen.

The oxygen atoms in the crystal appear to be key to its behaviour. 'Oxygen vacancies can move through the crystal and these defects are important,' says Banerjee. 'Furthermore, domain walls are present in the material and these move when a voltage is applied to it.' Numerous studies have sought to find out how this happens, but looking inside this material is complicated. However, Banerjee's team succeeded in using another material that is in a league of its own: graphene, the two-dimensional carbon sheet.

Conductivity

'The properties of graphene are defined by its purity,' says Banerjee, 'whereas the properties of STO arise from imperfections in the crystal structure. We found that combining them leads to new insights and possibilities.' Much of this work was carried out by Banerjee's PhD student Si Chen. She placed graphene strips on top of a flake of STO and measured the conductivity at different temperatures by sweeping a gate voltage between positive and negative values. 'When there is an excess of either electrons or the positive holes, created by the gate voltage, graphene becomes conductive,' Chen explains. 'But at the point where there are very small amounts of electrons and holes, the Dirac point, conductivity is limited.'

In normal circumstances, the minimum conductivity position does not change with the sweeping direction of the gate voltage. However, in the graphene strips on top of STO, there is a large separation between the minimum conductivity positions for the forward sweep and the backward sweep. The effect is very clear at 4 Kelvin, but less pronounced at 105 Kelvin or at 150 Kelvin. Analysis of the results, along with theoretical studies carried out at Uppsala University, shows that oxygen vacancies near the surface of the STO are responsible.

Memory

Banerjee: 'The phase transitions below 105 Kelvin stretch the crystal structure, creating dipoles. We show that oxygen vacancies accumulate at the domain walls and that these walls offer the channel for the movement of oxygen vacancies. These channels are responsible for memristive behaviour in STO.' Accumulation of oxygen vacancy channels in the crystal structure of STO explains the shift in the position of the minimum conductivity.

Chen also carried out another experiment: 'We kept the STO gate voltage at -80 V and measured the resistance in the graphene for almost half an hour. In this period, we observed a change in resistance, indicating a shift from hole to electron conductivity.' This effect is primarily caused by the accumulation of oxygen vacancies at the STO surface.

All in all, the experiments show that the properties of the combined STO/graphene material change through the movement of both electrons and ions, each at different time scales. Banerjee: 'By harvesting one or the other, we can use the different response times to create memristive effects, which can be compared to short-term or long-term memory effects.' The study creates new insights into the behaviour of STO memristors. 'And the combination with graphene opens up a new path to memristive heterostructures combining ferroelectric materials and 2D materials.'

Reference: Si Chen, Xin Chen, Elisabeth A. Duijnstee, Biplab Sanyal, and Tamalika Banerjee: Unveiling Temperature-Induced Structural Domains and Movement of Oxygen Vacancies in SrTiO3 with Graphene. ACS Appl. Mater. Interfaces, 11 November 2020

Turning heat into power with efficient organic thermoelectric material

by Rene Fransen (ScienceLinX)

Thermoelectric materials use a temperature difference between both sides of the material to create an electric current. Inorganic thermoelectric materials are already quite efficient, but they contain toxic or rare elements and are often brittle, which makes them unsuitable for everyday applications. By contrast, organic thermoelectric materials are safe to use, but their efficiency in converting a temperature difference into a current is not very good. A team of scientists led by Jan Anton Koster, Professor of Semiconductor Physics at the University of Groningen, has now created a much more efficient organic thermoelectric material that is made from buckyballs with organic side chains. Their flexible material could be used to power wearable electronics.

Thermoelectric materials can turn a temperature difference into electricity. Organic thermoelectric materials could be used to power wearable electronics or sensors; however, the power output is still very low. An international team led by Jan Anton Koster, Professor of Semiconductor Physics at the University of Groningen, has now produced an n-type organic semiconductor with superior properties that brings these applications a big step closer. Their results were published in the journal Nature Communications on 10 November.

The thermoelectric generator is the only human-made power source outside our solar system: both Voyager space probes, which were launched in 1977 and are now in interstellar space, are powered by generators that convert heat (in this case, provided by a radioactive source) into an electric current. 'The great thing about such generators is that they are solid-state devices, without any moving parts,' explains Koster.

Conductivity

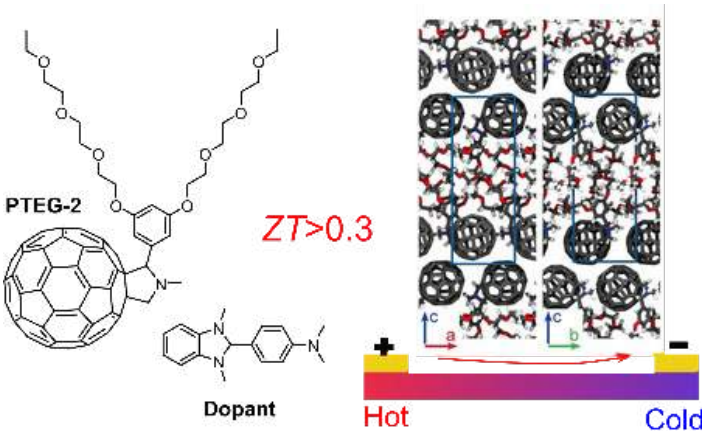
However, the inorganic thermoelectric material used in the Voyager's generators is not suitable for more mundane applications. These inorganic materials contain toxic or very rare elements. Furthermore, they are usually rigid and brittle. 'That is why interest in organic thermoelectric materials is increasing,' says Koster. Yet, these materials have their own problems. The optimal thermoelectric material is a phonon glass, which has a very low thermal conductivity (so that it can maintain a temperature difference) and also an electron crystal with high electrical conductivity (to transport the generated current). Koster: 'The problem with organic semiconductors is that they usually have a low electrical conductivity.'

> "The problem with organic semiconductors is that they usually have a low electrical conductivity"

Nevertheless, over a decade of experience in developing organic photovoltaic materials at the University of Groningen has led the team on a path to a better organic thermoelectric material. They focused their attention on an n-type semiconductor, which carries negative charge. For a thermoelectric generator, both n-type and p-type (carrying positive charge) semiconductors are needed, although the efficiency of organic p-type semiconductors is already quite good.

Buckyballs

The team used fullerenes (buckyballs, made up of sixty carbon atoms) with a double-triethylene glycol-type side chain added to them. To increase the electrical conductivity, an n-dopant was added. 'The



The chemical structure of the fullerene derivative used in our work improves the ordering of the molecules as shown (right) in the snapshots of the molecular packing. By using a suitable dopant, this material can convert heat into electrical energy.
Illustration: J.A. Koster, University of Groningen

fullerenes already have a low thermal conductivity, but adding the side chains makes it even lower, so the material is a very good phonon glass,' says Koster. 'Furthermore, these chains also incorporate the dopant and create a very ordered structure during annealing.' The latter makes the material an electric crystal, with an electrical conductivity similar to that of pure fullerenes.

'We have now made the first organic phonon glass electric crystal,' Koster says. 'But the most exciting part for me is its thermoelectric properties.' These are expressed by the ZT value. The T refers to the temperature at which the material operates, while Z incorporates the other material properties. The new material increases the highest ZT value in its class from 0.2 to over 0.3, a sizeable improvement.

Sensors

'A ZT value of 1 is considered a commercially viable efficiency, but we believe that our material could already be used in applications that require a low output,' says Koster. To power sensors, for example, a few microwatts of power are required and these could be produced by a couple of square centimetres of the new material. 'Our collaborators in Milan are already creating thermoelectric generators using fullerenes with a single side chain, which have a lower ZT value than we now have.'

The fullerenes, side chain and dopant are all readily available and the production of the new material can likely be scaled up without too many problems, according to Koster. He is extremely happy with the results of this study. 'The paper has twenty authors from nine different research groups. We used our combined knowledge of synthetic organic chemistry, organic semiconductors, molecular dynamics, thermal conductivity and X-ray structural studies to get this result. And we already have some ideas on how to further increase the efficiency.'

> "We have now made the first organic phonon glass electric crystal but the most exciting part for me is its thermoelectric properties."

Reference: Jian Liu, Bas van der Zee, Riccardo Alessandri, Selim Sami, Jingjin Dong, Mohamad I. Nugraha, Alex J. Barker, Sylvia Rousseva, Li Qiu, Xinkai Qiu, Nathalie Klasen, Ryan C. Chiechi, Derya Baran, Mario Caironi, Thomas D. Anthopoulos, Giuseppe Portale, Remco W. A. Havenith, Siewert J. Marrink, Jan C. Hummelen & L. Jan Anton Koster: N-type organic thermoelectrics: demonstration of ZT > 0.3 Nature Communications 10 November 2020

When going in circles helps you stay put:

How spin-orbit coupling leads to stable spins in color centers in materials

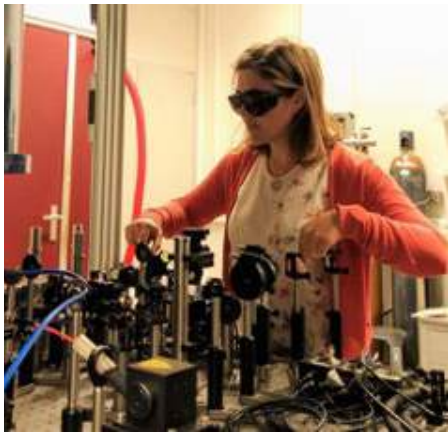
by Carmem Maia Gilardoni

Quantum computing and communication promise to revolutionize the way in which we process and transfer information, just like transistors and the internet did in decades past. Quantum information technology allows us to process information differently than classical computing and could enable fundamentally secure communication: according to the laws of quantum mechanics, it is impossible for a third party to eavesdrop on your quantum communication channel without you knowing.

The communication between remote quantum systems is most efficiently done using particles of light – so called photons. Thus, one of the big challenges in the field is to find materials that will efficiently hold onto their quantum information and transfer it into light particles on demand. Some of the major contenders in the field are tiny blinkers present in crystalline materials like diamond or silicon, called color centers. These color centers are almost omnipresent – in fact, they are responsible for the bright color of ruby, emerald and sapphire. They behave like artificial molecules trapped in the crystals: they vibrate and interact with light like a molecule would, but the shape of these 'artificial molecules' is determined by the crystal around it.

In a color center, electrons interact with external magnetic fields due to a fundamentally quantum mechanical property called spin. The spin can be used to store quantum information efficiently: generally, a spin interacts only with a magnet, which makes it relatively insensitive to the environment and allows it to live for a relatively long time. A photon emitted by such a color center can provide information about the quantum mechanical state of the electron spins in it.

Silicon carbide is an industrially mature semiconductor that hosts a variety of color centers, several of them interacting with light in the telecom band. This means that we can make use of the existing telecommunication infrastructure to transfer quantum information between these color centers. In some of these color centers the quantum mechanical spin property is strongly connected to the motion of the electrons (something that is called spin-orbit coupling). Since the motion of the electron is strongly influenced by its environment (the electron can bounce off other electrons or atoms, or interact with electric fields all around it), one would intuitively expect that the strong spin-orbit coupling would lead to faster loss of the quantum information stored in the spin. But this is not what researchers at the University of Groningen find, in their work published October



Carmem Maia Gilardoni working in the lab.

2020 in New Journal of Physics (*https://doi.org/10.1088/1367-2630/abbf23*).

In this work, the team lead by Caspar van der Wal investigates a type of color center containing molybdenum atoms in silicon carbide, which interact with light at the near-telecom range and are subject to strong spin-orbit coupling. The researchers used pulses of light to write and read the spin state in these color centers and tracked how long the stored spin information lived in these systems. They find that the spin information lived for very long in these color centers – several seconds when cooled to a temperature of 2 Kelvin (minus 270 Celsius). So, how do they explain their counter-intuitive result? In this particular 'artificial molecule', they crystal only allows the electrons to move in a circular path. Like a current in a coil, this circular motion creates an effective magnetic field, which interacts very strongly with the spin. Since this circular motion is pinned by the crystal, they find that spin-orbit coupling stabilizes the electron spin in these color centers, and this leads to the long-lived spins. At higher temperatures, they find that the additional vibrational motion of these 'artificial molecules' lead to additional interaction between the spin and the environment that destroys the spin quantum information in these systems.

Several color centers in various crystals have similar spatial properties to the Mo color center in SiC. Thus, the researchers conclude, 'these findings shine light into what processes are actually responsible for the loss of quantum information in this class of systems. Several suitable candidates have been overlooked in the past, partly due to their strong spin-orbit coupling. However, we find that they could have surprising and promising properties for the field of quantum communication'.

Dr. Bose, Dr. Raffa and Prof. Picchioni partners in EU's Horizon 2020 FET Open Program consortium

Dr. Ranjita K. Bose , Dr. Patrizio Raffa and Prof. Francesco Picchioni of the Engineering and Technology Institute Groningen (ENTEG) are partners in a consortium that received a European research council FET-Open 2018-2020 grant. The consortium's ' 5DNanoPrinting ' project has been awarded a grant of EUR 3.58 million, of which the UG's allocation is EUR 547,000. The goal of the project is to develop innovative smart materials and novel fabrication methods for micro and nano devices. The Italian Institute of Technology is coordinator.

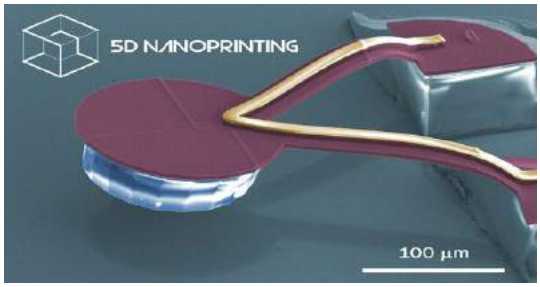
The project titled 'Functional & Dynamic 3D Nano-MicroDevices by Direct Multi-Photon Lithography' aims to develop fast and inexpensive functional 3D Nano- MicroDevices (NEMS/MEMS). MEMS, Micro ElectroMechanical Systems, are microscopic devices with moving parts which are capable of accomplish a specific task. They find applications in many fields such as consumer electronics, automotive and healthcare. The approach aspires to become a novel gold standard for micro/nano-technologies, similar to how 3D printing has become a cornerstone of manufacturing technologies in the last decade.

Novel polymers

The UG team of researchers will develop novel polymers, which will be used to make gradient structures with varying mechanical properties and crosslinking. The project's consortium includes academic and industrial partners from Italy, Austria, Ireland and the Netherlands. The partners will bring expertise in chemistry, material science, physics and engineering.

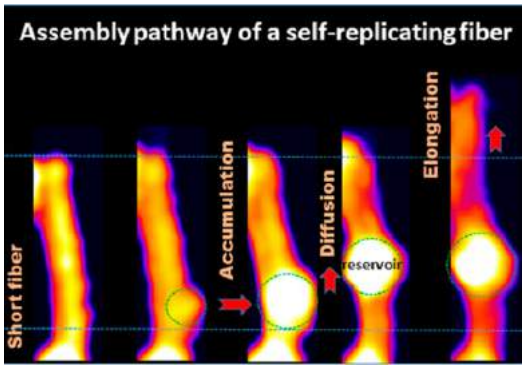
FET Open

FET Open supports the early-stages of science and technology research and innovation around new ideas towards radically new future technologies.



New High Speed AFM results featured as Spotlight in JACS

In an all Groningen research effort the groups of Prof. Marrink (GBB), Prof. Otto (Stratingh) and Prof. Roos (Zernike) have been able to follow fibre self-assembly in real-time at the nanoscale. Using a combination of High Speed AFM and Molecular Dynamics simulations the groups were able to scrutinize the nanomentre-scale mechanisms of self-replicating molecule assembly. The results appeared in the Journal of the American Chemical Society (JACS) and were featured prominently as a JACS Spotlight.



The goal of the project was to uncover the assembly mechanism of self-replicating molecules. While the Otto lab had already close to 10 years of experience with the studied system, within weeks of starting the project important and completely unexpected new insights into the mechanism of replication were found. In brief, it was already known that self-replication involved assembly of molecules into 1D-stacks, where the assembly process somehow drives the synthesis of the assembling material from smaller components (precursors). The combined High Speed-Atomic Force Microscopy (HS-AFM) and Molecular Dynamics (MD) Simulations revealed that the stacks play an active role in the process by binding the precursors at the sides of the stacks, where they accumulate in reservoirs, and guiding them to the ends from which the stack grow (see animated HS-AFM .gif illustration). During this reservoir-assisted growth process the free precursors are added to the growing fiber (see figure) and thereby converted into the molecules that replicate.

Putting the findings in perspective

The broader significance of these findings for the field of self-assembly can be summarized as follows. In the assembly of one-dimensional objects (stacks or fibers) there is an obvious but mostly overlooked problem: the assembling material needs to find the growing end of the fiber. This is a 3-dimensional search problem that causes assembly to be slow as the number of fiber ends tends to be small (often in the nanomolar range). The researchers discovered that fibers can bind the assembling material at their sides and guide this material to the ends, thereby turning a 3-dimensional search problem into a 1-dimensional one and greatly enhancing the efficiency of assembly. This finding constitutes a new mechanism for the assembly of one-dimensional objects. Mechanistic insight into assembly pathways, like the one unveiled here, are keenly sought after, but remain rare.

By combining the data from the different single-molecule and bulk experiments, the molecular dynamics simulations and the kinetic modelling, the authors were able to make this step in our understanding of self-assembly processes. The work was published in J. Am. Chem. Soc. where it was also highlighted as a JACS Spotlight. Please see below for the links to the article and Spotlight.

References: Sourav Maity, Jim Ottelé, Guillermo Monreal Santiago, Pim W. J. M. Frederix, Peter Kroon, Omer Markovitch, Marc C. A. Stuart, Siewert J. Marrink, Sijbren Otto, and Wouter H. Roos Caught in the Act: Mechanistic insight into Supramolecular Polymerization driven Self-Replication from Real Time Visualization; J. Am. Chem. Soc., 2020, Vol. 142, p. 13709–13717

First NWO ENW Team Science Award for Prof. Minnaard and Dr. Buter

Prof. Minnaard and Dr. Buter (UG, Stratingh Institute), together with Dr. van Rhijn (University of Utrecht) and Prof. Moody (Harvard), have been awarded the first NWO ENW Team Science Award. This cross-disciplinary team receives the award for the development of 'Comparative Lipidomics, a new strategy to study pathogenic bacteria that forms the basis for novel drug development, diagnostics and vaccines'.

The team is a cross-disciplinary team that has been working together for 14 years towards a common goal: to identify the key molecules that promote progression and response in tuberculosis. The team combines the strengths of synthetic and analytical organic chemistry, microbiology and immunology to reach their goals. An important detail is that the team does not focus on proteins but on lipids.

The team makes discoveries using an 'iterative approach': Moody discovers novel lipids by comparing pathogenic and non-pathogenic bacteria; Minnaard synthesizes the lipid(s); Van Rhijn studies their interaction with the human immune system, and Buter prepares new light-activatable drugs gleaned from these results. The combination of these complementary expertises and techniques is what makes the work of this team unique.

Besides pioneering in a new research field, the team has also made their discoveries open for researchers from all around the world. This knowledge and reagents sharing initiative benefits the advancement of lipid biology and sets a new scientific standard.

The assessment committee feels that it concerns a strong team that has been working together for a long time. The scientific goal of the team is clearly defined and there is a clear synergy between the team members and their expertise. Without this interdisciplinary character, the research would likely not be as effective. Additionally, the committee very much appreciates the fact that the newly synthesized lipids are freely available for everyone.

Prof. Sijbren Otto elected KNAW member

The Royal Netherlands Academy of Arts and Sciences (KNAW) has selected eighteen new members, one of which is from the Faculty of Science and Engineering (FSE) of the University of Groningen. It concerns Prof. Sijbren Otto, Professor of systems chemistry at the Stratingh Institute for Chemistry. The KNAW has approximately 550 members. They are chosen based on scientific achievements of researchers. The new Academy members will be installed later this year.

About Prof. Otto - systems chemistry

Prof. Sijbren Otto is a pioneer in systems chemistry, a new discipline in chemistry that studies networks of interacting molecules and their properties. Otto is using this approach to study the chemical basis of life. He succeeded in building systems with 'dead' molecules made in the lab that can make copies of themselves, with the aim to undergo Darwinian evolution. Mutations occur during replication, subsequently followed by selection depending on the chemical environment. This gives certain mutants the ability to replicate faster and win the race for resources available. Otto and his group also show how self-replicating molecules can use chemical energy to produce and maintain more complex structures: a first step towards metabolism.

National research programme led by University of Groningen professor Katja Loos

Polymer scientists cooperate with industry to create smart materials

by Rene Fransen (ScienceLinX)

Katja Loos, Professor of Polymer Chemistry at the University of Groningen, is conducting science while industry representatives are looking over her shoulder. Loos does not consider this scary. On the contrary, it inspires her and her colleagues from six other Dutch universities. Together, they make up the new virtual research centre for Soft Advanced Materials (SAM), which received a €3.6 million grant from the NWO (Dutch Research Council) and industry partners.

'Although our work is not focused on applications, we asked our industry partners to pick their favourites from over a hundred research ideas,' explains Loos. She wrote the programme proposal and is now the programme's coordinator. Twelve PhD students will work on the selected projects. 'The idea behind this is that the companies get to know the research groups at the different universities and that the young researchers get the opportunity to experience the industrial partner's R&D activities,' says Loos.

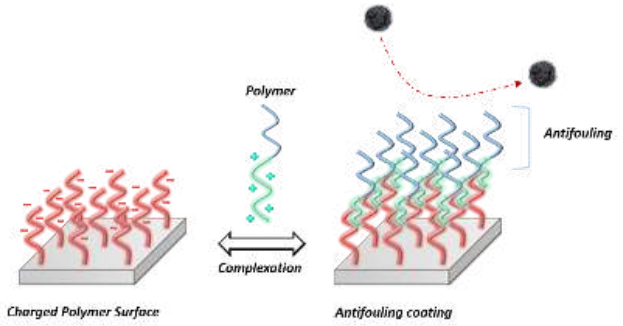
Progress

Four companies are participating in the SAM research centre: the Dutch chemical companies DSM (health, nutrition and materials) and Corbion (food and biochemicals), and Germany-based BASF (the second largest chemicals producer in the world) and BYK Altana (additives). Together, they are contributing €1 million to the programme.

The companies decided on the programme's general course by selecting 12 projects from a long list of research ideas. They are also involved in the annual review of each project. 'This allows them to indicate whether they feel that the project is still on the course that they envisioned at the start.' However, Loos stresses that the PhD supervisors make the final decision regarding the project's progress. 'If they disagree with the company representatives, it is up to me to find a solution.'

Curiosity driven

Most of the PhD students have started their projects. So far, Loos is excited about the interaction with the commercial partners. 'BASF is a German company but they don't really know what is happening in the chemical labs in the Netherlands within the fields of polymer science and soft matter. They are curious,



The polymer based anti-fouling system
Illustration Annemarie Maan

as is BYK Altana,' says Loos. And the companies are already interacting with the students. 'It is inspiring for the students to see a company representative interested in their work.'

So, over the course of the programme, the industry partners will learn more about what polymer scientists at Dutch universities are working on. The scientists will gain better insight into the companies' needs, while 12 curiosity-driven projects will have been completed.

Coating

The projects cover three main themes: adaptive materials, sustainability and platform science. Four PhD students from the University of Groningen take part in the SAM consortium. Loos is supervising two students with sustainability-themed projects, who will work on bio-based and on biodegradable polymers. The other two PhD students from Groningen are being supervised by Prof. Marleen Kamperman (adaptive materials) and Dr Giuseppe Portale (platform science).

The project that Kamperman is supervising (together with Prof. Wiebe de Vos from the University of Twente) aims to create a new coating to keep surfaces clean. If all works well, the coating can be regenerated. The first step is to create a polymer that will attach to a surface and that also has a charged section that sticks out. 'We then add a second polymer that has the opposite charge and properties that prevent fouling of the surface,' explains Kamperman. This second polymer will attach to the first polymer. 'The link between the two polymers can be broken by changing the acidity or the salt concentration. This would enable us to recycle the released polymer.'

The industry partners are interested in different applications. Anti-fouling materials could be used to keep a ship's hull clean or to prevent your office chair from causing stripes on the wall. 'The application determines the kind of polymers needed,' says Kamperman. Creating the right polymers will be the major challenge in this project. The joint experience of Kamperman and De Vos should help the PhD student to accomplish this.

X-ray machine

The project led by Giuseppe Portale is not aimed at creating new materials but at developing new characterization techniques to study them. In the Physics & Chemistry building's basement, Portale's group constructed a large, unique X-ray machine that can be used to study the nanostructure of materials (solution, bulk and thin films) in the 1-1000 nanometre range. One of the applications of this set-up is watching how paint dries in real time. Portale shoots X-rays at a sample, at small or wide angles, depending on the length scales to be investigated. These then bounce off and are focused on a 2D position-sensitive detector.

'The scattering pattern contains information about the surface structure of the films,' explains Portale. And not just about the surface. By adjusting the incident angle, X-rays can penetrate into the material to different depths before they get scattered. This means that he is able to study, for example, a 30-micrometre layer of coating or paint at different depths. Furthermore, the method is non-destructive and does not affect the sample, enabling him to watch coatings form during drying.

'That kind of information can help producers to understand the drying processes and can help them to refine coating formulations. My PhD student will look at different coatings that closely mimic the commercially available ones. All have the same ingredients but in different combinations.' Currently, changing the formulation is largely a trial-and-error process. The technique that Portale uses will help scientists to understand what factors determine the final structure and hence the coating's final properties.

It is a technique that he started to develop at the large European Synchrotron X-ray Facility (ESRF) in Grenoble (France). 'Synchrotron facilities such as the ESRF are much more powerful and we therefore use them in our research each time the system dynamics are faster than one second. The use of different X-ray tools allows us to study how atoms, molecules and nanoparticles assemble in space and time.'

More cooperation

With nearly all PhD projects underway, Katja Loos will be busy coordinating and mediating, while also conducting science. 'A major advantage of this programme is that all university partners are in the Netherlands. So, it is easy to meet up.' Furthermore, the companies involved are also located nearby. 'We even get spur-of-the-moment visits.' At the end of the programme, all partners will know each other better, which should lead to more cooperation between universities and chemical companies.

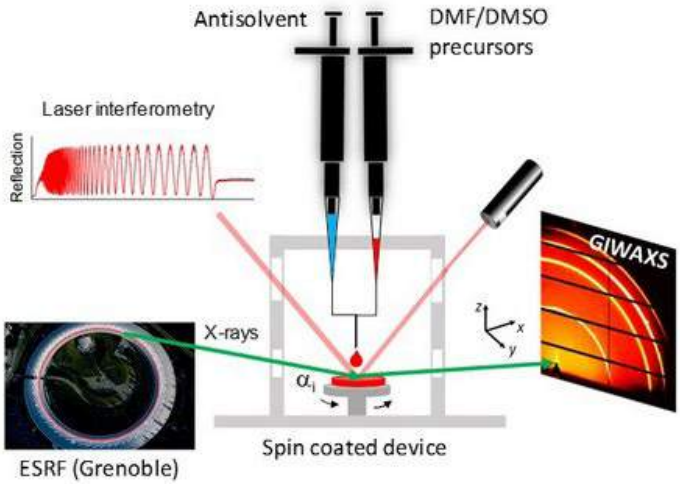
> "... companies get to know the research groups at different universities & young researchers get the opportunity to experience the industrial partner's R&D activities."

X-rays reveal in situ crystal growth of lead-free perovskite solar panel materials

by Rene Fransen (ScienceLinX)

Just over ten years ago, scientists discovered a new, promising material that could convert light into electricity: metal-halide perovskite. The first solar cell perovskites contained lead, which is toxic. Soon, perovskites were developed that were based on tin, but these were not very stable. A few years ago, scientists at the University of Groningen demonstrated that adding another type of perovskite – one that forms two-dimensional layers instead of three-dimensional crystals – increased the stability; however, it reduced efficiency. University of Groningen scientists have now 'watched' how thin films of tin-based perovskite crystals grow. They discovered that in mixtures of 3D and 2D perovskites, the 2D component helps to orient the 3D-like crystals but, at the same time, the 2D perovskite forms an insulating layer that is in contact with the substrate. By breaking up this insulating layer, it should be possible to create more efficient and stable tin-based perovskite solar panels.

Lead-based perovskites are very promising materials for the production of solar panels. They efficiently turn light into electricity but they also present some major drawbacks: the most efficient materials are not very stable, while lead is a toxic element. University of Groningen scientists are studying alternatives to lead-based perovskites. Two factors that significantly affect the efficiency of these solar cells are the ability to form thin films and the structure of the materials in the solar cells. Therefore, it is very important to investigate in situ how lead-free perovskite crystals form and how the crystal structure affects the functioning of the solar cells. The results of the study were published in the journal Advanced Functional Materials on 31 March.



Scheme of the experimental setup used to investigate the structural formation of perovskites thin films during spin coating.
Illustration G. Portale, University of Groningen

Photovoltaic cells that are based on hybrid perovskites were first introduced in 2009 and rapidly became almost as efficient as standard silicon solar cells. These materials have a very distinctive crystal structure, known as the perovskite structure. In an idealized cubic unit cell, anions form an octahedron around a central cation, while the corners of the cube are occupied by other, larger cations. Different ions can be used to create different

perovskites.

Spin coating

The best results in solar cells have been obtained using perovskites with lead as the central cation. As this metal is toxic, tin-based alternatives have been developed, for example formamidinium tin iodide (FASnI3). This is a promising material; however, it lacks the stability of some of the lead-based materials. Attempts have been made to mix the 3D FASnI3 crystals with layered materials, containing the organic cation phenylethylammonium (PEA). 'My colleague, Professor Maria Loi, and her research team showed that adding a small amount of this PEA produces a more stable and efficient material,' says Assistant Professor Giuseppe Portale [1]. 'However, adding a lot of it reduces the photovoltaic efficiency.'

That is where Portale comes in. Perovskites have been studied for a long time by Professor of Photophysics and Optoelectronics Maria Loi, while Portale developed an X-ray diffraction technique that allows him to study the rapid formation of thin films in real time during spin coating from solution [2] [3]. On a laboratory scale, the perovskite films are generally made by spin coating, a process in which a precursor solution is delivered onto a fast spinning substrate. Crystals grow as the solvent evaporates. At the beamline BM26B-DUBBLE at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France, Portale investigated what happens during the tin-perovskite film formation.

Interface

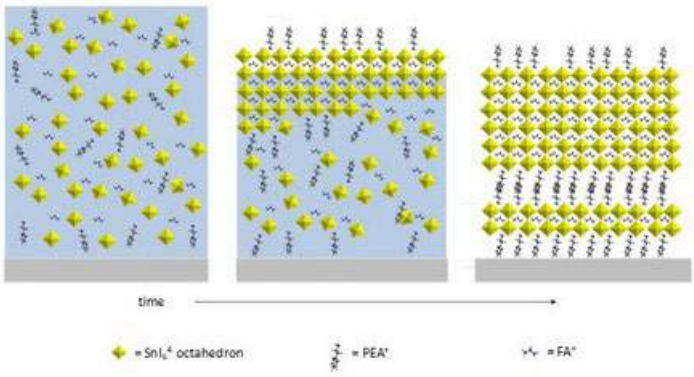
'Our initial idea, which was based on ex situ investigation, was that the oriented crystals grow from the substrate surface upwards,' Portale explains. However, the in situ results showed the opposite: crystals start to grow at the air/solution interface. During his experiments, he used 3D FASnI3 with the addition of different amounts of the 2D PEASnI4. In the pure 3D perovskite, crystals started to form at the surface but also in the bulk of the solution. However, adding a small amount of the 2D material suppressed bulk crystallization and the crystals only grew from the interface.

'PEA molecules play an active role in the precursor solution of the perovskites, stabilizing the growth of oriented 3D-like crystals through coordination at the crystal's edges. Moreover, PEA molecules prevent nucleation in the bulk phase, so crystal growth only takes place at the air/solvent interface,' Portale explains. The resulting films are composed of aligned 3D-like perovskite crystals and a minimal amount of 2D-like perovskite, located at the bottom of the film. The addition of low concentrations of the 2D material produces a stable and efficient photovoltaic material, while the efficiency drops dramatically at high concentrations of this 2D material.

Insulator

The experiments by Portale and Loi can explain this observation: 'The 2D-like perovskite is located at the substrate/film interface. Increasing the content of the 2D material to above a certain amount causes the formation of an extended 2D-like organic layer that acts as an insulator, with detrimental effect for the device's efficiency.' The conclusion of the study is that the formation of this insulating layer must be prevented to achieve a highly efficient and stable tin-based perovskite. 'The next step is to realize this, for example by playing with solvents, temperature or specific perovskite/substrate interactions that can break up the formation of this thick insulating layer.'

Reference: Jingjin Dong, Shuyan Shao, Simon Kahmann, Alexander J. Rommens, Daniel Hermida-Merino, Gert H. ten Brink, Maria A. Loi & Giuseppe Portale: Mechanism of Crystal Formation in Ruddlesden–Popper Sn-Based Perovskites. Advanced Functional Materials, 31 March 2020



Scheme of the mechanism of crystallization from DMF/DMSO solution during drying for the 2D/3D perovskite films.
Illustration G. Portale, University of Groningen

Researchers develop a new bioinspired polymer able to efficiently transport protons

Spider Silk inspires a new class of synthetic ion-conducting polymers for future energy applications

by Renee Moezelaar

Synthetic polymers have changed the world around us, and it would be hard to imagine a world without them. They have pervaded our life, making their way from simple plastic goods to sophisticated devices such as batteries and fuel cells. However, they do have their problems. It is for instance hard to precisely control their molecular structure from a synthetic point of view. This makes it harder to finely tune some of their properties, such as their ability to transport ions. To overcome this problem, a group of researchers headed by Dr. Giuseppe Portale from the University of Groningen (the Netherlands) decided to take inspiration from nature. The result was published in Science Advances on July 17: a new class of polymers based on protein-like materials and inspired to spider silk that work as proton conductors and might be useful in future bio-electronic devices.

'I have been working on proton conducting materials on and off since my PhD', says Portale. 'I find it fascinating to know what makes a material transport ions so I work a lot on understanding and optimizing structures at the nanoscale level to get greater conductivity.' But it was only a few years ago that he considered the possibility of making them from biological, protein-like structures. That was something the assistant professor came up together with Prof. Andreas Hermann, a former RUG-colleague now working at the DWI - Leibniz Institute for Interactive Materials in Germany and Prof. Kai Liu from Changchun Institute of Applied Chemistry at the Chinese Academy of Sciences: 'We could immediately see that proton conducting bioinspired polymers could be very useful for applications like bio-electronics or sensors.'

More active groups, more conductivity

What do spiders have in common with batteries? Nothing so far, but the material developed in the research published in Science Advances on July 17 by G. Portale and co-workers may change this in the future. The inset shows a robust membrane created using a spider silk inspired polyelectrolyte that is capable of efficiently transport protons.

But first they had to see if the idea would work. "Our first goal was to prove that we could precisely tune the proton conductivity of the protein-based polymers by tuning the number of ionic groups per polymer chain". A number of unstructured biopolymers that had different numbers of ionisable carboxylic acid (-COOH) groups was prepared. Their proton conductivity scaled linearly with the number of charged carboxylic acid groups per chain. 'It was not ground breaking, everybody knows this concept. But we were thrilled by the possibility to design something that worked

as expected' Portale says.

For the next step, Portale relied on his expertise in the field of synthetic polymers: 'I have learned over the years that the nanostructure of a polymer can greatly influence the conductivity. If you have the right nanostructure, it allows the charges to bundle together and increase the local concentration of these ionic groups and that gives a dramatic boost to the proton conductivity.' Since the first batch of biopolymers was completely disordered, the researchers had to switch to a different material. They decided to use a known protein having the shape of a nanosized barrel. 'We engineered a protein already existing in nature that has the structure of a barrel of few nanometers and added strands containing carbocyclic acid to its surface', Portale explains. 'This increased the conductivity greatly.'

A novel spider silk inspired proton conducting polymer

Unfortunately, the barrel-polymer was not very useful. It had no mechanical strength and it was difficult to process, so Portale and his colleagues had to look for another alternative. They landed on a well-known natural polymer: spider silk. 'This is one of the most fascinating materials in nature, because it is very strong but can also be used in many different ways', says Portale. 'During my time at the European Synchrotron laboratory, I have learned about the fascinating nanostructure of the spider silk. We have thus engineered a protein-like polymer that has the main structure of spider silk but was modified to host the strands of carbocyclic acid that we prepared before'

The novel material worked like a charm. 'We found that it self-assembles at the nanoscale similarly to spider silk while creating dense clusters of charged groups, which are very beneficial for the proton conductivity', Portale explains. 'And we were able to turn it into a robust centimetre-sized membrane.' A nice achievement if we consider that the measured proton conductivity is one order of magnitude higher than those of any previously known biomaterials.

What do spiders have in common with batteries? Nothing so far, but the material developed in the research published in Science Advances on July 17 by G. Portale and co-workers may change this in the future. The inset shows a robust membrane created using a spider silk inspired polyelectrolyte that is capable of efficiently transport protons.

But they are not there yet according to Portale: 'This was mainly fundamental work. In order to really apply this material, we really have to improve it and make it processable.'

Dreams

But even though the work is not yet done, Dr. Giuseppe Portale and his co-workers can already dream about applying their polymer: 'We think this material could be useful as a membrane in future energy devices. Maybe not for the large scale systems that you see in cars and factories, but more on a small scale. There is a growing field of implantable bio-electronic devices, for instance glucose-powered pacemakers. In the coming years we hope to find out if our polymer can make a difference there, since it is already bio-compatible.'

For the short term, Portale mainly thinks about sensors. 'The conductivity we measure in our material is influenced by the environment, like humidity, volatile chemical species or temperature. So changes in all these quantities can be measured using our material.' However, before all these dreams come true, there are a lot of questions to be answered. 'I am very proud that we were able to design, make and control these new materials on a molecular scale, and build them from scratch. But we still have to learn a lot about their capabilities and see if we can improve them even further.'

Reference: De novo rational design of a freestanding, supercharged polypeptide, proton-conducting membrane. Chao Ma, Jingjin Dong, Marco Viviani, Isotta Tulini, Nicola Pontillo, Sourav Maity, Yu Zhou, Wouter H. Roos, Kai Liu, Andreas Herrmann and Giuseppe Portale

Detailed model important step towards understanding Huntington's

by Renee Moezelaar

Huntington's disease is still a quite mysterious disease. It is genetic and causes brain cells to degrade over time. Many researchers have tried to figure out what happens, but no-one has been able to find a cure yet. But thanks to associate professor Patrick van der Wel this might be a step closer. He and his team of researchers came up with a new, more detailed and specific molecular model of the mutated part of huntingtin, the protein that plays a big part in this disease. The model was published in the Journal of Molecular Biology on June 27th.

'If you want to cure or find a medicine for a disease, you first have to understand how it works', says Van der Wel. Unfortunately this is not yet the case for Huntington's disease. 'For Huntington's we have a general idea, but details are not yet clear. That is why we started working on our model.'

Faulty gene

Van der Wel and his colleagues have been working on Huntington's disease for a couple of years now. 'We know that Huntington's is caused by a faulty gene that gives a mutation in the protein huntingtin', Van der Wel explains. 'Due to this mutation the patients get clusters of proteins in the brain, similar to what happens with Parkinson's or Alzheimer's.'

The clusters are associated with the development of symptoms, so researchers were eager to find out how they form exactly. Studying of this process revealed that the mutated huntingtin protein undergoes polymorphism: it can fold in different ways and have multiple structures. Van der Wel: 'In biology we often expect one protein to have one structure and one function. But huntingtin turns out to do good as well as bad things. We wanted to figure out how and why this happens.'

Folding and unfolding

In order to figure this out, Van der Wel's PhD student Jennifer Boatz used techniques like electron microscopy and NMR to learn more about the structure of the huntingtin protein and see how it folds. All this analysing resulted in a very elaborate model of clusters formed by the mutant Huntingtin protein, the most detailed so far. According to Van der Wel, the model is an important first step towards better understanding: 'Understanding the way the protein folds is very important for understanding the disease. And with this model the whole world can make more sense of what happens.'

However, the model is not the only important find. The researchers also discovered that the structure the protein formed depended on the concentration. 'This is very important to know, since we tend to use very high concentrations if we study this protein in the lab. But in our body the concentration is very low, so if we want to mimic the situation in our bodies we need to change our approach.'

New research

The associate professor hopes that all this information will lead to new and interesting research: 'We are looking at a number of different paths. It would be great if we could use our model to find molecules that can bind to the protein and prevent the wrong kind of folding. On the other hand we also want to look at diagnostics, and use the model to detect the clusters in a much earlier stage of the disease. And lastly I would really like to investigate what happens when one of these clusters forms and how it pushes other clusters to form.'

So there is still a lot of work to be done. For now, Van der Wel focusses on further improving the model. 'We are working with the campaign team Huntington to take the next step. We really want to go to the atomic structure, and understand all the details. Because the more we know, the better we can fight this disease.'

Reference: Protofilament Structure and Supramolecular Polymorphism of Aggregated Mutant Huntingtin Exon 1. Boatz, J.C., Piretra, T., Lasorsa, A., Matlahov, I., Conway, J.F. & Van der Wel, P.C.A. (2020) J. Mol. Biol., 432(16): 4722-4744. (Open Access)

Scientists create coatings from nature

UG and AkzoNobel join forces to develop the green chemistry of the future

Organic chemists from the University of Groningen and the Dutch multinational company AkzoNobel, a major global producer of paints and coatings, developed a process that allows them to turn biomass into a high-quality coating using light, oxygen and UV light. This process combines a renewable source with green chemistry and could replace petrochemical-based monomers such as acrylates, which are currently used as building blocks for coatings, resins and paints. A paper on the new process was published in the journal Science Advances on 16 December.

Coatings are everywhere, from the paint on your house to a protective layer on the screen of your smartphone. They protect surfaces from scratches, influences of the weather or everyday wear. Most coatings are made up of polymers based on acrylate monomers, with the global production of acrylate exceeding 3.5 million tonnes a year, all produced from fossil oil.

Biomass

To make these coatings more sustainable, scientists from the University of Groningen, led by Professor of Organic Chemistry Ben Feringa, teamed up with scientists from coating producer AkzoNobel. 'We wanted to use lignocellulose as the starting material,' says George Hermens, a PhD student in the Feringa group and first author of the paper in Science Advances. Lignocellulose makes up 20 to 30 per cent of the woody parts of plants and is the most abundantly available raw biomass material on Earth. Currently, it is mainly used as a solid fuel or used to produce biofuels.

Hydroxybutenolide

'Lignocellulose can be cracked with acid to produce the chemical building block furfural, but this needs to be modified to make it suitable for the production of coatings,' explains Hermens. He used a process that has been developed in their group to convert the furfural into a compound, hydroxybutenolide, that resembles acrylic acid. 'The chemical conversion uses only light, oxygen and a simple catalyst and produces no waste. The only side product is methyl formate, which is useful as a replacement for chlorofluorocarbons in other processes.'

Less reactive

Part of the structure of hydroxybutenolide is similar to acrylate, but the reactive part of the molecule is a ring structure. 'This means that it is less reactive than acrylate and our challenge was to further modify the molecule so that it would produce a useful polymer.' This was achieved by adding different green or biobased alcohols to the hydroxybutenolide, creating four different alkoxybutenolide monomers.

Coatings

These monomers can be transformed into polymers and coatings with the help of an initiator and UV light. 'Coatings are made up of cross-linked polymer chains. By combining different monomers, we could get cross-linked polymers with different properties.' For example, while all polymers would coat glass, one combination was able to also form a coating on plastic. And by adding more rigid monomers, a harder coating was formed, with properties comparable to those of coatings on cars. In this way, these coatings are adaptable for different purposes.

Patent

'We managed to create coatings from a renewable source, lignocellulose, using green chemistry,' concludes Hermens. 'And the quality of our coatings is similar to that of current acrylate-based coatings.' For two steps in the process, patent applications have been filed with AkzoNobel, the industrial partner in the project. Hermens is now working on a different building block derived from furfural to produce other types of polymer coatings.

Partners

The project was initiated by the Advanced Research Center Chemical Building Blocks Consortium (ARC CBBC), a Dutch national public-private research centre that develops new chemical processes and chemical building blocks for novel energy carriers, materials and chemicals

Continued on p. 23

Elisabetta Chicca new professor Bio-inspired Circuits & Systems

“If we cannot build neural networks, we can’t understand them properly”

Our brains are one of the most complicated machines we know, but little by little researchers are able to figure out more details. Some researchers are even able to translate the processes of the brain into electrical systems. Elisabetta Chicca is one of these researchers, and in August she joined the Zernike Institute as professor Bio-inspired Circuits & Systems.

“I am very excited about joining this team”, says the newly appointed professor. “I was welcomed with open arms and feel like a lot of people in the institute would like to cooperate with me, so there will be a lot of interesting new opportunities.”

Chicca’s work is said to be one of the missing pieces, the step that was so far missing from the institute: “A lot of people study the brain and make models of how certain processes work, but these models are often very abstract and they live in an ideal world. I work on the next step: actually building electrical circuits that mimic the processes of neurons and synapses.”

More interdisciplinary

Chicca started her career as a physicist at the University of Rome, but her research soon became more interdisciplinary. “When I started my PhD in Zurich I was only familiar with the theoretical physics side of building neural networks, so I had to learn a lot about neurobiology and electrical engineering. But this made me appreciate this field of research even more.”

The main reason Chicca wants to mimic the processes in the brain is to get a better understanding of how these processes work. “Feynman used to say: what I cannot create, I do not understand. I think this is true because when we build our neural networks it gives us many new insights. I’m not saying the environment is exactly the same, but we do encounter space and energy constraints that might also play a role in the brain.”

One of her favourite projects at the moment is that of PhD student Thorben Schoepe. In this project,

she is trying to understand insect navigation. "We look at the way a honeybee navigates through an environment, looks for flowers, and goes back to the beehive", she explains. "This sounds simple enough, but it requires a lot of different tasks to be performed simultaneously and in the right order. Just to keep flying is already very complicated."

Thanks to her collaboration with the group of professor Martin Egelhaaf at Bielefeld University, they were able to develop a computational system: "With the knowledge of the biologists, we developed a system which exhibits interesting behaviors comparable to that of the biological counterpart. We can use this system to verify the hypothesis about the computational role of bits and pieces of the insect brain."

Using this model, the researchers build a neural network that powers a small robot. Chicca: "When it encounters an obstacle, it will make a turn and avoid it." Unfortunately, the robot seemed to bump into the obstacles way more often than a bee would. The problem, as it turns out, was one missing neuron. "In nature, the bee slows down if the environment is too crowded. We added a single neuron to our neural network that senses how many obstacles

> "We look at the way a honeybee navigates through an environment, looks for flowers, and goes back to the beehive ..."

> "Feynman used to say: what I cannot create, I do not understand. I think this is true because when we build our neural networks it gives us many new insights."

are in the environment and used its output to change the speed of the robot. This was enough to substantially improve the performance of the robot."

Applying the system

Of course, these kinds of processes won't only yield fundamental insights. Chicca hopes she can also contribute to some real-life applications. "It would be great if we could build a system that does something artificial intelligence is not yet able to do. Our work can provide solutions for tasks that conventional computing can't manage because of the limited availability of resources like energy and data. We can for instance aim to equip small navigating agents running on batteries with cognitive abilities, so that they can navigate through complex environments and, for example, search for survivors in a rescue scenario."

But she also aims at investigating new technological solutions thanks to collaborations at Zernike. "Several groups here are exploring novel materials and their use for computation. The possibilities to collaborate with them open new exciting avenues for my research." Chicca is already busy setting up collaborations with colleagues at the Zernike Institute. "Besides the generous offer from the Zernike and CogniGron Institutes I also recently got some funding, so my group will be able to grow and take on more and more interesting projects."

One of the topics she would like to focus on is learning. "We know a bit about how people learn, for instance, that the synapse changes while we learn. But there is no general theory that can bring it all together. One of my dreams would be to find such a theory, and explain everything."

Meanwhile, she is getting used to living in Groningen. "I have been here so many times before, but it is still a bit unreal that I am actually living here now. I am getting to know the city even better now and enjoying the beautiful nature. I love it, and everybody is making such an effort to make me feel at home, both professionally and personally. I look forward to advancing my research here for many years to come."

Continued from p. 21

for sustainable chemistry. The ARC CBBC is a national initiative with partners from industry, academia and government.There are three universities involved (Utrecht University, the University of Groningen and Eindhoven University of Technology) and major industrial partners (AkzoNobel, Shell, Nouryon and BASF), as well as the ministries of Education, Culture and Science and of Economic Affairs and Climate Policy and the Dutch Research Council (NWO).

Ben Feringa

Hermens' supervisor, Ben Feringa, is one of the founders of this centre. Feringa: 'The programme entails all the steps from fundamental scientific discovery to process and product development. In this long-term partnership, universities and the chemical industry join forces to develop the green chemistry of the future.'

Simple explanation suffices for conduction in nickelates

by Rene Fransen (ScienceLinX)

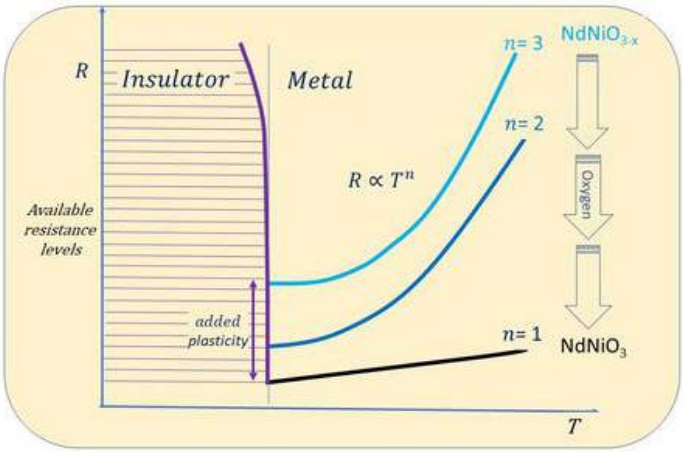
Scientists are looking for new materials to build computers that work in a similar way to a human brain. Such materials should be able to switch from being insulators to being conductors. Neodymium nickel oxide shows this behaviour yet it was unclear as to exactly what makes the electrons in the material move in the way that they do. It has been suggested that this is determined by interactions between the spins (a magnetic property) of the electrons of the nickel ions. However, University of Groningen scientists have discovered that a simpler explanation may suffice: strain and missing ions in the material increase the resistivity and can deceivably mimic the temperature dependence of the resistivity close to a magnetic phase transition. This improved knowledge will help in the development of electronics that can emulate neurons.

Some metal oxides, such as nickelates, have a tuneable resistivity, which makes them an interesting material for adaptable electronics and cognitive computing. These materials can change their nature from metallic to insulating. How exactly this metal-insulator transition takes place is a topic of great interest in condensed matter physics. However, even the metallic behaviour in nickelates seems unusual. Scientists from the University of Groningen, together with colleagues from Spain, have now found that it is not as complex as was previously assumed. The results were published on 11 June in the journal Nature Communications.

In a metal, electrons can move freely, whereas in insulators, they are strongly localized around the atomic nuclei. When a metal is heated, the ions' vibrations (called phonons) scatter the moving electrons and increase the resistivity. In contrast, heating can generate conductivity in some insulators, when electrons receive enough energy to be released and cross the energy band gap that otherwise prevents them from moving.

Exotic explanations

'In some oxides, such as nickelates, a transition from insulator to metal can occur but it is not clear how this happens,' says Beatriz Noheda, Professor of Functional Nanomaterials and Director of the Groningen Cognitive Systems and Materials Center (CogniGron) at the University of Groningen. She and her PhD student Qikai Guo are interested in nickelates because it is possible to tune their resistivity. They could be used in devices that



Materials close to a metal-insulator transition (MIT) have great potential in synaptic devices. The figure shows the behaviour of the resistivity of $NdNiO_3$ as a function of temperature upon changing its oxygen content: the exponent that describes the metallic state can be gradually tuned from n=1 to n=3, tuning at the same time the resistance change at the MIT.
Illustration: B. Noheda, UG

emulate the way that synapses in our brain work.

'Before we can do this, we should understand what the nature of the simplest state, the metal state, is. This means understanding how electrons move around in the material when an electric field is applied to them,' explains Noheda. A linear change in resistivity (an exponent of 1 in the curve that represents the resistivity as a function of temperature) can be explained by a simple model in which the electrons are impeded by the vibration of the ions. 'However, for an exponent that is not 1, more exotic explanations have been suggested, based on the presence of fluctuations in the spins of the nickel electrons and electron-electron interactions that occur when the system is close to a quantum critical point.'

Strain

However, in thin films of neodymium nickelate ($NdNiO_3$), Noheda and her team observed that the exponent was 1 in some samples, while in other samples of the same material, it was not. This suggests that the exponent is not an intrinsic property. Noheda: 'That led us to systematically look at samples grown on different substrates.' The results showed that in perfect films, the exponent is 1, which means that the resistivity is caused by phonons, as it is in normal metals. However, when the substrate that is used induces strain in the thin film, the exponent changes.

The strain leads to oxygen vacancies in the crystals and changes the forces between the ions and, therefore, the electronic energies. That in turn changes the materials' resistivity. 'What we found out is that we can control the amount of vacancies and continuously tune the resistivity exponent at will, which is a tuning knob that we did not know we had. Thus, understanding the metal state in these nickelates may not require exotic electron-electron interactions,' Noheda concludes.

Learning how to control the metal state and the transition to the insulator state will help scientists to design electronics based on nickelates, which can emulate the way that neurons work. That is the ultimate goal of Noheda and her team. 'We now know that these nickelates are more similar to normal metals than we previously thought. This means that they can be quite good conductors if we ensure that there are no ion vacancies in the crystal. In this way, the transition to the insulating phase brings about larger changes in resistance, leading to synaptic devices with improved plasticity.'

In these experiments, the change in resistivity in these nickelates was induced by an increase in temperature. 'This is of course not ideal when you want to make a device. Our next step is to design the material in such a way that we can tune resistivity using an electric field,' Noheda concludes.

Reference: Qikai Guo, Saeedeh Farokhipoor, César Magén, Francisco Rivadulla, and Beatriz Noheda: Tunable resistivity exponents in the metallic phase of epitaxial nickelates. Nature Communications, 11 June 2020

Provinces and SNN support research into production of plastic from sugar

How can we make bioplastics from sugar in an efficient way, so that the price becomes comparable to that of plastics from petroleum? This is what the University of Groningen with project leader Prof Gert-Jan Euverink of ENTEG and various companies and knowledge institutions will be researching over the next three years.

The province of Groningen, the province of Drenthe and the Samenwerkingsverband Noord-Nederland (SNN) jointly support the sustainable initiative with a subsidy of almost 1.2 million euros. More than 900,000 euros comes from a European EFRO subsidy. If the research shows that plastics from sugar can compete with plastics from fossil fuels, this can be a huge boost for the environment and the northern economy. If successful, the project can create 60 to 85 new jobs in a follow-up phase.

New assistant professor in our team - Jagoda Sławińska

"I think theorists can work more closely with experimentalists"

The University of Groningen has for a long time been among the top influencers globally in spintronics research. The reputation of the Zernike Institute for Advanced Materials has continued to attract the best talent, and recent years have seen some promising research in the spintronics field.

A newcomer preparing for her start at the institute in September, Jagoda Sławińska is an assistant professor with experience in spintronics and two-dimensional materials and a rare hands-on approach to research.
Although Sławińska has "plans for purely theoretical research," she is also keen to "work very closely with experimentalists" in her new role.

"My areas of interest are novel materials for spintronics and novel phenomena related to spin-orbit physics, taken in strong connection with low-dimensional systems and 2D materials," she added.

Spin-orbitronics' potential

Although there hasn't been a major breakthrough in the research of spin transistors in more than two decades, recent studies have shown that they could be used in logic-in-memory (LIM) applications. This architecture, popularised among others by researchers at the chipmaker Intel, may bring a significant performance boost to future CPUs.

As the name suggests, the main goal of LIM is to enable computational operations within a memory array, thereby reducing the time required to access the conventional memory and improving the energy efficiency of the system.

In 2018, researchers at Intel published a paper describing a magneto-electric spin-orbit (MESO) logic device with the potential to decrease the voltage required by 80 percent and overall energy consumption by as much as 97 percent compared to conventional complementary metal-oxide-semiconductors (CMOS).

This breakthrough inspired Sławińska to engage further with the topic and this research direction is now one of her main areas of interest. Her focus now is on exploring the applications of multiferroics and spin-orbit related phenomena with LIM arrays and seeking out the best materials to use in these devices.

Closer collaboration

Sławińska is also excited by the potential industrial applications of 2D materials — namely, heterostructures and hybrid systems — related to memories and novel computing architectures. She is currently researching methods of designing a new material with the properties needed for such applications through the stacking of different layers of atomically thin materials.

Sławińska plans to continue working on this topic in Groningen "as there are groups working on similar problems."

"We want to study 2D materials, including stacks of transition metal dichalcogenides (TMDC) that are broadly investigated in Groningen — but then I also want to go beyond that," she said.

Sławińska has emphasized the strength of experimentalist

groups at the Zernike Institute for Advanced Materials and their rich experience in growing 2D material layers. A researcher with a strong hands-on approach, she has become a major proponent of close collaboration between the theoretical and practical sides of academia and is always interested in industrial applications of her research.

"Often in theoretical papers, you'd find statements like 'it can be useful for spintronics applications,'" she added. "This is a general statement. […] What's different about me in this sense is that I have papers that are looking solely at new devices. The main goal of one of my recent papers was to describe and demonstrate that a specific device could be constructed and work.

"This is not common for a theoretician — and of course, it's also very risky; you can propose many things but it's hard to demonstrate that they will work. However, I still think that theorists can work more closely with experimentalists, with the industry. We can still contribute to the construction of some new devices. Maybe not in detail — but in general by proposing new phenomena and the ways of connecting several different effects to get specific functionality."

Sławińska is also no stranger to coding her way through complicated computations.

"I normally get involved in software development if I need to solve a particular problem," she explained. "So, my group won't be development-oriented — but I am looking for students who are prepared to code. If you need to measure something in an experiment, and that measurement is not implemented in any of the known libraries, then it's important that you can write your own module to do it."

"I'm used to working fast"

Sławińska obtained her PhD degree at the Department of Solid State Physics of the University of Łódź in Poland before working at the Spanish and Italian National Research Councils. Her latest postdoctoral position since April 2018 was in the Department of Physics at the University of North Texas. Her working experience of a wide range of institutions allows Sławińska to compare how the academic ecosystems function across the world.

"Generally, in the US the research-bound money is more mobile," she explained. "Sure, you pay more to attend conferences and so on, but at the same time, people are more active. I've been involved in more meetings and collaborations here; it's an environment that's not inert."

Now the researcher plans to use her international experience to embrace the best practices she has been exposed to over the years.

"For example, I believe that in the US people in and around academia act faster than elsewhere," she said. "Now, I'm used to working fast too."

"Often in theoretical papers, you'd find statements like 'it can be useful for spintronics applications. This is a general statement. The main goal of one of my recent papers was to describe and demonstrate that a specific device could be constructed and works. This is not common for a theoretician; it's also very risky."

Finding the missing mirror in spintronic nanodevices

When it comes to next-generation electronics beyond the current silicon-based technologies, spintronics is a top contender. It uses spin, the magnetic property of electrons, instead of their electric charge, to encode and decode digital information. A challenge surrounding spintronics is to efficiently convert between spin and charge signals. Usually, scientists use relatively large magnetic materials for this purpose, but a number of experiments in the past years seem to indicate that some tiny molecules with a certain shape can do the same trick too. You may wonder, can we then use these molecules in spintronic devices? If so, what kind of signals can we get? And what do these signals tell us about the molecules? This is exactly what PhD student Xu Yang, prof. Caspar H. van der Wal, and prof. Bart J. van Wees from the Zernike Institute for Advanced Materials (ZIAM, University of Groningen, the Netherlands) wish to answer with their new theory. Their results were recently published in the journal Nano Letters.

The Missing Mirror

The special thing about these molecules is that their mirror images are different from themselves. Think of it as your hands. The mirror image of your left hand is your right hand—and it cannot fit comfortably in your left-handed glove. These molecules are called chiral molecules, and they are widely available in nature, especially in living organisms. Being able to use them for spintronics has huge potentials. It not only allows for even smaller nanodevices, but can also dramatically reduce the cost of such devices. What's more, it opens up an avenue of using spintronic technologies for chemical and biological applications. This is exactly why it is so important to understand the link between these chiral molecules and spintronic signals coming from nanodevices.

Spintronic Signals

It turns out that, if one simply uses chiral molecules to replace a magnet in typical spintronic nanodevices, fundamental laws of nature would prevent the characteristic spintronic signal—the magnetoresistance (MR) signal—from arising in the linear regime (the common operating regime of electronic nanodevices). This was pointed out in an earlier publication from the same ZIAM physicists, and now in their new publication, they show that the MR signals can indeed emerge as we go beyond the linear regime.

'To generate the MR signals outside the linear regime, electrons with different energies must experience different environments as they travel through the spintronic nanodevice,' explains Yang, 'and they must lose some of their energy.' In this way, a nanodevice containing a molecule, a magnet, and two electrodes can indeed tell whether the molecule is chiral, and can even distinguish the opposite mirrored forms of such molecules. This result also goes beyond molecules, since the missing mirror symmetry is only about geometry, not the chemistry, which means it can happen for other materials as well.

Future Nanodevices

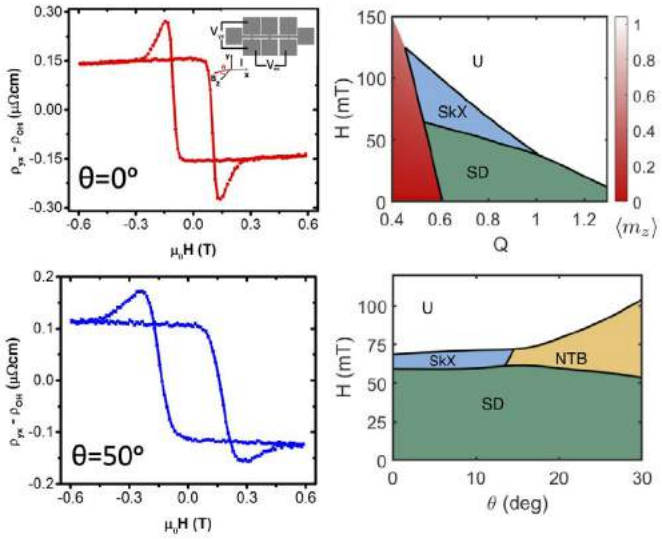
The ZIAM physicists also provide a new theoretical tool to model these spintronic nanodevices, and they can indeed largely reproduce signals that were observed in past experiments. 'Thanks to the new understanding beyond linear regime, we can now explain what determines the sign of these signals.' Moreover, they propose a completely new type of spintronic nanodevice—one that is fully built from chiral molecules, without using any magnetic materials at all. It relates the digital bits of 0 and 1 to the opposite mirror images of chiral molecules, and opens up the possibility of processing digital information by controlling the shape of these molecules. 'We hope these results bring further understandings to the fundamental connection between molecular chirality and electronic spin, and inspire the design of future spintronic devices.'

Reference: Xu Yang, Caspar H. van der Wal, and Bart J. van Wees, Detecting Chirality in Two-Terminal Electronic Nanodevices, https://pubs.acs.org/doi/full/10.1021/acs.nanolett.0c02417, Nano Letters, July 16, 2020.

Resilience and Adaptability:

New pathways with Skyrmion bubbles

Researchers from the University of Groningen and TU Wien have detected signatures of the skew scattering in the ferromagnetic conductor, SrRuO3, associated with topological magnetic bubbles. This effect showed a surprising adaptability to different substrate surfaces and unique resilience to variations of temperature, strength and direction of the applied magnetic field. This research was published on July 27, 2020, as a Rapid Communication in Physical Review Research.



Resilience and Adaptability: New pathways with Skyrmion bubble

Magnetic bubbles are cylindrically shaped islands with reversed magnetization that can be set into motion by electric current pulses. They have been discovered about fifty years ago and were immediately employed to store digital information in non-volatile memory that can withstand harsh environments.

The recent discovery that in chiral magnets the size of magnetic bubbles can be reduced to a few nanometers, spurred the interest in them. This extremely small dimension makes the bubbles highly suitable for novel high-density magnetic memory devices. The magnetic dipoles in the nanosized bubbles, also known as skyrmions, form a knot that cannot be easily unwound. This non-trivial topology gives rise to a skew scattering of electrons off skyrmions – the so-called Topological Hall Effect.

The detection of signatures of the skew scattering in the ferromagnetic conductor, SrRuO3, advances the field of skyrmionics. It provides significant opportunities to tailor device interfaces for new magnetic memory technologies and novel hardware components for alternative computing strategies.

This research is conducted by two research groups of the UG's Zernike Institute of Advanced Materials (ZIAM), led by Prof. Tamalika Banerjee (PhD students Ping Zhang and Arijit Das), Prof. Maxim Mostovoy (PhD students Evgenii Barts and Maria Azhar), and by researchers of the TU Wien, Austria.

New model helps to describe defects and errors in quantum computers

by Rene Fransen (ScienceLinX)

A summer internship in Bilbao, Spain, has led to a paper in the prestigious journal Physical Review Letters for Jack Mayo, a Master's student in Nanoscience at the University of Groningen. He has helped to create a universal model that can predict the number distribution of topological defects in non-equilibrium systems. The results can be applied to quantum computing and to studies into the origin of structure in the early Universe.

Jack Mayo is a student of the Top Master Programme in Nanoscience at the Zernike Institute for Advanced Materials at the University of Groningen. Last year, he received an email, circulated by one of the programme's supervisors, with a list of summer internships that were offered by the Donostia International Physics Center (DIPC) in San Sebastián, Spain. One project caught his eye. 'This was a theoretical project related to condensed matter, but it also had some clear technological relevance. I wanted to find out if this kind of work would suit me,' he explains. Mayo applied and was selected, so he spent his 2019 summer holidays on the Basque coast, immersed in theoretical physics.

Dr Luis Pedro García-Pintos, Dr Aurélia Chenu, Prof. Adolfo del Campo, Iñigo Perez, Léonce Dupays and Jack Mayo (left to right).

Ice crystals

The project that he participated in, together with the research group led by Professor Adolfo del Campo at the DIPC, was aimed at solving a problem in quantum computing – but it has much wider implications, from nanoscale magnets to the cosmos. In all these systems, the onset of order (for example, order induced by cooling) is almost always accompanied by the development of defects. 'Take a system in which particles have a magnetic moment that can flip between up and down,' Mayo explains. 'If you increase their attractive interaction, they will start to align with each other.'

This alignment will begin at certain uncorrelated points in a medium and then grow – like ice crystals in water. The alignment of each domain (up or down in the example of the magnetic moments) is a matter

of chance. 'Local alignments will grow outwards and at a certain stage, domains will begin to meet and interact,' says Mayo. For example, if an up-domain meets a down-domain, the result will be a domain wall at their interface – a symmetry-breaking defect in the ordered structure, leaving behind an artifact of the material in its higher-symmetry phase.

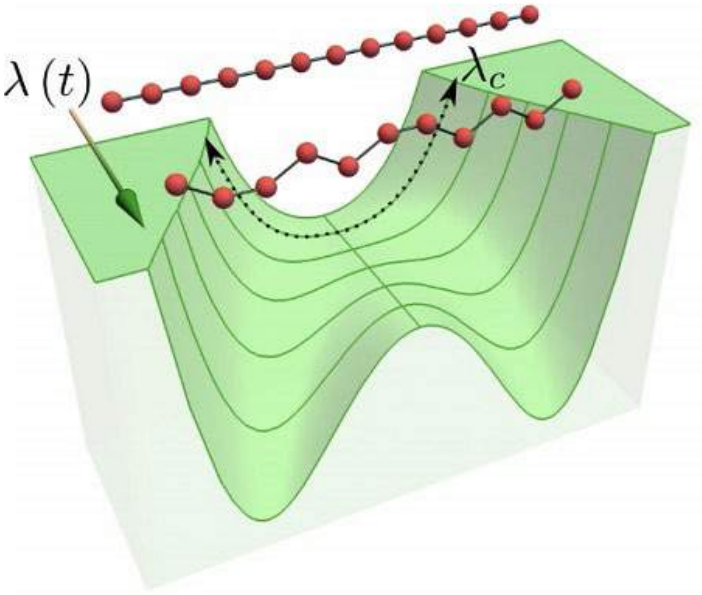
Travelling salesman

This annealing of a medium is described by the Kibble-Zurek mechanism, originally designed to explain how a phase transition resulted in ordered structures in the early Universe. It was subsequently discovered that it could be used to describe the transition of liquid helium from a fluid to a superfluid phase. 'The mechanism is universal and is also used in quantum computing based on quantum annealing,' explains Mayo. This technology is already on the market and is capable of solving complex puzzles such as the travelling salesman problem. However, a problem with this type of work is that defects that occur during the annealing process will distort the results.

Simulations

The number of defects that show up in quantum annealing depends on the time taken to pass the phase transition. 'If you have millions of years to slowly change the interactions between units, you do not get defects, but that is not very practical,' Mayo remarks. The trick is in designing finite-time – and therefore more practical – schedules to obtain an acceptable number of defects with high probability. The research project in which he participated was aimed at creating a model that could estimate the number of defects and guide the optimum design of these systems.

To do this, the physicists used theoretical tools to describe phase transitions and numerical simulations to estimate the defect distribution during cooling. As each domain can have one of two values (up or down in the example of the magnetic moments), they could estimate the chances of two opposite domains meeting and creating a defect. This led to a statistical model based on binomial distribution, which could be used to predict how a system should be cooled to create the smallest number of defects. The model was verified against independent numerical simulations and appeared to work well. This new model was described in a paper that was published on 17 June in Physical Review Letters and was accompanied by a 'Viewpoint' published in Physics, a comment on the results by the independent physicist Professor Smitha Vishveshwara from the University of Illinois at Urbana-Champaign.



At the point at which the energy landscape splits, the high symmetry chain decays into a lower symmetry state when the critical point is passed. In this case, a straight chain decays into a zig-zag configuration when the anisotropy \lambda(t) passes a critical value \lambda_{c}. Where two consecutive ions fall onto the same side, a state of higher energy locally, we observe a defect. | Illustration Fernando Gómez-Ruiz - Donostia International Physics Center

Amsterdam

Now, almost a year later, Mayo is finishing his Master's thesis in functional spectroscopy. He has learned that he has a taste for analytical work and, after graduating, he will start a PhD project intheoretical machine learning at the University of Amsterdam. 'I am finishing up work on a quasi-classical approach to model the defects, which was also started in Spain. But first things first.'

Reference: Fernando J. Gómez-Ruiz, Jack J. Mayo, and Adolfo del Campo: Full Counting Statistics of Topological Defects after Crossing a Phase Transition. Phys. Rev. Lett 17 June 2020

Transporting energy through a single molecular nanowire

by Rene Fransen (ScienceLinX)

Plants and photosynthetic bacteria catch sunlight via molecular antennas, which then transfer the energy to a reaction centre with minimal losses. Scientists would like to make molecular wires that can transfer energy just as efficiently. Scientists at the University of Groningen created tiny fibres by stacking certain molecules together. Single fibres transport energy, although they sometimes malfunction. Creating bundles of fibres (as is done with copper wiring) was thought to be the solution but this turned out not to be the case. Energy moves fast when spread out across several molecules. In single fibres, this works well but in bundled fibres, this spreading out is hampered as the molecules experience strain. These results can be used to better understand energy transport along molecular wires, which will help in the design of better wires.

Photosynthetic systems in nature transport energy very efficiently towards a reaction centre, where it is converted into a useful form for the organism. Scientists have been using this as inspiration to learn how to transport energy efficiently in, for example, molecular electronics. Physicist Richard Hildner from the University of Groningen and his colleagues have investigated energy transport in an artificial system made from nanofibres. The results were published in the Journal of the American Chemical Society.

'Natural photosynthetic systems have been optimized by billions of years of evolution. We have found this very difficult to copy in artificial systems,' explains Hildner, associate professor at the University of Groningen. In the light-harvesting complexes of bacteria or plants, light is converted into energy, which is then transported to the reaction centre with minimal losses.

Bundles

Five years ago, Hildner and his colleagues developed a system in which disc-shaped molecules were stacked into nanofibres with lengths exceeding 4 micrometres and a diameter of just 0.005 micrometres. By comparison, the diameter of a human hair is 50-100 micrometres. This system can transport energy like the antennas in photosynthetic systems. 'But we sometimes saw that the energy transport became stuck in the middle of our four micrometre-long fibres. Something in the system appeared to be unstable,' he recalls.

To improve the energy transport efficiency, Hildner and his colleagues created bundles of nanofibres. 'This is the same idea as that which is used in normal electronics: very thin copper wires are bundled together to create a more robust cable.' However, the bundled nanofibers turned out to be worse at transporting energy than single fibres.

Coherence

The reason for this lies in something called coherence. When energy is put into the molecules that make up the fibres, it creates an excited state or exciton. However, this excited state is not a packet of energy that is associated with a single molecule. Hildner: 'The energy is delocalized over several molecules and it can therefore move fast and efficiently across the fibre.' This delocalization means that the energy moves like a wave from one molecule to the next. By contrast, without coherence, the energy is limited to a single molecule and must hop from one molecule to the next. Such hopping is a much slower way to transport energy.

'In the bundles, coherence is lost,' explains Hildner. This is caused by the strain that the bundle imposes on each fibre within it. 'The fibres are compressed and this causes side groups of the molecules to crash into each other.' This changes the energy landscape. In a single fibre, the energy of the excited states of several neighbouring molecules are at the same level. In a bundle, the local environments of the molecules differ, leading to a difference in energy levels.

Bike tour

'Imagine that you are on a bike tour. The height profile of the tour represents the energy levels in the molecules that make up the

fibres,' says Hildner. 'If you are cycling in the Netherlands, you will arrive at your destination quickly because the terrain is flat. In contrast, in the Alps you must cycle uphill quite often, which is tough and slows you down.' Thus, when the molecules' energy levels in the fibres are different, transport becomes more difficult.

This discovery means that the team's original idea, to increase energy transport efficiency using bundles of nanofibres, turned out to be a failure. However, they have learned valuable lessons from this, which can now be used by theoretical physicists to calculate how to optimize transport in molecular fibres. 'My colleagues at the University of Groningen are currently doing just that. But we already know one thing: if you want good energy transport in nanofibres, do not use bundles!'

> "Imagine that you are on a bike tour. The height profile of the tour represents the energy levels in the molecules that make up the fibres"

Reference: Bernd Wittmann, Felix A. Wenzel, Stephan Wiesneth, Andreas T. Haedler, Markus Drechsler, Klaus Kreger, Jürgen Köhler, E. W. Meijer, Hans-Werner Schmidt and Richard Hildner: Enhancing Long-Range Energy Transport in Supramolecular Architectures by Tailoring Coherence Properties. J. Am. Chem. Soc. First online 11 april 2020

Newsflash

Prof. dr. Moniek Tromp elected vice-chair of the Young Academy of Europe

Prof. dr. Maria Antonietta Loi elected Fellow of American Physical Society

NEVAC prize for Brian Baker of the Stöhr group

NWO XS grant for Dr. Wlodarczyk-Biegun

Prof. dr. Rudolf partner in consortium that receives H2020 Marie Curie ITN-ETN grant

NWO KLEIN awarded to Prof. dr. George Palasantzas

JACS Spotlight on self-assembled monolayers of Prof. dr. Chiechi and Prof. dr. Rudolf

Prof. dr. Bart Kooi installed as Education Director of the Zernike Institute for Advanced Materials

Herman Duim Graduate Student Award recipient for the 2020 MRS Spring Meeting

ENW klein Grant for Prof. dr. Maxim Pchenitchnikov and Prof. dr. Thomas L.C. Jansen

IEEE Robert E. Newnham Ferroelectrics Award for Prof. Beatriz Noheda

Remco Havenith Nanoscience Teacher of the Year

Prof. dr. Koster partner in consortium that receives H2020 Marie Curie ITN-ETN grant

Dr. Amar Kamat wins FSE's Postdoc Prize

Annemarie Maan elected KNAW/De Jonge Academie Faces of Science

Prof. dr. Petra Rudolf appointed new Dean of Graduate Studies

Prof. Onck partner in ENW-GROOT project of EUR 2.7 million

KNG Juryprize for Björn Kriete

Prof. Marrink and Dr. Jansen partners in ENW-GROOT project of EUR 2.7 million

Heeres and Heeres receive Groene Groninger award

Jan Post project leader Northern Netherlands AI Hub

Jacquelien Scherpen awarded IEEE Fellow

Dr. Wlodarczyk-Biegun receives second NWO XS grant

Shirin Faraji Young Academy of Groningen board member

Bart van Wees featured in Physical Review B 50th Anniversary Milestones

CogniGron is two years along the path towards 'human' computers

by Eelco Salverda, Communication UG

The computer: our traditional powerful machine is rapidly approaching its limits, so researchers at the UG's CogniGron centre are working on developing the computer of the future. Two years into the project, Beatriz Noheda, director of CogniGron, takes stock. Although developing a new super-calculator is obviously a long-term project, CogniGron has already achieved a lot.

The computer of the future: it has almost become a holy grail that is being sought by researchers from every corner of the earth. Beatriz Noheda, Professor of Functional Nanomaterials at the UG, and her colleagues from the fields of materials science, physics, mathematics, computer science and artificial intelligence are working on new materials for the next generation of computers, inspired by the functioning of the human brain. The current generation is approaching the limits of its capacities. 'We need to change the way in which computers work if we are to keep up with the enormous amounts of data that are generated by the digital world,' explains Noheda. 'They cannot deal with big data efficiently, and they waste a lot of energy by doing so, forcing us to decide which data to process. This can and must become a more sustainable process, so that all of the useful information that is contained in the available data can be retrieved.'

Unused data

Noheda gives a few examples of data that currently goes unused. 'Take medical data. An analysis of symptoms reported by patients from all around the world could help to prevent diseases. And merging worldwide seismographic data could generate insight into potential earthquakes. Or take 'the internet of things'. We have been talking about fridges that tell the supermarket when you run out of milk for ten years now. These developments have ground to a halt because with the current computer design we are unable to process all of this data.' But this could be very different. Computers may be better chess players than humans, but there are still things that humans do better.

The brain is an example

Current computers send every bit of information from transistor to transistor, one step at a time. The human brain, however, is able to process lots of information simultaneously. This is called parallel processing. 'Take this room,' says Noheda to illustrate. 'If we sit here, you immediately know what to focus on. You listen to me and you don't pay attention to, or in other words waste energy on, information regarding the carpet and the chairs, for instance, despite that this information is also being sent to your brain. We can prioritize in a millisecond. This is because the neurons, our brain cells, have thousands of mutual connections and form networks that can transport the information through a multitude of paths. Brain cells process information, but at the same time they are also able to store information as

> "To take some of the pressure off humans, we created something that did not resemble a human. We are now going back to the drawing board, and using humans as our model."

being a memory. Computers use two separate systems to perform these two tasks. This makes our brain highly economical in terms of energy. A computer that works like this would be a real game changer.' Scientific coordinator Jasper van der Velde, who has now joined us, sums it up nicely: 'To take some of the pressure off humans, we created something that did not resemble a human. We are now going back to the drawing board, and using humans as our model.'

The search for the perfect material

We need new materials, electronic circuits and systems to be able to imitate the function and connectivity of neurons. It's not quite like looking for the proverbial needle in a haystack, but it certainly isn't easy. 'We have six research groups working at the Zernike Institute for Advanced Materials, each of which is studying two or three potentially suitable materials,' explains Noheda. 'The material we are looking for must satisfy a lot of conditions – and you also have to take long-term availability into account.'

Unique collaboration

'We soon realized that researchers from a single field wouldn't be able to do everything that we wanted to do,' Noheda continues. Whereas much of the research into new computers is carried out from within one single scientific discipline, the UG entered into a unique collaboration between the materials scientists from the Zernike Institute and the Bernoulli Institute for Mathematics, Computer Science and Artificial Intelligence. 'The computer scientists tell us exactly what is needed. The mathematicians make models of the properties, which the physicists then test on the new materials in their labs. Artificial intelligence researchers explain what the new hardware must be capable of. Algorithms developed within the field of Artificial Intelligence have proven to broaden our horizons, but the current generation of computers simply can't deal with them.' What was once a modern, useful machine is rapidly becoming the limiting factor.

> "Every discipline has its own way of working. People think differently. You have to learn each other's language."

Two productive years

CogniGron has existed for two-and-a-half years now. How are things going? 'Really well,' Noheda continues. 'Over thirty professors are now working on CogniGron related projects. We managed to recruit ten new professors. They were very keen to join us because they are equally enthusiastic about our vision and goals. In turn, CogniGron benefits from their expertise and global contacts. They are knowledge magnets.' And then there's the newly acquired transmission electron microscope (TEM), another flagship. There are only about ten of these microscopes in the whole world, and they can be used to study materials at the atomic level. 'That is a very important factor,' Van der Velde stresses. 'You have to know exactly how a material works before you can control it and make it work for you.' Finally, CogniGron has published around ten important articles in leading professional journals.

Learning to understand each other

Noheda explains that much of the initial years was spent generating understanding and trust. 'A collaboration between four disciplines requires a lot of brainstorming and discussions. What are we doing, how can we help each other? Only this way we can effectively combine the strengths of each discipline.' Noheda and her colleagues are based in Nijenborgh 4, which is the physics and chemistry building. One building further, you'll find the computer scientists, the mathematicians and the artificial intelligence researchers. They are only a few physical steps apart, but the metaphorical distance can be more difficult to span. 'Every discipline has its own way of working. People think differently,' explains Van der Velde. 'You have to learn each other's language.' But they managed. A shared vision and joint goal have helped to tear down walls and remove barriers. 'Sharing experiences helps you to grow,' says Noheda. 'It's healthy to look at things from the other side every now and then,' she laughs.

New generation of scientists

Working together means stepping out of your comfort zone. This can be a challenging, time-consuming business. Not everyone is flexible enough. All newly appointed professors therefore work in more than one field; they feel comfortable in two different worlds. In this respect, Noheda has high expectations of the PhD students working at CogniGron, where they grow up in a multidisciplinary environment. 'We are already seeing this with some of our Bachelor's and Master's students. They prefer broader-based course units, such as maths and physics, or physics and computer science. CogniGron is exactly what I was looking for, you hear them say.'

Experimenting

Fundamental research but with a practical goal – would that be a good description of Noheda's work? 'Yes, indeed,' she nods, 'because that computer is still a long way off. No, that's not frustrating. It's all about the ongoing learning process. We saw that we were getting closer after just six months. We're happy with every step in the right direction.' HP, IBM, Intel; they are all following CogniGron with great interest. These are the companies that will ultimately be manufacturing the computers. 'We work closely with companies like these but they can't diversify in their research as much as we can. Companies need to sell products and earn money. Researchers can be more adventurous, and try bolder ideas.' She is echoing Nobel Prizewinner Ben Feringa's words: 'Let universities be playgrounds'. 'Our mindset is broader,' adds Van der Velde. 'Some materials work best at extreme temperatures. A company won't investigate this, as the temperature would be too high for commercial purposes. So that's what we do. And if a material turns out to work, we start looking for workability at a more feasible temperature.'

Trendsetter

The multidisciplinary character of CogniGron also has a disadvantage. Research findings take longer to generate and are more difficult to publish as they fall outside the scope of field-specific scientific journals. But this hurdle is also being cleared. A new journal recently appeared: Neuromorphic computing and engineering. Three CogniGron researchers are closely involved in this journal, which just goes to show how things in academia are changing. And maybe how much of a trendsetter CogniGron is.

Ubbo Emmius Fund of the UG receives large donation from alumnus
Extra source of funds for academic research

A former student has donated a large sum via the Ubbo Emmius Fund to their alma mater, the University of Groningen (UG). At the end of October, as part of this donation, the Ubbo Emmius Fund received a sum of €35 million. It is expected that further sums will be received as part of this donation in the near future. The final donation amount is currently unknown because this depends on the return on the investments from which the donation was made. The donor has asked to remain anonymous; the UG and Ubbo Emmius Fund are respecting this wish.

According to the conditions attached to the donation, the funds must be used for scientific research at the UG. President of the Board of the University, Prof. Jouke de Vries: 'We are happy and thankful for this enormous donation to the Ubbo Emmius Fund. Never in our history has such a great sum been left to the University by an alumnus for the benefit of scientific research. It offers us the opportunity to substantially invest in fundamental and applied research. In addition, we will be able to give ambitious early-career academics the chance to further shape their scientific careers.'

€30 million for CogniGron

The donor selected the first recipient for part of the donation: the Groningen Cognitive Systems and Materials Center (CogniGron), which will receive a sum of €30 million. Under this project at the Faculty of Science and Engineering, researchers have been working on developing materials for the next generation of computers since 2018.

Prof Beatriz Noheda (right)

'It is important research because the demand made of computers to process and interpret enormous amounts of data will increase explosively over the coming years. At the UG, we can explore solutions to this challenge with a strong, multidisciplinary project comprising scientists from various disciplines. To show our thanks for this donation, we wanted to name CogniGron after the donor. But, of course, we are respecting their wish for anonymity', states Prof Beatriz Noheda, Director of CogniGron.

Fund

The donation is being managed by the Ubbo Emmius Fund. The Fund supervises the careful and correct allocation of donations in accordance with any conditions stipulated by donors. The intent is to deposit this donation into a so-called endowment fund, in which annual returns are paid out every year. In this way, the UG is ensured of a long-term, substantial extra source of income to benefit scientific research and PhD positions.

Virus assembly has been filmed

Spanish and Dutch researchers discovered how the HIV/AIDS virus is formed

Scientists in Groningen and Madrid have managed to capture unique images of the first steps of virus assembly. By using a very fast scanning probe microscope, they were able to film how HIV proteins begin to form a virus. It appears that the virus forming process does not proceed in a very orderly manner. At first sight, it seems very haphazard. Still, this process eventually leads to a regular virus particle. By figuring out how virus assembly takes place, research can be done in a more focused manner into anti-viral medicines that specifically hinder the forming of the virus.

Human immunodeficiency virus (HIV) causes AIDS, a disease that still results in the deaths of over half a million people per year. HIV packages viral genetic material into a capsule containing virus proteins, among other things. While highly clear images have been taken with an electron microscope that show how the proteins are bound to one another, until recently, no methods have been able to demonstrate how they bind together. After all, electron microscopes cannot capture moving images. However, a very fast atomic force microscope recently entered the market: the High Speed Atomic Force Microscope (HS-AFM), with which videos can be made. This microscope has made it possible to study molecular processes by touch , but scientists had not yet succeeded in following the incredibly dynamic process of virus assembly.

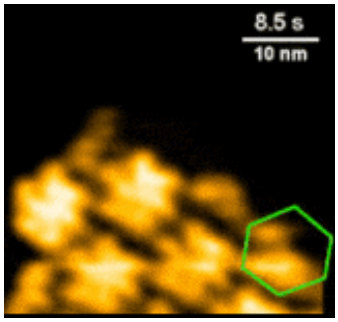
Through intensive collaboration between a research group specializing in HIV at the Universidad Autónoma de Madrid and the Molecular Biophysics research group led by Prof. Wouter Roos at the University of Groningen, who have a version of the high-speed microscope in their lab, it became possible to follow virus assembly in real time. 'A technical masterpiece', exclaims Prof. Wouter Roos.

Completing the puzzle

The researchers demonstrated that virus assembly does not proceed in a very ordered manner at all. It appears more like completing a jigsaw puzzle, in which puzzle pieces are added at different spots but also taken away again if they do not appear to fit. In this way, the process seems like an apparently haphazard coming and going of proteins, with some sort logic hidden beneath this. Finally, an ordered grid of proteins is created, which forms the basis of the virus particle. It is likely that other viruses use a similar process to build virus particles.

Coronavirus

The results of the research have been published in scientific journal ACS Nano. Now that it is clear how the first stages of virus forming take place, the researchers from Groningen and Spain want to shed light on the next steps. In this way, they hope to create a complete image of the process,



Single molecules building

from the creation of the individual building blocks at the start, to the formation of a whole infectious virus particle. As well as providing fundamental insights into the biology of viruses, this work also has functional applications. Once it is clear how virus particles are made up, highly targeted research can then be done into anti-viral medicines that focus on interrupting the assembly of the AIDS virus. At a later stage, it is also hoped that these methods can be used to investigate other viruses, such as the coronavirus strain that caused the outbreak of COVID-19.

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