Scientia

EXCITING INNOVATIONS IN PHYSICAL SCIENCE AND TECHNOLOGY

HIGHLIGHTS:

- Reducing Atmospheric Carbon Dioxide Through Direct Air Capture
- Developing Sustainable Water Purification Technologies
- Understanding the Nature of Matter through Quark Gluon Plasmas
- Advancing Quantum Computing to Accelerate Scientific Research

EXCLUSIVES:

- The European Chemical Society
- The American Association of Chemistry Teachers

Issue: #138

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WELCOME...

In this inspiring new edition of Scientia, we are delighted to feature some of the most ground-breaking research findings and innovations across the diverse fields of chemistry, materials science, physics and computer science.

Our opening section explores the weird and wonderful world of chemistry. Here, we begin with a focus on chemistry education, before highlighting a selection of research projects in this fascinating branch of science. From developing chemical methods to remove carbon dioxide from the atmosphere, to devising inexpensive strategies for synthesising pharmaceuticals, this section shows how chemistry continuously offers solutions to an array of societal challenges.

Next, we report on some exciting developments in the critical field of materials science. In this section, we meet scientists who are creating cutting-edge materials for advanced technologies – from nanoporous membranes that remove bacteria from drinking water, to graphene foam that promotes tissue repair in the treatment of various medical conditions, including osteoarthritis.

In the third section of this exciting edition, we delve deeper into the nature of matter. Here, we highlight the latest discoveries and innovations in the world of physics – from understanding how matter behaved in the early universe, to creating gigantic atoms with sizes comparable to grains of sand.

Our final section celebrates innovation in computing technology – a field that has completely transformed human society in just a few decades. Here, we introduce researchers who are spearheading tomorrow's breakthroughs in computer science – from optimising virtual reality technology, to bringing the power of quantum computing to research labs across the globe.

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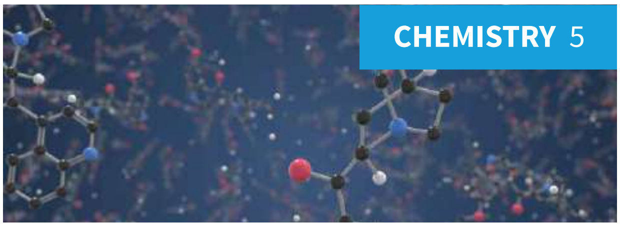

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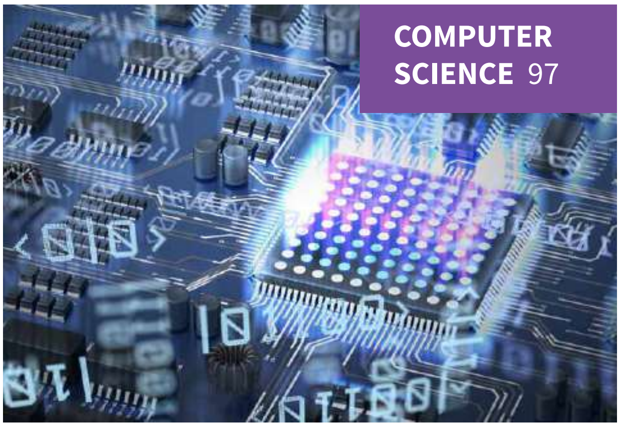

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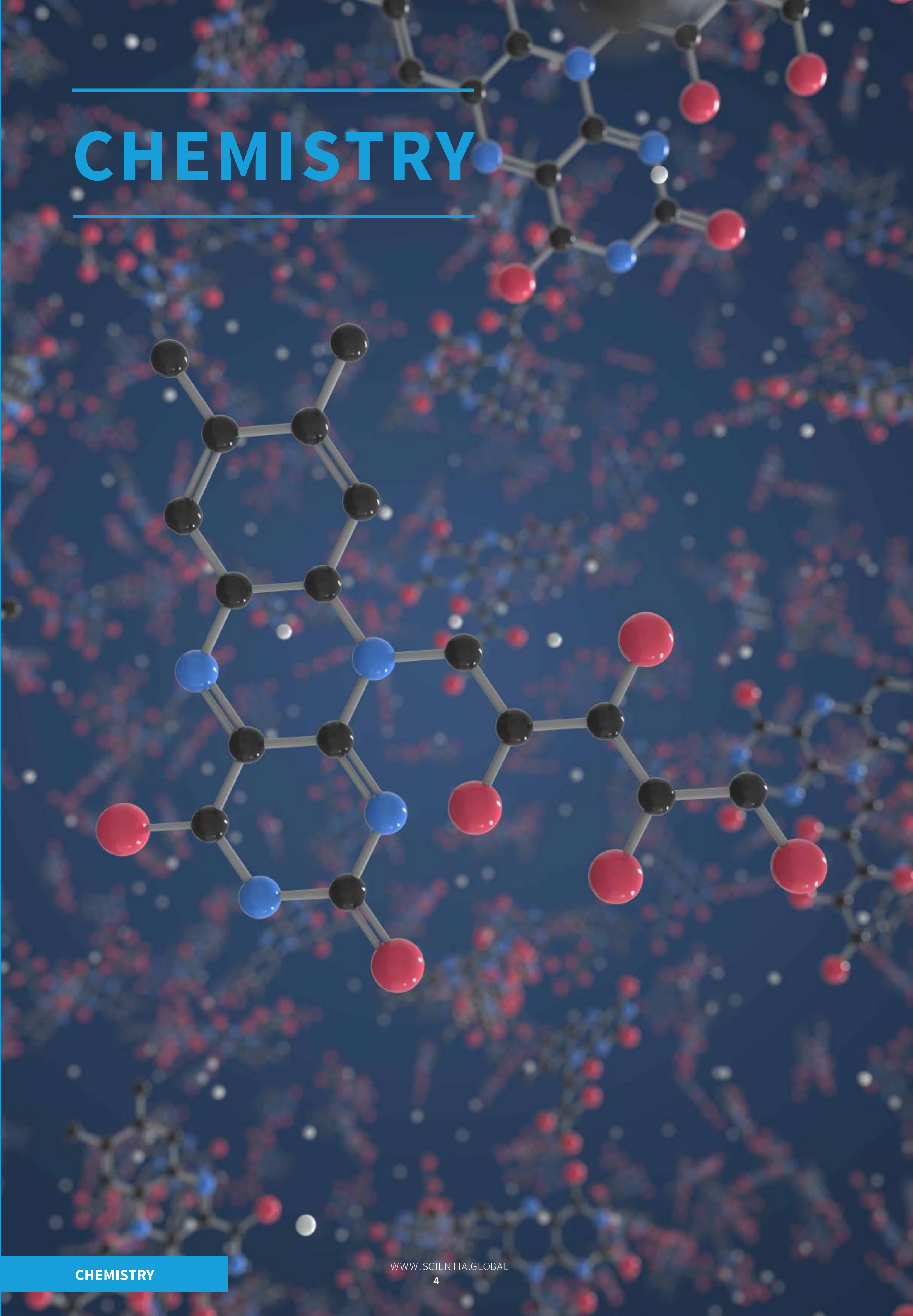
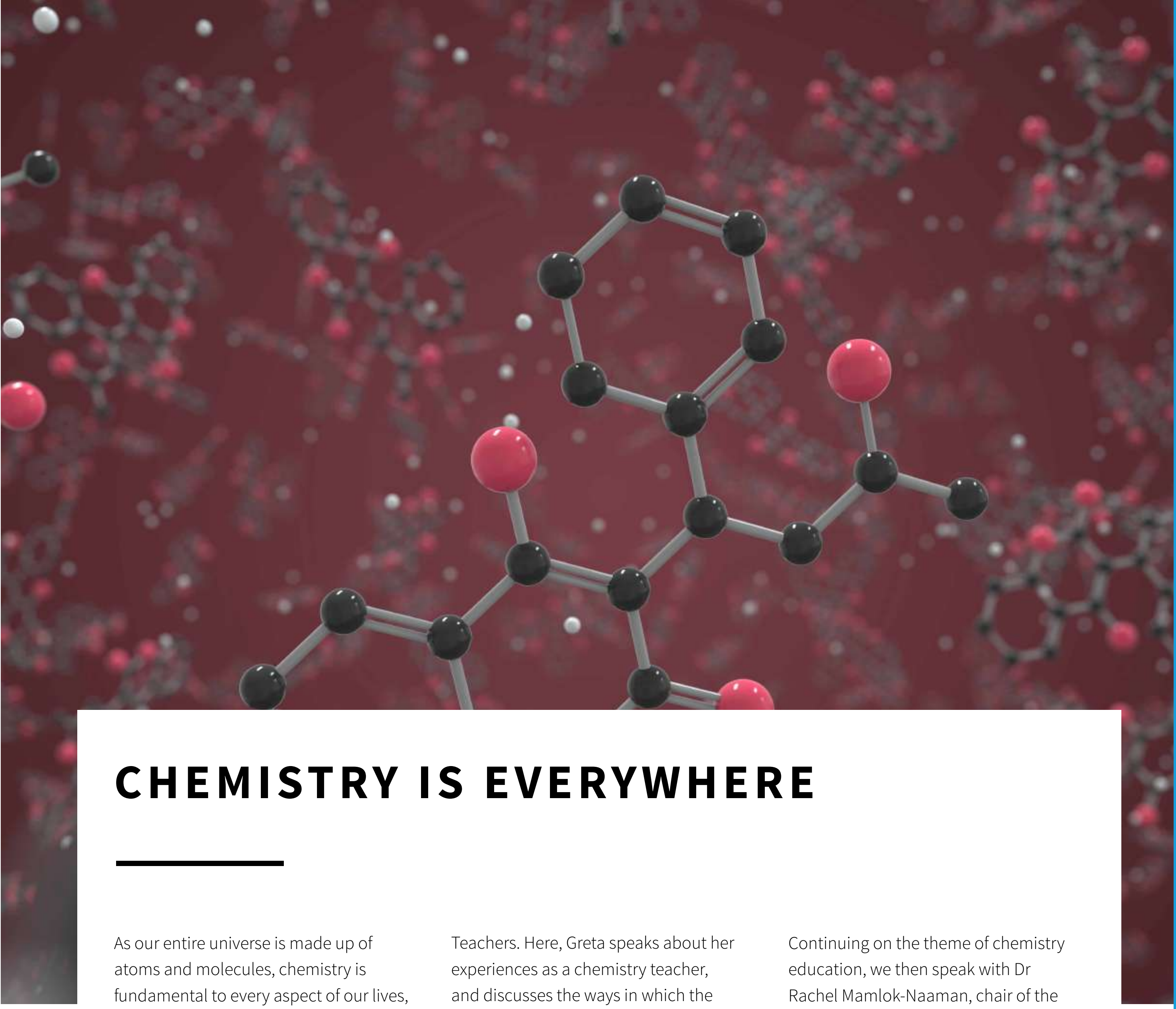
CHEMISTRY





CHEMISTRY IS EVERYWHERE

As our entire universe is made up of atoms and molecules, chemistry is fundamental to every aspect of our lives, from keeping our bodies functioning, to our food, our possessions and the weather. As such, the scientific field of chemistry offers us a deeper understanding of the world around us.

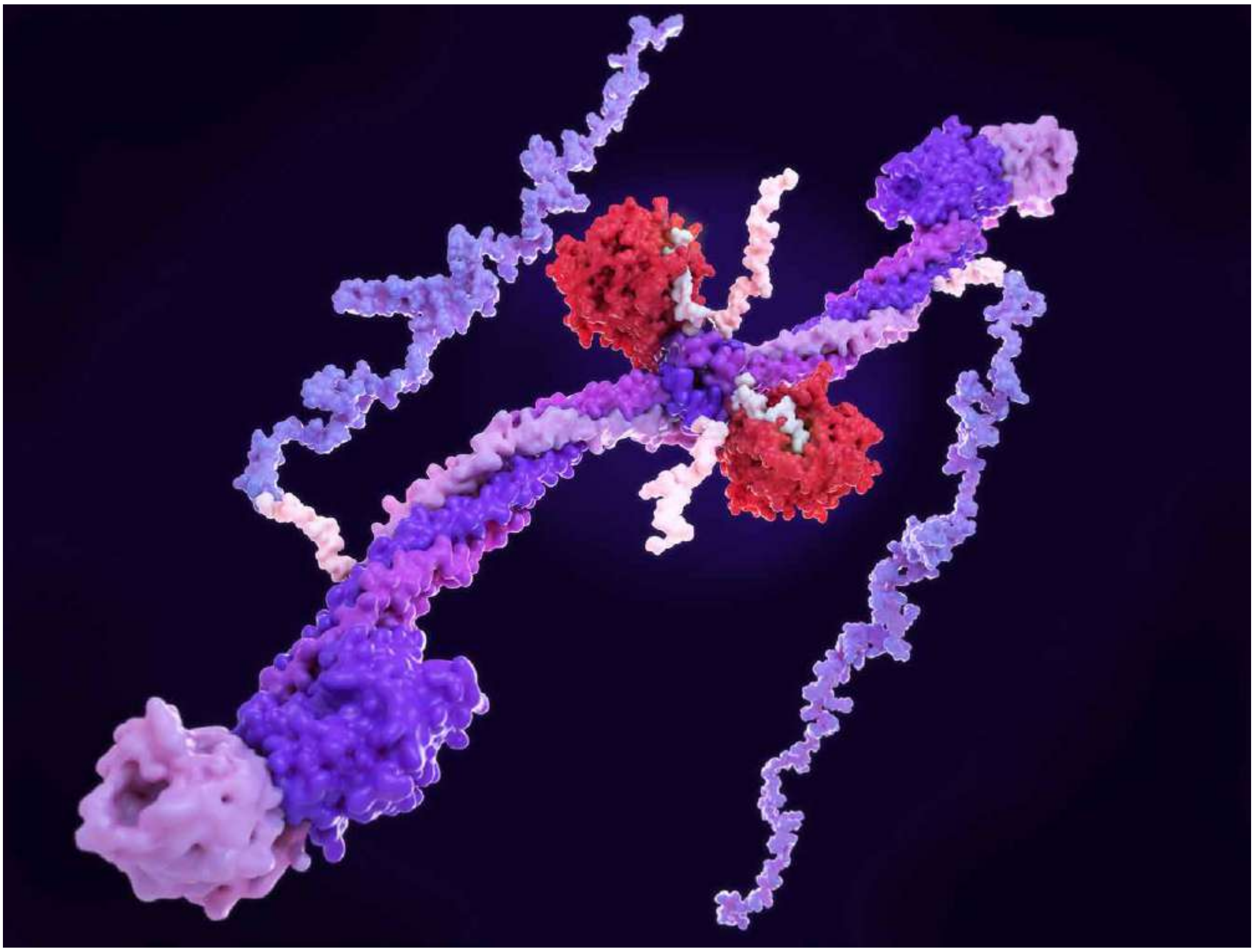
In addition, chemistry research has been improving our quality of life for centuries, by providing solutions to various societal problems, in areas from healthcare and sanitation, to energy and environmental protection. Therefore, the world needs more highly-skilled chemists to address the urgent issues facing humanity today.

That's why we decided to open this section with a focus on chemistry education. First, we feature an exclusive interview with Greta Glugoski-Sharp, the Governing Board President of the American Association of Chemistry Teachers. Here, Greta speaks about her experiences as a chemistry teacher, and discusses the ways in which the Association empowers teachers to provide their students with the best possible chemistry education.

To ensure better outcomes for all chemistry students, Dr Marcos Caroli Rezende and Dr Carolina Aliaga Vidal at Universidad de Santiago de Chile have been developing visual learning methods. In their recent work, which we'll feature in this section, they have focused on helping students to visualise a complex chemical process known as phase-transfer catalysis. By using visual learning to help students grasp abstract chemistry concepts, such teaching approaches could enable more students to graduate with chemistry degrees, towards fulfilling the demand for graduates in this important field.

Continuing on the theme of chemistry education, we then speak with Dr Rachel Mamlok-Naaman, chair of the European Chemical Society's Division of Chemical Education. In this exclusive interview, she discusses the Division's work, exciting new approaches teaching chemical science, and her own fascinating research in the field of science education.

Next, we meet one researcher who uses her vast experience and knowledge of chemistry to tackle two pressing societal problems: the rise of antibiotic-resistant bacteria and mercury pollution. Dr Maria Ngu-Schwemlein and her colleagues at Winston-Salem State University are addressing these issues by developing molecules that can bind toxic mercury ions, and creating molecular scaffolds that can enhance the effects of antibiotics.



Also addressing an increasingly urgent societal problem is Dr Radu Custelcean at Oak Ridge National Laboratory, who has been developing new chemical methods to remove carbon dioxide from the atmosphere. As this greenhouse gas is the primary driver of global climate change, Dr Custelcean's work comes at a critical time.

Our next featured chemist is Dr Hyun-Joon Ha from Hankuk University of Foreign Studies in the Republic of Korea. His team is developing new ways to transform molecules called aziridines into a range of important medicinal compounds called alkaloids. As alkaloids are typically naturally occurring, many of them are in short supply. Therefore, Dr Ha's new synthetic methods will increase the availability and reduce the cost of these important compounds, towards improving people's access to life-saving medicine.

Dr Oscar Verho and his team at Uppsala University are also developing innovative new methods for synthesising known drug molecules in an efficient and cost-effective manner. To do so, these researchers are figuring out ways to 'activate' the carbon-hydrogen bonds that are commonly found in drug molecules, so that such molecules can be synthesised in a rapid fashion.

Our next two articles in this section focus on biological molecules, and we first home in on proteins. Protein molecules are a fundamental building block of all living organisms. Therefore, detecting them and monitoring their interactions is vital in numerous fields, from food science to pharmacology. In this section, we meet Dr Anne Kleinnijenhuis of TRISKELION, who specialises in developing innovative analytical techniques for measuring proteins. Recently, he has designed improved methods that have far-reaching applications in food preparation, pharmaceuticals and blood analysis.

Although protein molecules are critical to many processes in our bodies, countless other biological mechanisms rely on small molecules and ions, and specifically, their movement across cell membranes. However, these processes can be extremely intricate and complex, making them frustratingly difficult to study.

Dr Evelyne Deplazes and her team at the University of Queensland and the University of Technology have been investigating these processes by combining the best elements of experimental and computational membrane biophysics. Their research, which we feature in the final article of this section, helps us better understand the way our bodies work, with exciting implications for biotechnology and drug development.

THE AMERICAN ASSOCIATION OF CHEMISTRY TEACHERS

Under the auspices of the American Chemical Society, the American Association of Chemistry Teachers (AACT) was established in 2014 as a professional community for chemistry teachers in schools across the US. AACT supports educators by providing quality resources, professional development, and valuable networking opportunities. In this exclusive interview, we speak with **Greta Glugoski-Sharp**, AACT's Governing Board President, who speaks about her experiences as a chemistry teacher, and discusses the ways in which the Association empowers teachers to provide their students with the best possible chemistry education.

What inspired you to become a chemistry teacher?

I was born and raised in San Francisco, California. I graduated from the University of California at San Cruz and majored in chemistry, and after I graduated, I had the opportunity to work as a staff research associate in an HIV research lab at the University of California at San Francisco, School of Medicine.

Even though the research I was a part of was exciting, I decided to become a volunteer with the University's Science Health and Education Partnership program. In this program, volunteers were partnered with high-school science teachers to create science curriculum and to bring their students into the lab so that they can see science being done first hand. The visits were designed with the goal of providing students with exposure to scientist role models and connections to science.

My interactions with the high-school students involved developing demos and experiments and teaching them how to do inquiry-based labs. As I watched the students expand their curiosity and thinking, I realised that teaching was something I was good at, and I really enjoyed doing. I really wanted to bring that love for learning science to young people.

How does AACT inspire and empower chemistry educators in schools across the USA?

Chemistry teachers often feel isolated in their classrooms for various reasons. It could be that they are teaching in a school where they are the only chemistry teacher, or they could be a teacher who is interested in incorporating new ideas and wants to share their ideas with others but doesn't have anyone in the school to connect with.

AACT is there for those chemistry teachers. It not only provides resources to help its teachers with their curriculum, but also fosters a strong sense of community, so that teachers can connect and share their successes and failures and learn from each other. Sometimes these connections have led to friendships.

AACT strives to provide teachers of chemistry with the best teaching resources. Most of our Classroom Resource Library is made up of content from great teachers who create and share their own work. Currently, there are over 900 classroom resources available in the library for K-12 teachers of chemistry to use in their classrooms. The library is organised into three grade bands (elementary, middle and high).

A large collection of multimedia resources, including animations, simulations and videos, is also available for teachers to use. Additionally, select resources are highlighted as part of themed resource collections. All of the available teaching resources are classified in the library by topic, subtopic, and resource type. We also have External Teaching Resources from the chemistry community to connect our teachers with additional outside teaching resources.

Explain why it is so important to teach chemistry in a culturally responsive way. What's involved in this approach, and how does AACT encourage its members to be culturally responsive in their classrooms?

As a Latina Chemistry Educator, I understand the importance of diversity, equity, and inclusion in STEM fields, and the need to increase the number of underrepresented students' interest in STEM.

As a Latina Chemistry Educator, I understand the importance of diversity, equity and inclusion in STEM fields, and the need to increase the number of underrepresented students' interest in STEM. I believe that experiences which can spark an interest in STEM are extremely important and that mindful lesson planning is needed to promote greater cultural responsiveness and improved STEM career expectations.

Cultural responsiveness in the chemistry classroom is a powerful approach that would allow teachers to improve engagement and equity in their classrooms – a way for teachers to bridge the cultural divide that can sometimes occur. Culturally responsive teaching recognises students' cultural background and uses those cultural resources to empower all students to excel in the sciences and to increase interest in pursuing a career in a STEM field.

Chemistry educators have a responsibility to create a classroom culture of inclusion, collaboration, and cultural sensitivity. To accomplish this, we need to develop classroom level curricula that lessens the cultural disparities between educators and their students. The ultimate goal would be a chemistry curriculum that is totally inclusive and celebrates the achievements of ALL.

How has AACT supported its members throughout the COVID-19 pandemic, which has been a very challenging time for educators and students alike?

From the start of the COVID-19 pandemic, chemistry teachers all over the world took their new situation seriously and pretty much thought of their students before anything else. They figured out the best practices for distance learning and continued on with teaching the best they could under the strenuous and unpredictable situation.

From the beginning of the pandemic, AACT was there for its teachers. We immediately opened up our site and gave teachers free access to the AACT teaching resource library. This included lesson plans, labs, demos, simulations, animations, student passes, videos and even webinars. Because many face-to-face science conferences were cancelled during this time, AACT hosted a Virtual Summer Symposium in which many top chemistry educators were featured. They presented and shared their successes and resources.

As we emerge from the pandemic, what are you the most excited about for the future of AACT and chemistry education in general?

The COVID-19 pandemic has clearly changed the way we teach chemistry. The immediate switch to distance learning forced teachers to adapt and reshape the way they taught without a chance to even think about it. Many of AACT's experienced chemistry teachers immediately contributed valuable resources to our AACT resource library.

The support system that AACT provided during this time was invaluable, thanks to our members. During this time our membership grew, mostly due to the fact that teachers realised the need to be able to connect with other teachers and share their success and failures as well as their resources.

As we emerge from the pandemic, we are now being given a new opportunity to reflect on what we teach our students and why we do so. Our students are not the same people they were before the pandemic. Even though we may have advanced in some areas of virtual learning, we have regressed back on others. We must now take the time to reflect upon what concepts and lab activities are the most beneficial and relevant for our students, so that they will be better prepared as citizens who can understand and deal with uncertainty and change if another pandemic were to occur.

www.teachchemistry.org

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American Association of Chemistry Teachers

ENHANCING SCIENCE EDUCATION THROUGH VISUAL CHEMISTRY

Chemical scientists are vital to numerous important areas of society – from pharmaceutical drug development to solar energy conversion. To prepare for their future careers, it is critical for chemistry students to gain a deep understanding of complex molecular processes. However, chemistry is full of abstract concepts that can be difficult to grasp, causing many students to fall behind. To address this issue, **Dr Marcos Caroli Rezende** and **Dr Carolina Aliaga Vidal** at Universidad de Santiago de Chile have been developing visual learning methods to improve the quality of chemistry education, and ensure better outcomes for all students. In their recent work, they have focused on helping students to visualise a complex chemical process known as phase-transfer catalysis.

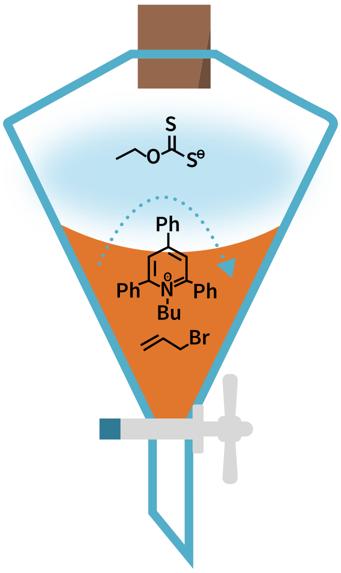
Education Through Visualisation

Anyone who has sat through a long chemistry lecture will tell you that understanding complex chemical processes is no small undertaking. Like many scientific disciplines, chemistry involves abstract concepts that must be understood before anything else fits into place. Grasping such abstract concepts can be a challenge for students, especially those with a greater affinity for visual learning methods. This can leave many students confused, resulting in higher rates of dropout.

Practical experiments in the laboratory aim to help students develop a better understanding of the abstract concepts they learn in the classroom. Unfortunately, although some experiments involve processes that are easy to conceptualise, many do not. As a result, students may simply follow the practical steps outlined in their instructions, without understanding the underlying chemical processes that are taking place. This can lead to a disconnect, where students do not fully understand the relationship between the steps they take in an experiment, and the chemistry happening in the background.

Because of this, there has been a push to develop visual methods of teaching chemistry. Such methods would allow more students to grasp abstract chemistry concepts, particularly visual learners. In turn, this would ensure greater inclusivity in chemistry education, allowing all students to reach their full potential. As chemistry graduates are needed in a range of important fields – from vaccine development to forensics – achieving greater inclusivity will help to meet the growing demand for skilled chemical scientists.

Towards this aim, Dr Marcos Caroli Rezende and Dr Carolina Aliaga Vidal at Universidad de Santiago de Chile have been developing visual learning methods for chemistry students, and investigating their effectiveness in achieving better educational outcomes. Their focus is to demonstrate how complex chemical processes can be visualised, so that students can gain a deeper understanding of how they work at a molecular level.



Understanding Phase-Transfer Catalysis

As part of their efforts, Dr Caroli Rezende and Dr Aliaga Vidal developed a strategy to help students to grasp the mechanisms involved in phase-transfer catalysis. In this process, a molecule acting as a catalyst transports one or more reactants from one phase, such as water, into another phase, such as oil, where the reaction occurs and the product is formed. As the phase-transfer catalyst is a key factor in allowing chemical reactants to cross the phase boundary, it is therefore an integral part of the reaction.

Phase-transfer catalysts have been used across various industries for almost half a century, where they facilitate the synthesis of various pharmaceutical drugs, agricultural chemicals and soaps. They have also been used in wastewater treatment and remediation of environmental pollutants. Because of the widespread applications of phase-transfer catalysis, it is important that students understand the mechanisms that drive this process, to prepare them for their future careers.

Visualising the Catalytic Process

Usually, when phase-transfer catalysis is taught, there is an emphasis on the reaction that is being catalysed, rather than the catalyst itself. This makes sense from a manufacturing standpoint, as there are many different important reactions that use catalysts to synthesise valuable chemical products. In this sense, the catalyst is just a means to an end; it is a tool that allows the chemist to achieve a reaction and synthesise a product cleanly and in high yield.

However, this outlook can cause difficulty when teaching undergraduate students about catalytic reactions. By focusing on the reaction and not the catalyst itself, some students will fail to fully understand the role of the catalyst in the chemical reaction. 'The actual catalysis is not directly observed, but only inferred by the student,' explains Dr Aliaga Vidal. On top of this, the concepts involved in phase-transfer catalytic reactions are abstract and can therefore be difficult to conceptualise.

Dr Caroli Rezende and Dr Aliaga Vidal decided to tackle this problem from the opposite direction. Instead of focusing on the conversion of reactants into a product, they set up an experiment that allows the student to visualise the stages that the catalyst itself goes through.

They achieved this by using a cation as a catalyst that can also form a 'charge-transfer complex' when paired with an anion. Though the cation and anion are colourless when apart, they form a coloured complex when paired in solution. Dr Aliaga Vidal and Dr Caroli Rezende chose this type of phase-transfer catalyst for its colour-changing ability, as students would be able to monitor the colour change as the reaction progressed, and determine the state of the catalyst at each stage in the reaction.

The team then designed an experiment involving the reaction of 3-bromo-1-propene and potassium xanthate to produce a chemical called O-ethyl-S-2-propenyldithiocarbonate, as an example of a common organic transformation called a nucleophilic

substitution reaction. The phase-transfer catalyst they chose was a pyridinium salt, which is capable of forming a charge-transfer complex with the xanthate anion. They conducted the reaction in a flask containing two immiscible solvents, water and dichloromethane. As water is the less dense liquid, it sits on top of dichloromethane, forming two separate phases.

Introducing Students to the Experiment

To test the effectiveness of their designed experiment, the team then conducted practical classes with second-year chemistry undergraduates at the University of Santiago de Chile. Before the students began the experiment, they were given a short lecture explaining what will happen to the catalyst at each stage in the reaction. These abstract concepts would then be explored visually during the experiment.

Then, in the laboratory, the students began by dissolving potassium xanthate in water and adding dichloromethane. At this stage, both the water and dichloromethane phases were colourless. However, when the students added the catalyst, something interesting occurred. Xanthate ions interacted with the pyridinium catalyst, forming a yellow charge-transfer complex that could move from the water phase into the dichloromethane phase. As a result, the dichloromethane layer had become yellow, while the water layer on top remained colourless.

Once the students had formed the yellow complex, they could then move on to the next stage. They added the next reactant – 3-bromo-1-propene – to the mixture, and watched the flask as the yellow colour disappeared. The return to a colourless state indicated that xanthate had reacted with 3-bromo-1-propene in the dichloromethane phase to form O-ethyl-S-2-propenyldithiocarbonate, and that the catalyst had returned to its original state.

The key point here is that the colour changes observed were due to the disappearance of the charge-transfer complex, as the xanthate anion was consumed in the reaction. While the students could infer what was happening in terms of the reaction, they could actually visualise the catalyst moving across the two phases and, as the colour changed, how the transferred xanthate anion was consumed, giving a much better indication of how the mechanism worked in one cycle.

The whole process and the colour change could be repeated by simply shaking the mixture and allowing the two phases to separate again. The students could thus notice that the catalytic process was a sequence of small steps that were repeated until all of the chemical reactants were consumed.

Alongside their visual observations, the students also monitored the reaction using UV-vis spectroscopy, which they used to measure the presence and amount of the yellow charge-transfer complex. Once the experiment was complete, they could identify the product that they had synthesised in a rather pure state by employing another spectroscopic technique, called nuclear magnetic resonance.

Student Feedback

Once the practical classes were complete, Dr Caroli Rezende and Dr Aliaga Vidal wished to assess the educational benefit of their visual approach to chemistry education. To do so, they asked each of the students to complete a questionnaire to evaluate their experience of the experiment.

The responses were overwhelmingly positive, with 100% of students strongly agreeing that the experiment had enabled them to understand phase-transfer catalysis, and that visualisation had helped them to easily understand abstract concepts. On top of this, the majority of students agreed that they could make connections between what they had learned in the lab and other types of chemical reactions.

These results undeniably demonstrate the great success of the laboratory class designed by Dr Aliaga Vidal and Dr Caroli Rezende. The team hopes that their visual approach will be adopted by chemistry teachers in other universities, towards achieving better outcomes for their students. By making chemistry more accessible for visual learners, such teaching approaches could enable more students to graduate with chemistry degrees, towards fulfilling the demand for graduates in this important field.

Beyond improving chemistry education, Dr Caroli Rezende is also keen to relate chemistry with many aspects of the wider world. 'Science teaching should help students understand and become more critical of the world in which they live,' he explains. 'As an example, phase-transfer catalysis can be regarded as a chemist's trick to bypass a natural boundary. These continuous, small-scale processes are found everywhere. They ensure that – for better and for worse – we all live in one global world, where isolating frontiers prove ineffective in the long run.'

Meet the researchers

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Dr Carolina Aliaga Vidal earned both her master's degree and PhD from the University of Chile in 1995 and 2000, respectively. After this, she went on to work as a postdoctoral researcher at the University of Ottawa from 2001 to 2004. Today, she works as a Professor at the Universidad de Santiago de Chile, where her research focuses a variety of spin and fluorescent probes to monitor hydrogen-transfer reactions. Dr Aliaga Vidal is also a research fellow of the Centre of Nanoscience and Nanotechnology, and the Chilean Agency for Science and Technology.

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Dr Marcos Caroli Rezende completed his BSc and MSc at the Universidade Federal do Rio de Janeiro and Universidade Federal de Santa Catarina, respectively, before moving to the UK to complete his PhD at the University of East Anglia. He then returned to Universidade Federal de Santa Catarina where he worked as a professor, before moving to the Universidad de Santiago de Chile, where he holds his current position. Dr Caroli Rezende has contributed to over 180 papers in peer-review journals, ranging in topic from organic synthesis and mechanisms, all the way to developing chemical dyes and sensors.

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FURTHER READING

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THE EUROPEAN CHEMICAL SOCIETY'S DIVISION OF CHEMICAL EDUCATION

Representing more than 160,000 chemistry professionals, the European Chemical Society (EuChemS) is an umbrella organisation representing chemistry societies and organisations across Europe. One of the professional networks within EuChemS is the Division of Chemical Education, which aims to advance chemistry learning in Europe and beyond. In this exclusive interview, we speak with chairperson **Dr Rachel Mamlok-Naaman**, who discusses the Division's work, exciting new approaches teaching chemical science, and her own fascinating research.

To begin, please tell us a bit about the European Chemical Society's Division of Chemical Education. What are the Division's goals?

The main goals of the Division of Chemical Education are to find new activities in order to promote chemical education research and practice in Europe, and to disseminate chemistry education information.

We achieve this through conferences, national reports, working groups, publications, bi-annual meetings, and cooperation with professional networks, such as the Committee on Chemistry Education of the International Union of Pure and Applied Chemistry (CCE IUPAC).

In your opinion, what are the main challenges experienced by chemistry educators?

Chemistry education faces many challenges. Firstly, chemical studies are not easy for some students, and many students are not aware about the variety of career opportunities for chemistry graduates. Secondly, many people claim that chemistry is responsible for certain disasters in the world, such as those associated with chemical weapons. Finally, there is a belief that by studying subjects such as finance, economics and computer sciences, students will have better career opportunities, and their salaries will be higher. Therefore, there is quite a lot to be done in the pursuit of addressing these beliefs.

Describe some exciting approaches teaching chemistry, which are advocated by the Division of Chemical Education.

One of the approaches advocated by the Division of Chemical Education is the use of the historical approach to chemistry teaching and learning. The use of the historical approach may help students to achieve a better understanding of the essence of scientific phenomena, scientific methodology, and overall scientific thinking. Students who study according to this approach become familiar with the fact that explanations of different phenomena have changed over decades due to new data, new technological developments, and changes in the scientific community's perceptions. Students draw timelines and denote scientific developments together with technological, cultural and societal developments. They learn that science is an ever-developing entity, and that it is associated with societal, economic and technological happenings.

Another approach is education for sustainable development. For example, some of our members in Israel developed and researched learning materials for high-school chemistry studies by incorporating inquiry-type socio-scientific issues from the chemistry industry and from green chemistry. Their goal is to educate students about sustainable development and environmental issues using inquiry-based learning, for example, asking questions, postulating, drawing conclusions, and using argumentation. These learning materials were developed both for students and for teachers, integrating chemistry with environmental, health, economic and societal aspects. As a former high-school chemistry teacher, I always try to incorporate relevance, context-based, and inquiry-type socio-economic issues in my teaching.

Explain why inclusive education that fosters diversity is so important in STEM disciplines such as chemistry.

Approaches for inclusive science teaching currently tend to focus on only one dimension of diversity at a time. This neglects the fact that diversity is multidimensional in nature and the consideration of only one dimension of diversity can yield inclusive practices of only limited scope.

The goal of inclusive education that fosters diversity is, therefore, to promote inclusive teaching practices for dealing with several dimensions of diversity simultaneously. Science learning should be part of the education of those who will eventually be 'future citizens'. We should consider personal needs, societal issues, career awareness and academic preparation.

This approach may be enacted through integrating STEM in teaching and learning, since the goal of the STEM curricula is to enable the learner to build greater knowledge through disciplinary connections and practices. It has the potential to give learners a broader range of access to learning, a more complex understanding of authentic and relevant phenomena, and perhaps enhance learning outcomes given the same amount of time as studying each individual subject. Thus, it will help in shaping the character of science-literate citizens, who will be able to make important decisions about current problems and issues of a scientific origin, and personally act as a result of these decisions. As a consequence, citizens who understand how science, technology and society mutually interact will be able to use their knowledge in handling the problems and issues that they confront. By learning through this approach, all students are taught about natural phenomena in a way that links science with the technological and social world of the student.

What does your own research focus on?

My work focuses on topics related mainly to research on students' learning and to teachers' continuous professional development. My research can be described as a 'spiral' procedure, referring to the diversity facets of chemistry education, which are integrated into each other. The findings on student learning and motivation guide me in designing and revising curriculum materials and professional development programs for chemistry teachers, since they are the key to any success of their students, implementation of new curricular materials, or reforms in education.

More specifically, the professional development programs and models that I have developed, implemented and researched over the last 20 years are based on research into students' conceptions and misconceptions regarding chemistry learning, inquiry-based skills and activities, including relevance in chemistry education, or teaching and learning in different cultures. These programs involve topics that are relevant to chemistry education, such as education for sustainable development (for which I was selected as a 2018 Awardee for the *ACS-CEI Award for Incorporation of Sustainability into the Chemistry Curriculum)*, the history of chemistry, systems thinking in chemistry education, and inclusion and diversity in chemistry education.

All the programs, workshops, and courses are followed by research. My research design is based on mixed methods, including both quantitative and qualitative tools, questionnaires disseminated among teachers and their students, interviews with teachers and students, observations and video-taping of lessons, and written minutes. The use of

a variety of tools enables an adequate triangulation of data analysis.

The conclusions and discussions lead to recommendations for further actions. For example, my studies referring to three cycles of chemistry teachers' action research workshops (10 teachers in each cycle), revealed that models of professional development in which teachers bring evidence to their work, or research their own work, are highly efficient in enabling teachers to gain a sense of ownership of their teaching, and in increasing their self-efficacy.

In recognition of my work, I was elected by IUPAC as one of the *2020 twelve distinguished women in chemistry*.

The Division recently hosted the 9th European Variety Conference in Chemistry Education. Tell us a bit about this event.

The Division hosts two bi-annual conferences: The European Conference on Research in Chemistry Education (ECRICE), and European Variety Conference in Chemistry Education (EUROVARIETY). ECRICE is the forum for researchers and teachers to exchange experiences on research in chemical education carried out at every education level – from primary school up to graduate studies. The EUROVARIETY conference is devoted to practical aspects of chemistry education at university level. It provides a forum for sharing of good practice and innovation related to teaching and learning chemistry at university degree level. This year it was an online conference, organised by the Faculty of Education at the University of Ljubljana, Slovenia.

The conference enabled chemistry lecturers and educational professionals to share and showcase best practice in the field, and network across the community. We encouraged participants from all levels, from those working in the field of chemistry education research, to practicing educators and doctoral students involved in teaching and research, to join us and present their own impressions and conclusions gained during their teaching experiences.

Finally, as we begin to emerge from the COVID-19 pandemic, what are you most excited about for the future of chemistry education?

In January 2021, I initiated an online meeting with the Division delegates. We discussed the situation of teaching and learning in the light of the COVID-19 pandemic. The discussion enabled an exchange of ideas, and even highlighted positive aspects regarding online communication. I felt that looking at the benefits of the technological advancements during these challenging days was beneficial to everybody. Moreover, it helped us all in conveying the conclusions to the chemistry teachers in their countries, encouraging them, and highlighting some positive aspects of this period.

We all stressed the point that we hope that these aspects will be sustained, and the educational system will benefit from the fact that teachers have developed a more advanced technological literacy (albeit due to problematic times).

The discussions lead to several points. For example, we discussed the possibility of customised learning through the division into breakout rooms. It is possible to give a task to the class and in the plenum to teach a lesson to the students who have missed it or are having difficulties. Due to the fact that the teacher moves between different rooms, students can try to solve problems themselves while waiting for the teacher. In a face-to-face class there is a greater temptation to ask the teacher for the answer. Another benefit for example is for students who are diagnosed with ADHD. During the lesson, students with ADHD who have difficulty working in the hustle and bustle of the classroom can enter a breakout room alone, and work quietly on their assignment.

We also discussed how our acquaintance with a diversity of technological tools and online communication strategies encourages international discussions and collaborations between schools, teachers and students. Finally, the development of online school chemistry experiments may be a solution for schools that do not have proper laboratories.

Additional benefits include greater inclusion at international conferences and meetings. More scientists can attend online conferences, without worrying about financial means or family responsibilities, and the talks can be broadcasted to a larger population all over the world.

EuChemS
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DEVELOPING MERCURY IMMOBILISERS AND ANTIBIOTIC ENHANCERS

The rise of antibiotic-resistant strains of bacteria and the ubiquitous nature of mercury in the environment are two major health hazards and concerns faced today. **Professor Maria Ngu-Schwemlein** and her team from the Winston-Salem State University, USA, are addressing these issues by developing biomolecules that can bind and immobilise toxic mercury ions more effectively. Together with Professor Ngu-Schwemlein's collaborators, the team is also investigating carbon nanodots as molecular scaffolds to enhance antibiotics in combating antimicrobial resistance.

Finding and Enveloping the Target

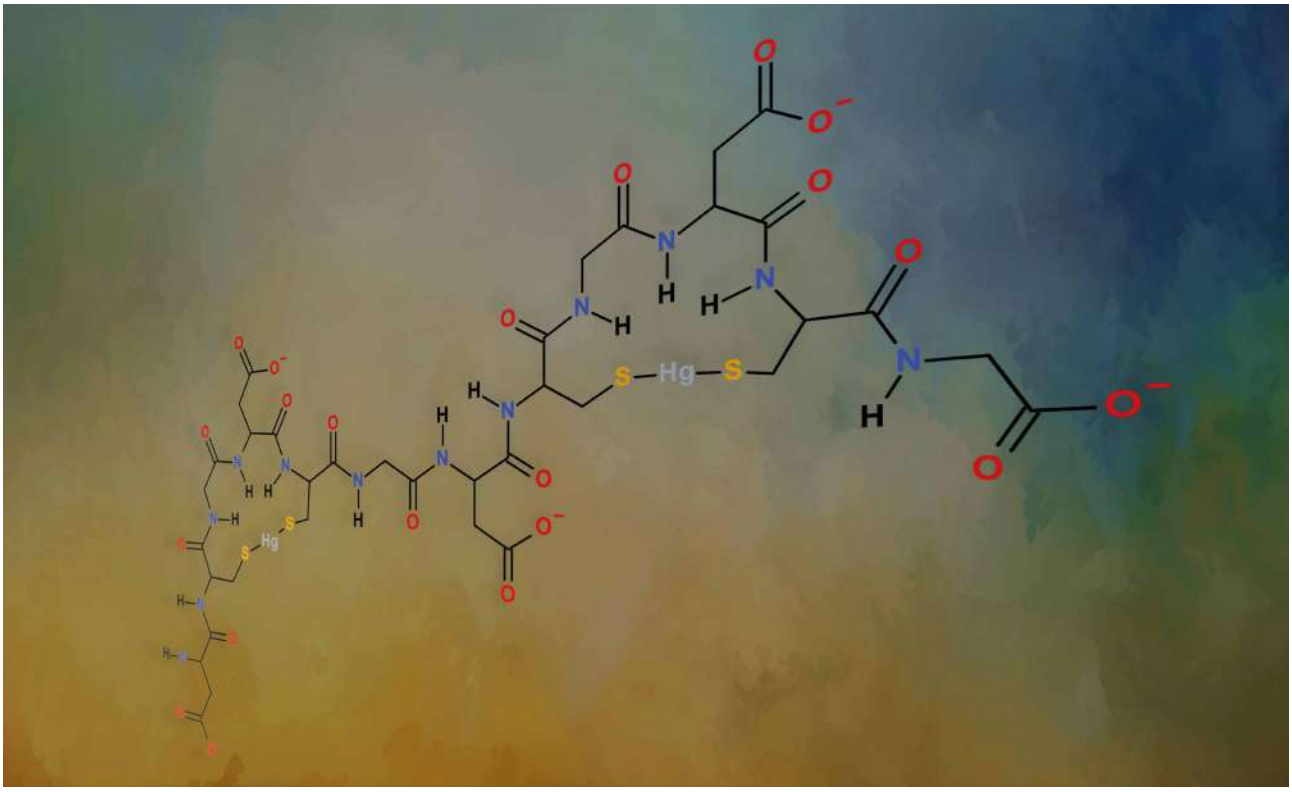
Mercury and many other heavy metals can be found in water as positively charged ions. Typical concentrations of metal ions in untreated water supplies are usually quite low and not all metals are harmful – indeed, some are vital. Some metal ions are required for a multitude of biochemical reactions taking place within living organisms while others, such as mercury, are toxic. Therefore, developing methods that can reliably target and remove mercury ions, over other metals, is a major undertaking.

Because of the health hazards posed by mercury, highlighted by the public health disasters in Iraq and Minamata Bay in Japan, many international efforts have been initiated to remediate contaminated sites, protect human health, and reduce mercury pollution. Although various technologies have been developed, there is still a need for compounds that can effectively bind to mercury – a process called 'immobilisation' – so that it can be more easily removed. Medical researchers are also constantly trying to develop new therapies that can target and effectively immobilise mercury ions so that they can be removed from patients.

In addition to the health hazards posed by mercury, the rise of antibiotic-resistant bacteria is another global challenge threatening human health. As a result, the World Health Organization (WHO) has endorsed a global action plan, which aims to not only prevent but treat infectious diseases with effective medicines that can target and kill harmful, antibiotic-resistant bacteria.

Professor Maria Ngu-Schwemlein and her team from the Winston-Salem State University are designing new compounds that tackle both of these challenges. In one of their research projects, they have modified and improved existing molecules that can target mercury ions for safe remediation. In their second research direction, the team has also devoted time to find compounds that can enhance the effect of antibiotics on resistant strains of bacteria.

The mechanism by which each type of compound binds to a metal ion or a bacterium is similar. Take, for example, an insect-eating sundew plant; this species is an effective carnivore partly because its tentacles can envelope their prey. Each point of contact is comparatively weak, but in combination, they provide a very firm grip on their target. This behaviour is somewhat analogous to the binding action of the molecules designed by Professor Ngu-Schwemlein and her



colleagues. In general, the team first identifies which atom or group of atoms bind to their target. They then start modifying the surrounding structure in order to maximise the number of points of contact or bonds formed.

Caged Mercury Ions

Sulphur atoms have a particularly high affinity for mercury ions. Some sulphur-containing compounds, including those found naturally in proteins, comprise not one, but several sulphur atoms. This means that each compound can form multiple contact points or bonds with a single mercury ion. There are other atoms, such as oxygen and nitrogen, that can also bind to mercury, though this tends to result in a relatively weak interaction.

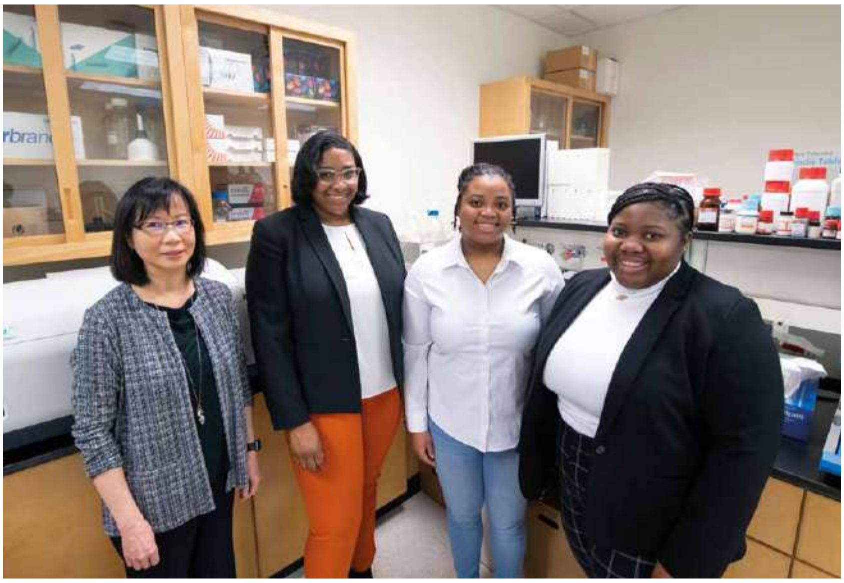
The sulphur-containing compound that binds to a mercury ion with two or more contact points is an example of a ‘chelator’. One of the goals of Professor Ngu-Schwemlein’s research is to develop a chelator that can wrap around a mercury ion. The wrapping of mercury immobilises it and prevents it from interacting with other biological molecules. In principle, this approach should protect the body from the toxic effects of mercury. While there is an understanding about how chelators behave, the team believed that more could be done to build more effective mercury deactivators.

As part of a preliminary investigation, Professor Ngu-Schwemlein’s group determined how sulphur-containing units in a compound could bind mercury ions. By using a technique called ‘electrospray ionisation mass spectrometry’ to analyse these interactions, they found that tethering multiple sulphur-containing units to a chelator compound can enhance the binding efficiency through the compound’s ability to bind more than one mercury ion. The compound that forms when a chelator is bound to a metal ion is known as an ‘adduct’.

For the next phase of the study, the team was interested in finding out how the ratios of the chelated mercury ions would change with time. In other words, do they convert from one type to another, and if so, how does this affect the strength of the interaction? In addition, the team wanted to explore the effect of incorporating other atoms that could bind to mercury.

The researchers narrowed their study to a class of naturally occurring peptide chelators that contain a sulphur group at each end. The chelator is symbolised here as SXS, where X is a group of atoms that connect the two sulphur groups (S), which can bind to mercury. The team prepared two types of SXS compounds, one in which X contains oxygen atoms that could also bind to mercury, and another variant where X is not expected to bind to mercury.

After multiple experiments, the team found that both variants bound to mercury in a ratio of 1:1. The team also found that the presence of the oxygen atoms at X appeared to speed up the formation of the adduct. This shows that the oxygen atoms enhanced the interaction between the chelator SXS and the mercury ion. More specifically, the oxygen atoms formed a type of bond with mercury, which helped to bring the chelator closer and more tightly to mercury.



In collaboration with Dr John Merle, the group also performed computational studies. Their calculations and simulations also confirmed that the extra oxygen atoms would result in a stronger, more tightly formed adduct.

Indole Rings and Spatial Orientation

Following the success of the above investigation, Professor Ngu-Schwemlein and her team turned their attention to studying more structurally diverse groups of atoms at X and how these groups influence the chelation of mercury. The team wanted to learn more about how a fused network of atoms, known as an 'indole ring', would shield the chelated mercury ion from reacting with other molecules. One can visualise this interaction by holding a tennis ball above the face of a tennis racket. The racket frame represents the indole ring, and the tennis ball represents the mercury ion. Indoles have an appreciable amount of negative electron density and are attracted to positively charged mercury ions. When an indole ring is bound to a mercury ion, it forms a barrier on one side of the mercury ion.

The researchers compared two variants of SXS, both of which contained an indole ring. The only difference between the variants was the direction in which the rings were pointing. Interestingly, the team confirmed that only one of the indole-containing variants, with the ring pointing towards the mercury ion, interacted strongly. The specific orientation of the indole rings was also supported by computational studies. The researchers are currently working on incorporating two indole rings into the variants to 'sandwich' and shield the chelated mercury ion, thereby creating a barrier on both sides of the mercury ion. Such chelators may provide a valuable tool for immobilising toxic mercury ions more effectively. They hope that these findings will be useful for applications including environmental remediation, and human health protection.

Combatting Antibiotic-Resistant Bacteria

Another major part of Professor Ngu-Schwemlein's research is the development of compounds that combat antibiotic-resistant bacteria, with the assistance of compounds known as 'dendrimers'. Dendrimers can be viewed as compounds where identical branches of atoms extend from a central point, like the tentacles of an octopus. What makes their selected dendrimers behave similarly to chelators, is that along each branch of the dendrimer are positively charged nitrogen that can, under appropriate conditions, bind to the cell walls of bacteria. When this happens, the cell walls are weakened and, in a few cases, broken down, killing the bacteria.

The effectiveness of dendrimers as antibacterial compounds is limited, and this is thought to be due to the low concentration of nitrogen groups. Consequently, the team wanted to find a way of packing more nitrogen groups into a small space, thereby increasing the chances of disrupting the cell walls on contact.

In order to pack more of these groups into a smaller space, Professor Ngu-Schwemlein and her collaborator Dr Suk-Fun Chin utilised a class of materials known as 'carbon nanodots'. As the name implies, carbon nanodots are small particles of carbon. The team chose carbon nanodots derived from starch as a central framework, because they have the surface properties needed to attach multiple dendrimers.

Once the nanodots were grafted with dendrimers, the team targeted two common types of bacteria, *E. Coli* and *S. aureus*, as well as three other bacteria that have evolved resistance to antibiotics. The team was pleased to discover that these dendrimer-bound carbon nanodots were effective at killing all types of bacteria.

Given that the team's dendrimer-bound nanodots were able to disrupt the cell walls of bacteria, the researchers then decided to combine them with some existing common antibiotics. In many antibiotic-resistant bacteria, the cell walls form a barrier to these common antibiotics. Much to their delight, the researchers found that the antibiotics were indeed made more effective when administered with their nanodots.

These results are highly significant. It shows that there are other treatments, well within reach, that can be utilised to combat antibiotic-resistant bacteria. Professor Ngu-Schwemlein and her team hope that their findings will encourage others to build on their success.

Meet the researcher

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Professor Maria Ngu-Schwemlein was awarded her PhD from the Australian National University in 1989. After working at many notable institutes, including ETH Zürich, Louisiana State University and Lawrence Livermore National Laboratory, she joined Winston-Salem State University in 2006 as an Associate Professor, before becoming a full Professor in 2010. Her recent research interests focus on designing second-generation chelators for toxic metal ions and developing antimicrobials to combat antibiotic-resistant bacteria. Professor Ngu-Schwemlein is passionate about training undergraduates in research skills, and she involves them in her projects, providing them with invaluable research experience. In recognition of her contributions at Winston-Salem State University, Prof Ngu-Schwemlein was awarded the Wilveria Atkinson Distinguished Research Award and the John Fountain Master Teaching Award.

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WINSTON-SALEM
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REDUCING ATMOSPHERIC CARBON DIOXIDE THROUGH DIRECT AIR CAPTURE

Climate change is mostly the result of elevated carbon dioxide emissions. Over the past two decades, research groups have been searching for new technologies that capture carbon dioxide from the atmosphere as an effective way of reversing climate change. **Dr Radu Custelcean** and his colleagues at the Oak Ridge National Laboratory in the US specialise in this endeavour. The team is developing novel materials and methods that filter carbon dioxide out of the air in an energy-efficient manner.

The Challenges Ahead

There is a range of strategies that attempt to address climate change, many of which are focused on reducing our carbon dioxide emissions. Another promising approach is known as the 'direct air capture' method, for removing carbon dioxide from the atmosphere. In this process, air is filtered through a solution or solid matrix, referred to as the 'sorbent', to absorb or 'capture' carbon dioxide. The filtered air is then returned to the atmosphere.

Direct air capture methods have the potential to remove over 10 billion tonnes of carbon dioxide per year. Currently, however, the technology is still considered to be underdeveloped. Dr Radu Custelcean and his team at Oak Ridge National Laboratory in the US have been researching new direct air capture methods that could provide a simple, energy-efficient and environmentally friendly technology for atmospheric carbon dioxide removal.

Once captured, carbon dioxide presents several potential options. It can be transported through pipelines before being either injected underground, or supplied to industries that use it. As such, it's important for Dr Custelcean's team to develop sorbents that not only capture carbon dioxide efficiently, but also release it in a controlled, energy-efficient and sustainable way.

There are plenty of challenges for Dr Custelcean and his team. A sorbent that can strongly bind to carbon dioxide is advantageous for the absorption stage of the process, but much less so for the release stage. Additionally, although atmospheric carbon dioxide levels have risen substantially over the past few decades, its overall concentration is still very low, at about 0.04%, thereby requiring very large volumes of air to be handled. Furthermore, other gas molecules, including water and nitrogen, can also become absorbed as air is passed through the sorbent. Therefore, the ideal sorbent would need to be able to selectively separate low concentrations of carbon dioxide while letting other gases pass through, and then release carbon dioxide with a low energy input when needed.

Trapping and Releasing Carbon Dioxide

One class of sorbents that has been previously explored is an 'inorganic alkaline' solution of sodium hydroxide and calcium hydroxide in water. The overall procedure involves two connected cycles. During the first 'absorption' cycle, carbon dioxide reacts with the solution and produces dissolved sodium carbonate. During the second 'regeneration' cycle, calcium hydroxide then reacts with sodium carbonate to produce solid calcium carbonate while regenerating sodium hydroxide. Since calcium carbonate is solid, it can be filtered from the sorbent. It can then be heated to release carbon dioxide and regenerate calcium oxide, which when mixed with water, regenerates calcium hydroxide. The sorbents are thus recycled and the capture, regeneration, and release steps are repeated.

Inorganic alkaline solutions are known to quickly react with carbon dioxide, despite its low concentration in air. However, these solutions can be corrosive, and the temperatures (around

900°C) and energy demands needed to heat calcium carbonate to release carbon dioxide are quite high.

Alternatives to inorganic alkali sorbents are organic, amine-containing sorbents. Amines are nitrogen-containing organic compounds, which produce an alkaline solution when dissolved in water. There are, however, disadvantages to using amines. They are volatile, toxic compounds, and eventually evaporate to the atmosphere over time. There have been efforts to bind amines to solid frameworks to prevent them from evaporating, but these solid-supported amine sorbents are slow to absorb carbon dioxide and found to degrade in air over time.

Dr Custelcean's team recently discovered a class of organic sorbents known as 'bis(iminoguanidines)', abbreviated as BIGs, which partly resemble amines in structure, and dissolve in water to produce an alkaline solution. The alkaline solution of BIG can react with carbon dioxide and form an insoluble carbonate salt. The solid salt, when filtered from the sorbent, can be heated at relatively low temperatures (around 100°C) to release carbon dioxide and regenerate the BIG sorbent. Unfortunately, the carbon dioxide capacity and rate at which it is absorbed is low; therefore, modifications are needed to increase the amount of carbon dioxide captured and speed up carbon dioxide absorption.

Amino Acids as Sorbents

Dr Custelcean's team considered the two-cycle approach and decided to investigate the pairing of 'amino acids' with BIG compounds as the sorbent mixture, analogous to the sodium hydroxide and calcium hydroxide mixture. That is, amino acids are involved in the absorption cycle and BIG compounds are involved in the regeneration cycle. Amino acids are the building blocks of proteins and therefore have a much lower toxicity than inorganic alkalis. They are also far less volatile than amines.

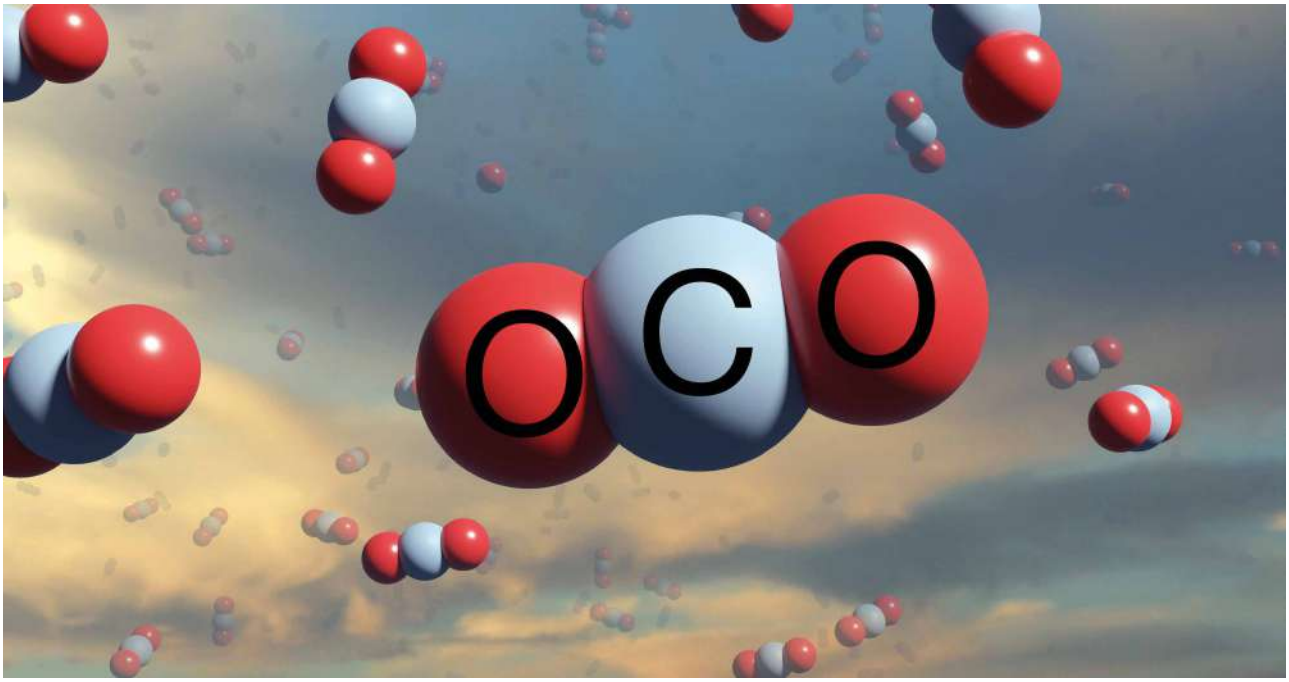
In a study published in 2018, Dr Custelcean's team found that the reaction between atmospheric carbon dioxide and aqueous amino acid solutions was very fast, on par with that between carbon dioxide and sodium hydroxide or amines. The resultant carbonate ions could then be crystallised using a BIG derivative, called PyBIG, at room temperature. Encouragingly, the team found that the PyBIG-carbonate salt, when heated to 120°C for 30 minutes, released most of the carbon dioxide and was converted back to PyBIG in near quantitative yield. This result demonstrates that sorbent regeneration could be achieved at temperatures much lower than those needed when using inorganic alkalis, with negligible loss of material.

The group then heated a sample of the PyBIG-carbonate salt in air for one week, equivalent to 336 30-minute heating cycles, to test the chemical stability of the PyBIG sorbent. They then added the regenerated PyBIG sample to an amino acid-carbonate mixture to detect whether prolonged heating or usage would affect the carbon dioxide capture efficiency. The group's results indicated only a very small difference compared to freshly prepared PyBIG, demonstrating that the sorbent would have a long life-cycle.

Heating methods that avoid the use of energy sources that emit carbon dioxide are an important consideration in direct air capture technologies. As part of their PyBIG study, Dr Custelcean's team demonstrated the use of concentrated solar power as a source of sustainable energy to heat the PyBIG-carbonate salt and release nearly all of the captured carbon dioxide.

Other Derivatives of BIG

Following the successful proof-of-concept studies with amino acids and PyBIG, Dr Custelcean's team then looked to further their investigation by exploring other derivatives of BIG that are cheaper and more effective than PyBIG. Their next target was a derivative referred to as BBIG. Structurally similar to PyBIG, BBIG has a single nitrogen atom replaced with a pair of carbon and hydrogen atoms. This minor structural modification means



that BBIG is much cheaper to prepare compared to PyBIG. However, a downside is that the BBIG-carbonate solid formed is less crystalline and more sludge-like, making filtration more difficult. This observation is important to note particularly as the methodology could eventually be scaled up from a laboratory gram-scale to an industrial tonne-scale. On the other hand, the heating conditions required to release carbon dioxide from BBIG-carbonate are very similar to those involved in the PyBIG study.

In another investigation, Dr Custelcean's team explored the carbon dioxide capture abilities of GBIG, one of the simplest and oldest BIG derivatives, first reported by German scientists at the end of the 19th century. While the team found that GBIG was quite an effective and energy-efficient sorbent for carbon dioxide capture from more concentrated streams, such as the flue gas emitted from coal-burning power plants, it was not very efficient at direct air capture. Unlike PyBIG and BBIG, GBIG formed less stable crystals with carbon dioxide. While the lower crystal stability led to a smaller regeneration energy, it also reduced the direct air capture efficiency of GBIG.

These findings contribute to the overall understanding of the structural and thermodynamic factors that determine the suitability of a sorbent for direct air capture. Based on this fundamental understanding, very recently Dr Custelcean's team demonstrated that when combined with small peptides, GBIG led to an effective direct air capture process with significantly lower energy requirements compared to state-of-the-art technologies.

Correlating Structure with Direct Air Capture Function

Following Dr Custelcean's GBIG publication, the team then focused on the development of new BIG sorbents with improved direct air capture performance, by incorporating one or two 'methyl' groups into GBIG (they use the label 'methyl-GBIG' to refer to these new compounds). A methyl group is composed of one carbon atom and three hydrogen atoms.

In most cases, a methyl group is thought to repel water and make the given molecule less water-soluble. Surprisingly, the team found that methyl-GBIG was much more soluble in water than GBIG, leading to the expectation of a significant increase in the carbon dioxide capture efficiency. Solid precipitates generally form when dissolved molecules cluster together and start resembling a pure solid. Based on X-ray and neutron diffraction measurements, Dr Custelcean's team reasoned that the methyl groups prevented the methyl-GBIG molecules from self-assembling in solution and packing efficiently in the crystals.

On the other hand, Dr Custelcean's experimental and computational analyses of the carbonate salts of methyl-GBIG derivatives showed that, unlike GBIG, the methyl-GBIG derivatives form stable carbonate crystals that are relatively insoluble in water. Thus methyl-GBIG derivatives, like PyBIG, are suitable as direct air capture sorbents. Their thermodynamic properties, such as temperatures and energies of regeneration, are very similar to those of the PyBIG prototype.

Moving forward, Dr Custelcean's team is interested in scaling-up these direct air capture systems, optimising their performance, and testing them over multiple capture-release cycles, with the ultimate goal of developing an energy-efficient, sustainable direct air capture technology that can help address climate change. Towards this goal, Dr Custelcean seeks to team up with industrial partners and attract capital investments for moving this promising scientific discovery from the laboratory bench to the real world.

Meet the researcher

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Dr Radu Custelcean is a Senior Research Scientist at Oak Ridge National Laboratory. He received his PhD in Chemistry from Michigan State University in 2000 under the supervision of Professor James E. Jackson, followed by postdoctoral training with Professor Michael D. Ward at the University of Minnesota. Dr Custelcean started his independent career in 2003 at Oak Ridge National Laboratory, where for the past 18 years has been pursuing research in the areas of self-assembled molecules and materials for environmental and energy applications, crystal engineering, separation science and technology, anion recognition, and carbon capture. In 2008, he received the Margaret Etter early career award from the American Crystallographic Association.

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BUILDING DIVERSE MEDICINAL COMPOUNDS FROM AZIRIDINES

The artificial synthesis of medicinal compounds that are typically derived from natural sources helps scientists to better understand how they function and deduce whether they can be enhanced. Unfortunately, the work involved in synthesising such natural compounds and their analogues is extremely difficult. **Professor Hyun-Joon Ha** and his team from Hankuk University of Foreign Studies in the Republic of Korea are exploring ways to transform compounds called aziridines into a range of biologically active molecules.

From Aziridines to Alkaloids

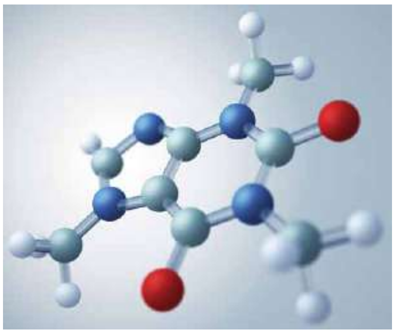
A class of nitrogen-containing organic compounds, known as 'alkaloids', represent the majority of all naturally occurring medicinal compounds – from morphine to numerous anti-cancer drugs. Alkaloids have repeatedly been shown to treat a large variety of ailments and conditions. Unfortunately, the supply of naturally occurring compounds is very limited. Additionally, in the case of many alkaloids, the way in which they function is largely a mystery.

Artificially synthesising alkaloids is one way to address the short supply of these important compounds, while also providing scientists with a better understanding of how they work. The path, however, to prepare copies of naturally occurring alkaloids involves multiple stages and is quite challenging.

Part of the challenge is due to the complex 'stereochemistry' of alkaloids. Stereochemistry refers to the relative spatial arrangement of atoms within a molecule. It describes how two molecules made up of the same number and types of atoms can, for example, exist as a 'left-hand' version and a 'right-hand' version. In this analogy, both hands have the same number and types of fingers, but they have different three-dimensional structures.

Stereochemistry is a fundamental component of biological systems. With the multitude of biochemical processes taking place at any given time, stereochemistry allows for control over which processes are triggered. This can be realised if a biochemical process requires a specific 'hand', in other words, a molecule with a unique three-dimensional form, in the same way as a mechanical lock requires a specific key. This is why all biologically active alkaloids have stereochemical properties: to ensure greater control.

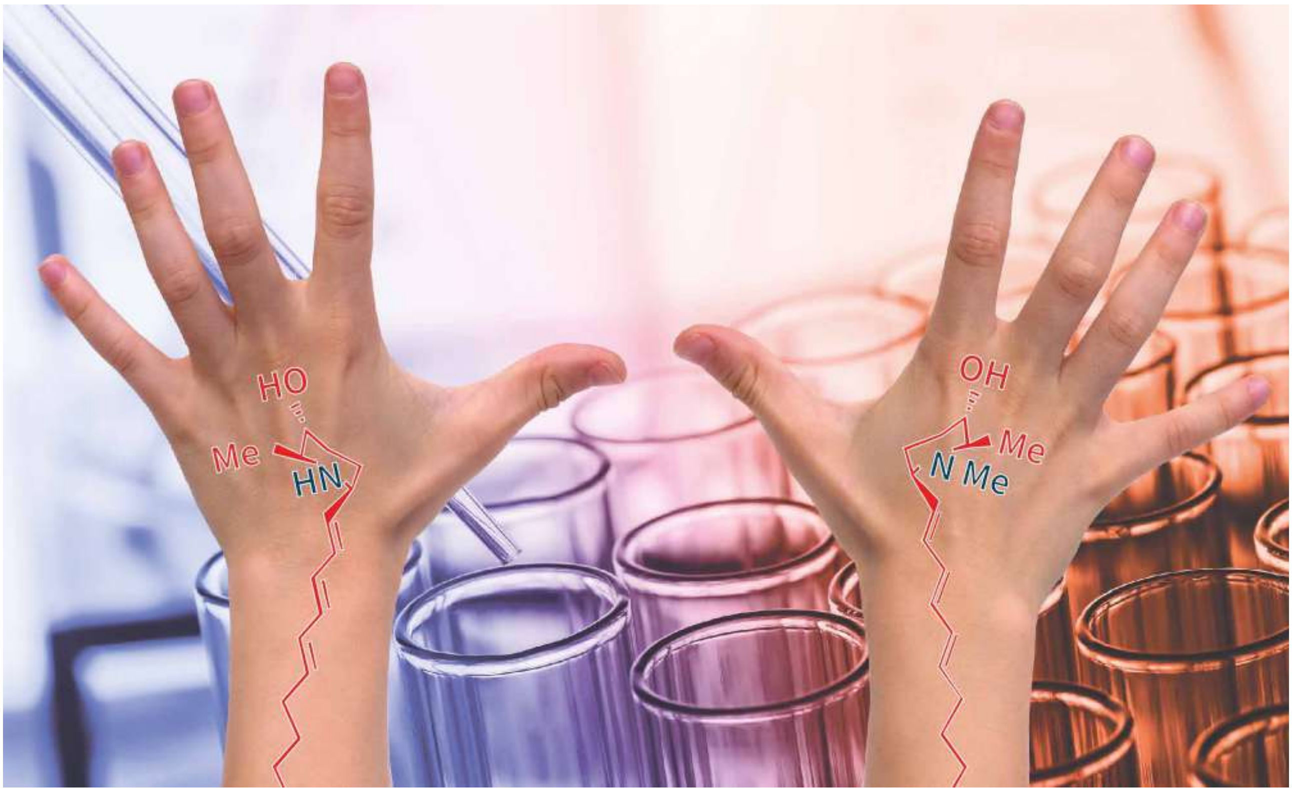
A significant challenge faced by synthetic chemists is that the pathway needed to produce the desired 'hand' often results in a mixture of both right and left hands. When both versions of a molecule are produced in the same mixture then considerable effort is required to separate them.



To get a head-start, some chemists start with smaller, more readily available compounds that already have some of the stereochemistry required to build the desired version of an alkaloid. Professor Hyun-Joon Ha and his team from the Hankuk University of Foreign Studies in the Republic of Korea are interested in the development of new routes to alkaloids, by starting the synthetic process from a class of compounds known as 'aziridines'.

Left- and Right-hand Aziridines

Aziridines are compounds containing a ring composed of two carbon atoms and one nitrogen atom. They, like alkaloids, can possess stereochemical properties. Some aziridines can exist



as a left-hand version and a right-hand version. Atoms bonded to the ring reside on one side of the ring only, introducing stereochemistry to the molecule.

As part of Professor Ha's synthetic route to prepare alkaloids, the aziridine ring must be opened. When this occurs, the orientation of the atoms bonded to the ring is preserved. This is what makes aziridines particularly useful in the preparation of alkaloids. Professor Ha's team utilises the stereochemical properties of aziridines that bear spatially unique groups to help them synthesise alkaloids with the desired stereochemistry.

Another challenge for the team is to choose an appropriate aziridine that will eventually lead to the required alkaloid. As is the case with many research projects of this scope, Professor Ha and his colleagues plan each step by first considering the chemical structure of the alkaloid they want to synthesise. They then work backwards from the product, rearranging the bonds on paper to visualise what the previous step would look like. This analysis is repeated until they reach a compound that looks like an aziridine. The overall analysis, referred to as 'retrosynthesis', helps the team to decide which aziridine to use.

Cancer Treatment and Mosquitos

One of the alkaloids of interest to Professor Ha's team is known as 'Microgrewiapine A'. This compound is known to target cancerous colon cells in humans while ignoring healthy cells. Microgrewiapine A can be extracted from the stem bark, branches and leaves of the orange jasmine tree, which is commonly found in many parts of south Asia.

Regarding the chemical structure, the Microgrewiapine A molecule contains a ring composed of five carbon atoms and one nitrogen atom. An aziridine ring is composed of three atoms, so during the synthesis, the team had to open the aziridine ring and then close a chain of atoms to form a larger, six-membered ring. Impressively, they were able to isolate the left-hand and right-hand versions of Microgrewiapine A. Through a detailed analysis, the team confirmed which version exists in nature by comparing the natural form of Microgrewiapine A with their synthetic forms.

The overall process of converting the required aziridine compound into Microgrewiapine A is significant undertaking. Quite often, chemists will aim to synthesise one alkaloid while remaining open to the possibility of synthesising other alkaloids with similar structures. This approach takes advantage of the lessons learned in making one alkaloid, and can be more productive from a research standpoint.

During the synthesis of Microgrewiapine A, Professor Ha and his colleagues were also able to record the preparation of other alkaloids that contain a six-membered ring. The team achieved this by making very small adjustments to some of the steps involved. One of the other alkaloids produced is known as 'Microcosamine A'. This alkaloid was first extracted from the leaves of a shrub found in China called Microcos paniculate, and is used in traditional medicine to treat digestion related ailments. Microcosamine A is also known to have insecticidal properties

and can effectively target the larvae of mosquitos. Remarkably, the only difference in the chemical structure of these two alkaloids is the presence of a few additional atoms bonded to the six-membered ring in Microgrewiapine A.

‘However, we found versions of handedness, as left-hand and right-hand versions of natural Microgrewiapine A and Microcosamine A are opposites,’ says Professor Ha. ‘This was achieved with measurements of the optical rotation of the molecules.’

The synthesis of both Microgrewiapine A and Microcosamine A was a first for the community and a major achievement for Professor Ha’s team. The process involved at least eight steps starting from the required aziridine. The complexity of this feat also demonstrates the power and control of plants, which can produce such diverse compounds, using only water, carbon dioxide, sunlight and minerals drawn from the soil.

Spruce Trees, Fire Ants and Bacteria

The six-membered ring described above is also a key component of many other alkaloids. Professor Ha and his colleagues have published the synthetic pathway needed to produce the compounds ‘dihydropinidine’ and ‘isosolenopsin’. Dihydropinidine is an alkaloid that functions as a defence chemical of evergreen spruce trees found in North America, and can also be found in the Mexican ladybird beetle. Isosolenopsin can be extracted from fire ants’ venom and is known to exhibit numerous properties. These include the breakdown of red blood cells, antibiotic activity against bacteria as well as antifungal properties.

Structurally, both dihydropinidine and isosolenopsin have the same six-membered ring found in Microgrewiapine A and Microcosamine A, described previously. The key steps involved in the synthesis of dihydropinidine and isosolenopsin were also similar. The team had to open the aziridine ring and then eventually close a chain of atoms to form the six-membered ring.

To keep the synthetic procedures as simple as possible and reduce chemical waste, they performed many of the reactions in one vessel. This approach to chemical synthesis is known as a ‘one-pot’ procedure and is generally much quicker and easier than performing each step in a different vessel. About 50% of the aziridine was converted into the alkaloid, which is a commendable achievement given that the process involves at least four steps.

Another significant finding for Professor Ha and his team was the synthesis of ‘biemamide B’ and ‘biemamide D’, which was another first for the community. Both alkaloids have been extracted from bacteria and are known to prevent the transformation of healthy human cells into cancerous cells. This time, the ringed structure found in both alkaloids is composed of four carbon atoms and two nitrogen atoms.

As with all other examples presented, the researchers started from the required three-membered aziridine ring and, following multiple stages, eventually synthesised the desired biemamide alkaloid. In addition, the team was able to confirm which hand was present in nature, by comparing the analytical data of their synthesised forms of bienamide B and D with the naturally derived forms of each alkaloid.

A Promising Future

In conclusion, Professor Ha and his colleagues have made significant progress in the synthesis, structural identification and understanding of a range of medicinal alkaloids, built using commercially available aziridines. They hope that their work will increase the availability and reduce the cost of these important compounds, towards improving people’s access to life-saving medicine.

Meet the researcher

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Professor Hyun-Joon Ha earned his PhD in chemistry in 1987 from Brown University in the US. Following his postdoctoral work at Stanford University, he joined the Chemistry Department at Hankuk University of Foreign Studies in Seoul, South Korea, in 1991. Professor Ha's research interests include the exploitation of new methods in organic synthesis. He has recently become interested in medicinal chemistry for drug discovery, process development for pharmaceuticals, and the design and synthesis of radiopharmaceuticals. He has also taken up several, fixed-period, senior administrative assignments, as the Dean of Natural Science at Hankuk University of Foreign Studies and as the 51st President of the Korean Chemical Society.

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OPTIMISING CARBON-HYDROGEN BOND ACTIVATION FOR EFFICIENT ORGANIC SYNTHESIS

Choosing which drug molecule to build is only one part of pharmaceutical research; medicinal chemists also need to know how to synthesise drug molecules in an efficient and cost-effective manner. **Dr Oscar Verho** and his team at Uppsala University in Sweden have made significant progress in this area and are aiming to reduce the time and resources needed to make drug compounds. The team is researching methods to 'activate' the carbon-hydrogen bonds that are commonly found in organic molecules to ultimately shorten the synthetic route to the required compound.

Building Drug Compounds in Fewer Steps

The synthesis of drug compounds almost always involves multiple steps, and therefore requires a lot of thought. The synthetic procedures for these chemicals must be economically viable and result in minimal chemical waste.

Each intermediate step of a synthetic pathway involves the incorporation of atoms at a specific site of the molecule. This iterative process continues until the final product is built. At the end of each step, the reaction mixture is usually purified, requiring solvents and other chemicals, before being analysed to confirm its structure and purity. Overall, the synthetic process can be long and complex.

Nearly all organic compounds contain both carbon and hydrogen atoms, often bound to one another in carbon-hydrogen bonds. In many synthetic methods, chemists prefer to directly swap a hydrogen atom in an organic compound for another atom or group of atoms. Unfortunately, this is not easy to achieve because carbon-hydrogen bonds are quite unreactive, and so are difficult to break. Furthermore, many molecules are made up of several carbon-hydrogen bonds, which means that a synthetic procedure must also be selective for a specific carbon-hydrogen bond.

For the past two decades or so, chemists have developed efficient methods that exchange hydrogen for the desired atom or group of atoms in a few steps. Dr Oscar Verho and his team from Uppsala University in Sweden are part of a community of chemists who develop methods that aim to substitute hydrogen atoms more directly from carbon-hydrogen bonds.

Carbon-hydrogen bonds, hereinafter referred to as 'C-H bonds', are difficult to break. Dr Verho's research attempts to resolve the unreactive nature of the C-H bond by temporarily changing the chemical structure of the molecule by introducing a chemical group near the bond.

'Introducing this so-called "directing group" works as a guide for a catalyst, pointing it to a specific C-H bond,' explains Dr Verho. The catalyst can then break the C-H bond, in a step known as 'activation', allowing the chemist to replace the hydrogen atom with another atom or group. 'However, as the directing group itself has no value in the product, it often must be removed afterwards, which constitutes another important chemical step for which new synthetic methods are needed,' Dr Verho adds.

Detaching the Directing Group

Central to Dr Verho's work presented here is an organic compound known as '8-aminoquinoline', abbreviated as AQ, which is composed of a ring-like structure of carbon, hydrogen and nitrogen atoms. The team's plan is to incorporate AQ as a directing group, use it to mediate the substitution of the hydrogen atom of the C-H bond, and then remove it.

It is already known that AQ can facilitate the activation of C-H bonds and greatly simplify the processes through which organic compounds are built, particularly drug molecules. Techniques to remove the AQ group from the molecule, once the hydrogen atom has been replaced, have also been developed, but these methods are often harsh and can sometimes lead to the precious molecules breaking down. Before developing new AQ-based methods for the C-H bond activation of unexplored drug-like compounds, Dr Verho and his group first looked at the latter stages of the overall pathway, that is, the removal of AQ.

An arrangement of bonded atoms known as the 'amide' group is commonly found in many drug molecules. Both amide and AQ groups contain nitrogen. As such, AQ can connect to the amide group through its nitrogen atom. Substituting the nitrogen-containing AQ group with a different nitrogen-containing group (for example, an amine compound) breaks the link between AQ and the amide, freeing AQ from the molecule and forming a new amide bond with the incoming nitrogen-containing group. Gratifyingly, Dr Verho's team showed how AQ could be substituted and removed under mild reaction conditions to form many new types of amide compounds that are useful in medicinal chemistry.

Overall, the team's work produced some very encouraging results, demonstrating that AQ can be removed from a wide range of compounds that had been subjected to C-H activation.

AQ as a Viable Director

Dr Verho's research team continued their pursuit of simpler and more efficient synthetic methods by using AQ to assist in the activation of the C-H bonds in compounds derived from a class of chemicals known as 'terpenes'. Terpenes are readily-available and inexpensive organic compounds derived from turpentine which can be sourced from wood pulping processes. To chemists, terpenes are considered a natural source of ready-made, structurally diverse organic compounds that contain atoms arranged in interesting ring shapes. Terpenes are useful in the pharmaceutical industry, and in the production of fragrances and polymers, among other compounds.

Using a terpene named verbenone, the Verho group could produce a molecule containing a ring of four carbon atoms, called 'cyclobutane'. Each carbon atom in a cyclobutane ring is usually bonded to at least one hydrogen atom. However, many sought-after compounds are composed of a cyclobutane ring bonded not to hydrogen, but to other

atoms. Synthesising such compounds is unfortunately quite challenging, as it requires complex reactions involving C-H activation to be carried out. Dr Verho's team was particularly interested in the potential for AQ to help in the activation of the C-H bonds of cyclobutane, enabling them to substitute the hydrogen atoms for other groups under mild conditions.

Dr Verho and his group started with the major components of turpentine and followed a five-step process to produce a compound containing both a cyclobutane ring and an AQ group. With this compound in hand, the team attempted to substitute a hydrogen atom bonded to the cyclobutane ring with other ring-containing organic groups. Much to their delight, the researchers found that they could activate a specific C-H bond in cyclobutane using a palladium catalyst with the aid of AQ, allowing for a range of ring-containing groups to be introduced in the place of the hydrogen atom.

The products obtained by the team also exhibited another noteworthy property – that of 'stereoselectivity'. If two or more products have the same number and types of atoms and bonds, but these atoms and bonds are arranged in different ways, then the molecules are distinct, and can have different properties. These different variations of a molecule are known as 'stereoisomers'.

What is impressive about Dr Verho's findings is that their synthetic method resulted in the production of one specific stereoisomer. The preferential production of one stereoisomer over the other is commonplace in nature, but is quite difficult to control in the laboratory. Indeed, there are lots of examples of pharmaceuticals where only one stereoisomer will lead to a required medicinal response.

'In this project, we made use of ozone to activate the AQ so it could be removed under mild conditions using dimethylsulfide and ammonium hydroxide,' says Dr Verho. In this way, his team was also able remove AQ in a series of steps at temperatures no higher than room temperature, converting and recovering 65% of the maximum possible amount of product.

One-pot Reactions

Another commonly occurring organic structure found in pharmaceuticals is 'benzofuran', a ring structure of carbon, hydrogen and a single oxygen atom. Following the success of their work with AQ-assisted activation of C-H bonds in cyclobutane, Dr Verho and his team investigated the application of AQ towards C-H bond activation in benzofurans.

Dr Verho's team proceeded to bond AQ to a benzofuran-containing compound through an amide group. The newly incorporated AQ group can guide a palladium catalyst to activate the C-H bonds of benzofuran for subsequent hydrogen substitution. 'Similar reactions to introduce ring-containing groups like in the case of cyclobutane could be done for benzofuran as well,' says Dr Verho. 'This showcases the generality and power of the 8-AQ C-H activation approach, as it can be carried out in high efficiency on many, vastly different organic compounds.' The amide link between the benzofuran and the AQ also provided the team with an easy way to remove the AQ.

The removal of AQ and the formation of the final AQ-free product requires two stages. Instead of carrying out each stage independently, Dr Verho's team performed both stages in the same reaction vessel, as a so-called 'one-pot' procedure. Essentially, the starting compounds for the first stage are mixed together, and after a certain time has passed, those for the second stage are added. The team found that the one-pot process could be completed in less than 11 hours and resulted is yields of over 60% after both stages. This approach saves time and minimises waste.

Dr Verho and his team have made considerable advances concerning the activation of C-H bonds, and developed strategies where the directing group, AQ, can be readily attached and detached when required. Their one-pot synthesis also makes AQ removal simpler to execute, and provides access to a range of interesting amide compounds. Evidently, their work will benefit all sorts of chemical industries, particularly pharmaceuticals, allowing for the efficient production of drug intermediates.

Meet the researcher

Dr Oscar Verho
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Dr Oscar Verho earned his PhD in Organic Chemistry from Stockholm University in Sweden. Following this, he worked as a Researcher at the same university and then moved to the Broad Institute of MIT and Harvard in the US to take a position as a Postdoctoral Research Fellow. He then returned to Stockholm University for three years, before moving to Uppsala University, where he currently works in the Department of Medicinal Chemistry. Dr Verho's research group focuses on the development of novel synthetic methodologies that can be used for the preparation of biologically active compounds and structurally diverse compounds. Throughout his career, Dr Verho has presented his work in numerous countries around the world, including the US, Australia, Japan and across Europe.

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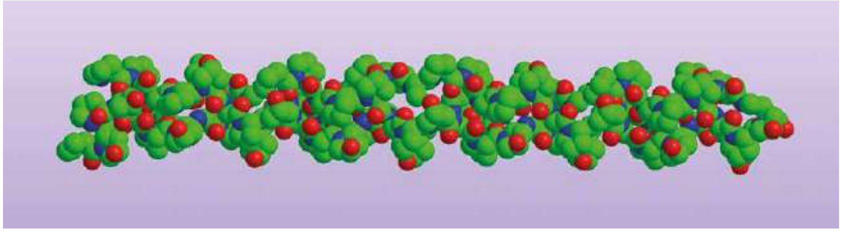
DEVELOPING RELIABLE METHODS FOR DETECTING PROTEINS

Proteins are a fundamental building block of all living organisms. Knowing how to detect and quantify them and monitor their interactions is therefore vital in numerous different fields, from food science to pharmacology. **Dr Anne Kleinnijenhuis** and his colleagues at TRISKELION in The Netherlands specialise in the development of innovative analytical techniques for measuring proteins. Recently, they have been designing improved methods that have far-reaching applications in food preparation, pharmaceuticals and blood analysis.



Merging Analytical Methods

TRISKELION, part of DUCARES B.V. in Utrecht, the Netherlands, is an innovative contract research organisation whose purpose is to develop methods and products that improve people's health and wellbeing. With clients in the pharmaceutical, food, feed and agrochemical industries, TRISKELION recognises that health and safety of humans, animals and the environment are all interconnected.

Dr Anne Kleinnijenhuis is a senior scientist at TRISKELION, who specialises in the development of Liquid Chromatography Mass Spectrometry (LC-MS) techniques for detecting proteins. His team has developed innovative LC-MS methods that can detect a range of proteins found in food and medications.

LC-MS is a combination of two techniques: liquid chromatography (LC) and mass spectrometry (MS). With LC, the sample mixture is separated into its constituent components and the relative amount of each component can be measured. The underlying mechanism behind LC is similar to how the different pigments in a spot of dried ink can become separated by water, migrating across a piece of paper. As the water spreads out over the ink on dry paper, it pulls the ink along with it and separates the ink into coloured bands, each of which represents a different component.

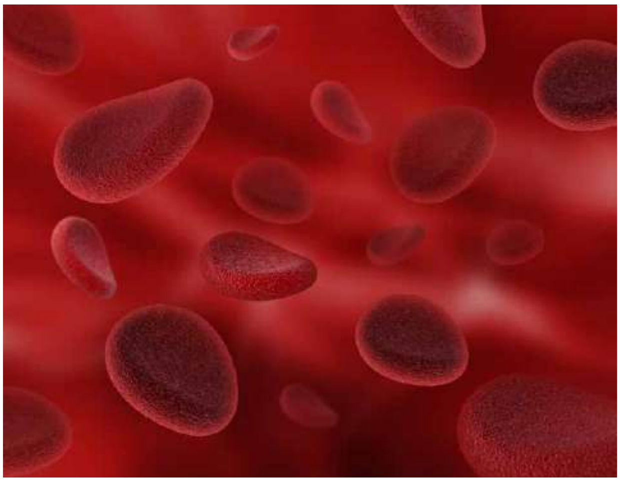
Each component is then processed at the next stage, namely MS, to determine the mass of each of the molecules present. The MS instrument works by turning the sample received into a cloud of charged, gaseous particles. These particles are then fired inside electric and/or magnetic fields towards a detector. An operator can then change various instrument settings to control how particles reach the detector and ultimately use the instrument settings to deduce the mass of the particle.

Applications in Food Science

Consumers with specific dietary requirements or preferences often want to know about the origin and composition of food products. While biochemical analysis has played a prominent role in providing this information, there is still much room for improvement. Analytical chemists are constantly seeking and designing methods that minimise sample degradation and waste, and reliably determine not only what substances are present but also how much is present and in what form.

A significant part of Dr Kleinnijenhuis's research is the detection and quantification of gelatine, a commonly used foodstuff. Gelatine is a more water-soluble derivative of a structural protein, collagen, taken from the skin and bone of cattle and pigs. There are nearly 30 known variations of collagen.

‘Our greatest achievement is to improve consumer knowledge about the products they consume!’



Following detailed work, Dr Kleinnijenhuis and his group published a quantitative method that can distinguish between gelatine derived from pigs and that derived from cattle using LC-MS, while taking into consideration the variety of gelatine materials in use. Their collagen portfolio contains many more collagen types and animal species.

‘We developed a method to quantify gelatine from different animal species; this method is important for consumers who want to avoid eating certain animal species such as pig,’ explains Dr Kleinnijenhuis. ‘Our greatest achievement is to improve consumer knowledge about the products they consume!’

Detecting Protein-based Drugs

In the development of new pharmaceuticals, researchers must be able to quantify the amount of drug that will ultimately end up in a patient’s bloodstream and cells, in order to optimise its therapeutic effects. Bioavailability data and dosage is vital in animal studies and subsequent clinical trials, which are both needed before a therapeutic drug can be brought to the market.

The researchers have recently published updated LC-MS procedures that can detect protein-based drugs. As a demonstration, the team applied their methodology to detect a drug called infliximab (Remicade®), which is made up of protein. This therapeutic is used to treat a range of autoimmune diseases, including Crohn’s disease and rheumatoid arthritis.

Previously developed procedures can detect infliximab at concentrations in the range of 100–250 nanograms (one nanogram is one billionth of a gram) per millilitre of solution. Dr Kleinnijenhuis modified the sample preparation stages and utilised more advanced LC-MS instrumentation to detect infliximab at concentrations as low as 75 nanograms per millilitre of solution. In addition, he derived a formula to improve the performance assessment of protein LC-MS methods.

Monitoring Haemolysis

The breakdown of red blood cells, known as haemolysis, can occur in an organism when there are underlying physical conditions or when certain drugs are taken. Haemolysis can also take place externally whenever a blood sample is processed prior to analysis. In all cases, the breakdown of the red blood cells releases more substances into the test sample, complicating the analysis of other targeted substances.

Measuring the extent of haemolysis is sometimes subjective. A lab technician can visually inspect the sample and compare how much the red colour intensifies as the degree of haemolysis increases. Other more precise methods are available: one can measure how much ultraviolet and visible light is absorbed by a sample, using a technique called UV-Vis spectroscopy, though this method requires relatively large additional amounts of sample.

Dr Kleinnijenhuis and his team found a more objective approach to measuring the extent of haemolysis. They developed a method based on LC-MS that monitors the changes to red blood cell levels. Like some of the group’s other methods, this particular approach is based on monitoring a protein fragment known as ‘tryptic peptide’. The team was able to apply their procedures and analyse blood derived from different animal species.

It turned out that UV-Vis and LC-MS techniques returned similar results when analysing blood samples with known amounts of tryptic peptide. However, one of the disadvantages of visual and UV-Vis inspections is that they are both dependent on the colour of the sample, which can also be influenced by the presence of residual fat molecules, or ‘lipids’. Lipids are

commonly found in blood samples, especially shortly after an individual has eaten, and cause the samples to appear cloudy. Dr Kleinnijenhuis demonstrated that lipids interfere with both visual and UV-Vis analyses, while LC-MS analysis readily reveals the levels of tryptic peptides regardless of whether the sample was cloudy or not. This shows that LC-MS is a more universal technique.

Following the Course of Protein Uptake

Protein supplements can take one of many forms. Of particular interest to Dr Kleinnijenhuis and his group are 'collagen hydrolysates'. These are smaller, broken-down forms of collagen. Collagen hydrolysates and other protein hydrolysates are quickly absorbed in the gut and can be of significant benefit to individuals who cannot absorb proteins readily.

The researchers continued their work on LC-MS protein analysis and assessed the state of hydrolysates at three different stages: pre-digestion; post-digestion and pre-uptake (before entering the blood stream at the gut); and post-uptake. The team found that the resultant changes to collagen hydrolysates were very complex.

To assist with the processing and interpretation of the data, they carried out a series of preliminary LC-MS analyses, known as non-targeted analyses, to help them design targeted LC-MS analyses. A non-targeted analysis is concerned with detecting a broader range of substances, revealing as much information about the entire sample as possible. The main drawback with non-targeted analysis is the sheer size and complexity of the dataset produced. Targeted analyses tend to focus on a much narrower range of substances and usually involves comparing the signals produced by the sample with those produced by a standard containing known amounts of a substance. The problem with targeted analysis, however, is that it becomes all too easy to exclude potential experimental data that may be vital to the investigation.

The overall two-stage analysis is intended to eliminate as much bias as possible, by observing nearly everything during the first stage, before homing in on more specific results. By considering both stages, the team's study outlined a pathway describing how collagen hydrolysates are broken down into smaller units, known as 'tri- and dipeptides' and 'amino acids'. 'The formation of many different collagen tri- and dipeptides and their role after uptake is particularly interesting and is actively investigated, while in the past there has been a more limited focus on free amino acids,' explains Dr Kleinnijenhuis.

The work of Dr Kleinnijenhuis and his colleagues has not only proved valuable to their community but also more long-term to the consumer. Their achievements will carry across to other domains wherever proteins are involved and have set another foundation for others to build on.

Meet the researcher

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Dr Anne Kleinnijenhuis is a senior scientist at TRISKELION, part of DUCARES B.V. in Utrecht, The Netherlands. His main interest is analytical method design and, specifically, the quantification and characterisation of proteins in biological matrices using a wide variety of sample preparation and LC-MS techniques. Dr Kleinnijenhuis has a scientific background in fundamental and applied biomolecular mass spectrometry and other related fields, including biochemistry. Before joining TRISKELION, Dr Kleinnijenhuis carried out his PhD research at the Institute for Atomic and Molecular Physics and at Utrecht University. Following this, he worked as a postdoctoral researcher at the University of Southern Denmark and as a project manager at TNO.

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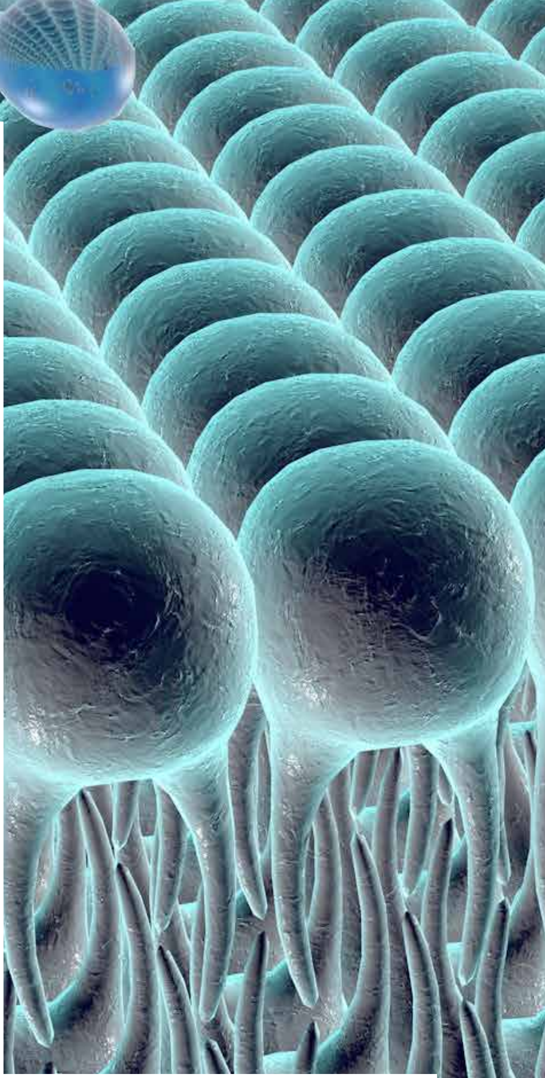
COMBINING SIMULATIONS & EXPERIMENTS TO EXPLORE INTERACTIONS BETWEEN MEMBRANES & SMALL MOLECULES



Many important processes in our bodies rely on the transport of small molecules and ions across cell membranes. However, these processes can be extremely intricate and complex, and are frustratingly difficult to study. **Dr Evelyne Deplazes** and her team at the University of Queensland and the University of Technology have been investigating these processes by combining the best elements of experimental and computational membrane biophysics. This research could help us better understand the way our bodies work, with exciting implications for biotechnology and drug development.

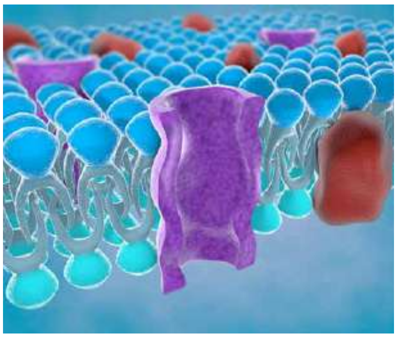
Movement of Ions and Molecules

Of the many complex processes that take place in our bodies, one of the most important is the transport of ions and small molecules into and out of our cells. Each of our cells is enclosed by a membrane made up of fatty molecules called phospholipids, which protects the cell's interior from the external environment, and controls which substances can pass through. When an ion or molecule interacts with the surface of a cell, the membrane can allow it to pass through under the right conditions. However, the nature of these interactions is not yet fully understood.

Naturally, scientists have been searching for new ways to study these processes in order to learn more about them. Such improved knowledge would be invaluable for numerous different research fields – from understanding how certain diseases develop to designing effective methods for delivering drug molecules into cells.

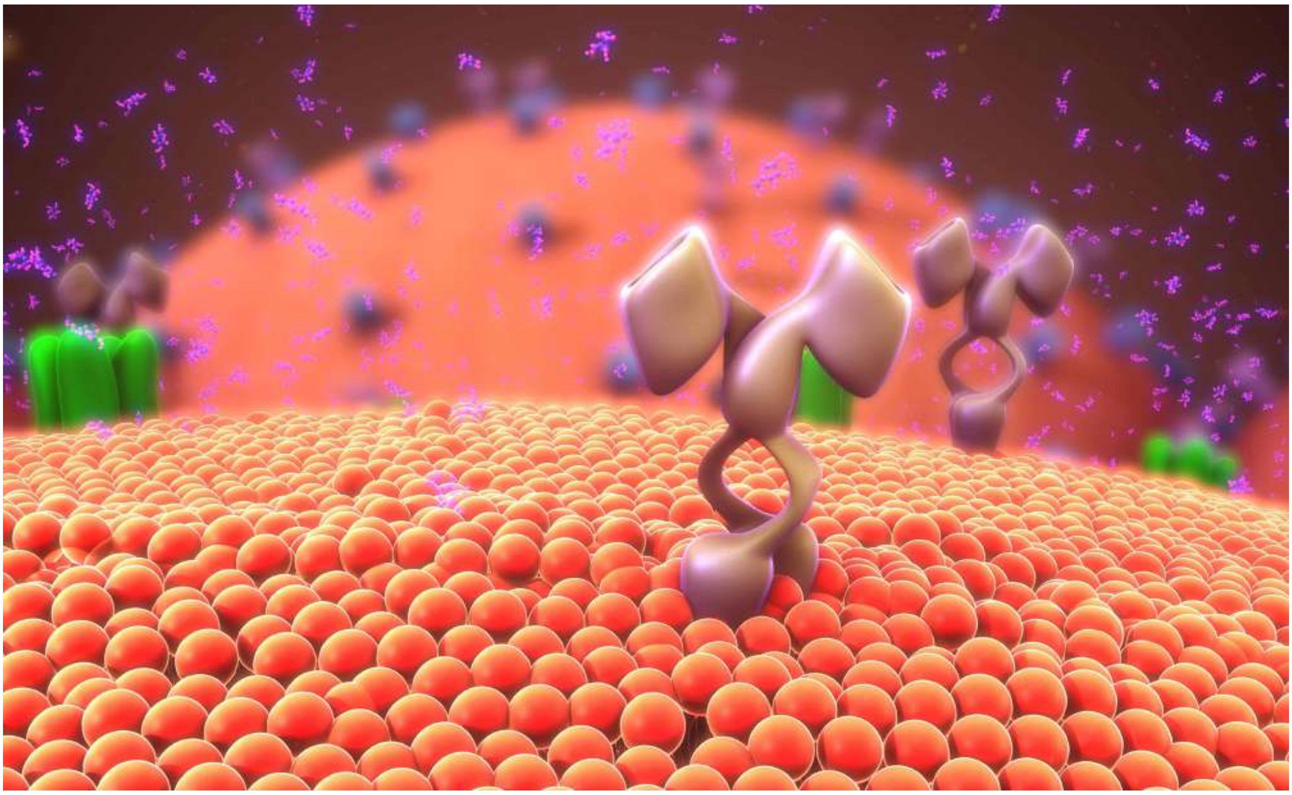
'The transport of small molecules across membranes is important to understand both fundamental biological processes as well as for many applications in biotechnology and drug development,' explains Dr Evelyne Deplazes, researcher at the University of Queensland.

Unfortunately, due to their complexity, these interactions are extremely challenging to study in the laboratory. Computational chemists have developed simulations that allow for more in-depth analysis, but these are not without their own limitations based on processing power and computation time. These simulations also need to be validated, ideally by comparing their results to experimental data collected from the system being simulated. Dr Deplazes and her colleagues have been tackling these issues by using a unique combined method.



Exploring Sodium and Potassium Transport

Dr Deplazes and her colleagues began their investigations by using 'tethered membranes', which are essentially phospholipid molecules anchored to a substrate made of pure gold. These model membranes mimic the fluidity that would be found in a cell membrane, but in an environment where lipid composition and other variables such as pH and ion concentrations can be controlled. This allows the team to isolate different effects in a way that is usually not feasible using cell membranes.



By measuring the electrical properties of the membrane in the presence of different concentrations of sodium and potassium ions, the team was able to learn more about how these two important ions interact with the surface. Sodium and potassium ions play key roles in countless biological processes, including water regulation, muscle contraction and the transmission of nerve signals.

At low concentrations, the researchers found that sodium decreased the membrane's electrical conductance, while potassium increased this property. However, they only observed this effect with certain types of phospholipid membranes, and not others, implying that the effect was caused by specific interactions between the phospholipid molecules and the ions.

To further investigate this phenomenon, the team implemented molecular dynamics simulations. This computational approach is used in chemistry research to simulate the ways in which molecules interact with each other. From these simulations, the team gathered data showing that sodium was more likely to interact with multiple phospholipid molecules than potassium. Sodium was also more likely to be found at the surface of the membrane. Dr Deplazes explains that these differences could be leading to a change in the way the molecules are able to move on the surface, hence a change in conductance.

This study has not only generated valuable information on the way in which our cells can interact with ions, but also made a strong case for the effectiveness of combining computational and experimental methods for probing biophysical mechanisms.

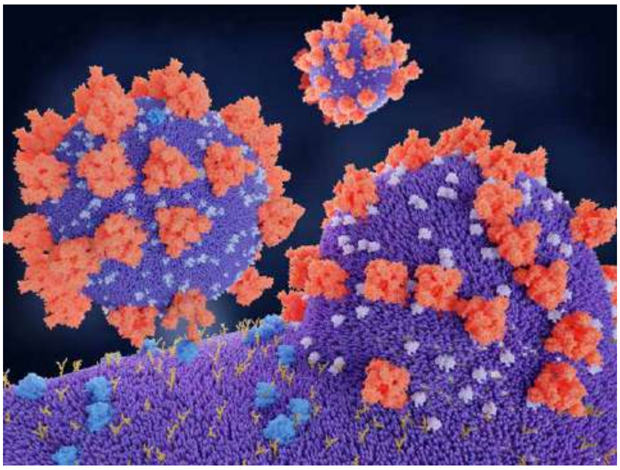
Membrane Pores

Nearly every disease-causing virus we know about interacts with our bodies in a similar way: by entering our cells through the outer membrane. Once the virus is inside a cell, it can start hijack the cell's machinery and start replicating itself, allowing it to spread to other cells. This is done by all kinds of viruses, including HIV, measles, and the virus that causes COVID-19.

The process of viruses taking over the body's cells is referred to as viral-membrane fusion. Scientists have studied this process extensively, to better understand how exactly viruses can pass through the cell membrane. Understanding how the virus does this may help scientists to identify ways to prevent it from happening. An improved understanding of this process would also be invaluable for vaccine research, as many of today's vaccines – including some of those for COVID-19 – deliver genetic code to our cells inside a harmless viral 'shell'.

Scientists have previously explored how viruses penetrate the cell membrane using a special molecule called 'GALA' – a synthetic protein designed to mimic the way viruses interact with phospholipid membranes. Dr Deplazes and her team have been investigating how GALA molecules are able to open pores in the cell membrane, by using a combination of experiments and molecular dynamics simulations.

It was already understood that, under acidic conditions, GALA molecules would assemble and insert themselves



into the cell membrane to create an open pore. It was previously believed that each of these pores was made up of 8–12 individual GALA molecules. Dr Deplazes and the team have demonstrated that it is more likely that these pores are made up of 6 molecules instead. This is important information, as it tells us more about the size of the pores and what they could let through. 'This combined approach, for the first time, directly provides structural information to estimate the size of pores formed by a peptide similar to the ones found in viruses,' explains Dr Deplazes.

Furthermore, the team found the pores showed selective permeability – allowing some ions to enter more easily than others. Their results could represent an important step in learning more about how GALA, and thus viral fusion peptides, operate.

How Can Small Molecules Alter Membranes?

Understanding how small molecules interact with phospholipid membranes is important for many different applications, including drug development and biotechnology.

By integrating molecular dynamics simulations and experiments with tethered membranes, Dr Deplazes and her team have developed a powerful approach to gain valuable insights into molecule–membrane interactions at the molecular level. The lab's ongoing research includes studying the membrane-altering effects of steroids, steroid-like molecules and phenolic acids.

Phenolic acids are molecules that are commonly found in plants. Present in many plant-based foods, phenolic acids have been extensively studied for their antioxidant, anti-inflammatory and pro-coagulant properties.

Some of these biological activities are related to the interaction of phenolic acid molecules with cell membranes. However, compared to their activities inside cells, very little is known about how these molecules interact with the cell membrane.

Dr Deplazes and her team's tethered membrane experiments show that certain phenolic acids, such as caffeic acid, caffeic acid methyl ester and kojic acid, change the permeability of phospholipid membranes to varying degrees. In contrast, other phenolic acids with similar structures, including p-coumaric acid, gallic acid and syringic acid, do not alter membrane permeability.

To understand why certain phenolic acids can alter membrane structures, while others cannot, the research team performed experiments with different types of phospholipid, to study specific interactions between phenolic acid molecules and the lipid component of phospholipid molecules. They used the data they collected to validate simulations that provide structural information on these interactions. 'Our results from these simulations suggest that membrane disruption is related to the phenolic acids inducing local and temporal changes at the water-phospholipid interface without changing the overall shape of the membrane,' says Dr Deplazes.

In another study, her team investigated the interaction of steroids and steroid-like molecules with phospholipid membranes. Steroids include molecules that naturally occur in our body, such as progesterone and testosterone, and drugs used to treat inflammatory conditions including arthritis, eczema and asthma. The team's tethered membrane experiments showed that these clinically used steroids directly alter the permeability of cell membranes. Their results will be useful for designing more effective steroid-based drugs for a range of inflammatory diseases.

A Winning Combination

Throughout her research, Dr Deplazes has demonstrated how a combination of computational and experimental chemistry can answer questions that one method alone could not. 'Our lab is one of the few labs where biophysical experiments and molecular dynamics simulations are directly combined,' she says.

Her team's simulations and tethered membranes are highly effective for studying molecular interactions in systems where conditions can be controlled. To translate their findings into living systems, however, the team collaborates with microbiologists, molecular biologists and molecular biophysicists.

In collaboration with these researchers, the team's unique approach continues to provide deep insights into the behaviour of cell membranes, with important implications in numerous fields, including drug delivery, vaccine development, and treatments for infectious diseases, cancers and neurological disorders.

Meet the researcher

Dr Evelyne Deplazes
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Dr Evelyne Deplazes earned her PhD in computational biophysics from the University of Western Australia in 2012, before being awarded early career fellowships by the Swiss National Science Foundation and the Australian National Health and Research Council. She worked as a research fellow at the University of Queensland, Curtin University and the University of Technology Sydney, before returning to the University of Queensland, where she holds her current position as Senior Lecturer. As a biophysical chemist, Dr Deplazes' research integrates wet-lab and computational approaches to study how small molecules such as drugs or peptides interact with membranes. She uses this knowledge to further our understanding of biological and (bio)chemical processes and to facilitate the development of pharmaceuticals and drug delivery systems. In addition to her research, Dr Deplazes is passionate about training up the next generation of scientists and teaching them how to be critical thinkers. Through her mentoring and leadership activities, she is actively involved in promoting diversity, equity and inclusion in STEM and higher education.

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MATERIALS SCIENCE

SOLVING SOCIETAL CHALLENGES WITH NEW MATERIALS

Although there is much overlap between the fields of chemistry and materials science, we felt that the latest material innovations deserved their own unique section in this edition of Scientia. When studying materials, chemists tend to exclusively focus on the atomic or molecular properties, while materials scientists focus on physical characteristics at any level – from chemical interactions at the molecular level, to quantum phenomena at the nanoscale, all the way up to macroscale properties such as mechanical strength and elasticity.

Materials science has proved critical in tackling our most urgent societal problems. For instance, materials scientists have been behind the development of platforms for detecting SARS-CoV-2 and those needed for delivering COVID-19 vaccines. Equally important has been the development of materials for renewable energy technologies. The widespread use of these technologies, such as solar cells, will hopefully soon allow us to put an end to our reliance on fossil fuels.

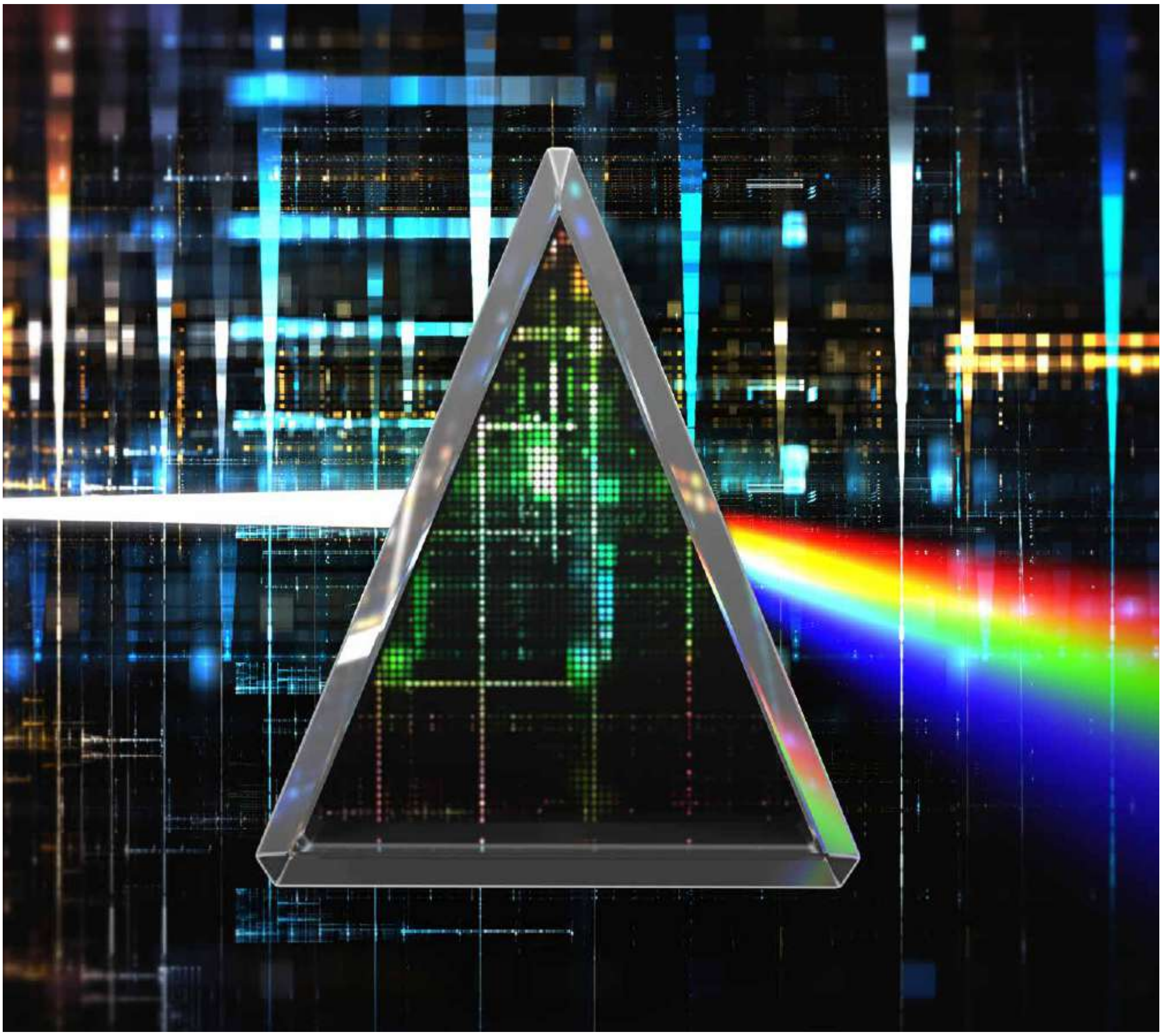
In this section, we showcase the work of talented materials scientists, who are addressing diverse challenges through the creation and optimisation of new materials.

First, we meet researchers from the Nanotechnology Enabled Water Treatment (NEWT) Center, which is headquartered at Rice University. By developing and researching nanostructured membrane materials, these researchers are developing cutting-edge purification technologies that can provide communities with access to clean and safe drinking water.

Dr Matthew Lasich at Mangosuthu University of Technology in South Africa is also researching materials for purification purposes. Specifically, his team utilises computational modelling to discover how clay-based materials can be used to purify fuel gas mixtures. Such new and improved methods for purifying fuel gases can both improve their efficiency and reduce their environmental impact.

Meanwhile at the University of Illinois at Urbana-Champaign, Dr Jean-Pierre Leburton conducts both computational modelling and experiments to explore the application of nanoporous graphene materials to DNA sensing applications. His DNA detection platforms could have widespread medical applications, enabling early disease diagnosis and prompting effective treatment, as well as providing invaluable technologies for assisting with DNA sequencing.

Another exciting application of graphene is its use as a scaffold material for promoting tissue growth



in the treatment of various medical conditions, including osteoarthritis. This is the theme of our next article, in which we introduce Dr Julia Oxford and Dr David Estrada at Boise State University, USA, and Dr Solov'yov at Carl von Ossietzky University in Oldenburg, Germany. By gaining a greater understanding of the interactions between graphene and cells, the team hopes to develop implantable graphene-based devices that can rebuild damaged tissue.

Dr László Forró and his team at Ecole Polytechnique Fédérale de Lausanne combine graphene with another exceptional material, called perovskite, to create high-performance sensors that have the ability to detect a single photon of light. Because of their outstanding sensitivity, the team's technologies are leading to new applications ranging from more sensitive medical diagnostics, to safer nuclear reactors.

Next, we showcase the work of Dr Hiroaki Nishiyama and his team at Yamagata University in Japan, who have developed a new approach to 'Direct Laser Writing' – a technique used to deposit intricately patterned materials onto surfaces. By harnessing the unique properties of nanoparticles when they are illuminated with laser pulses, the team's approach can create highly sophisticated nanoscale structures, for applications ranging from biomaterials to semiconductors.

While traditional 'inorganic' semiconductors are typically made from silicon, organic semiconductors are an emerging technology composed of organic molecules, which mainly comprise carbon and hydrogen atoms. Organic semiconductors can be found in the latest television screens and smartphone displays, and even in low-cost solar cells. In the next article, we introduce Dr Masahito Oh-e at the National Tsing Hua University in Taiwan, who studies the intriguing properties of these materials, towards developing more efficient and high-performing technologies for the future.

Our final article in this section also highlights exciting research into organic materials. Here, we meet researchers at the NASA Glenn Research Center, who are designing flexible organic materials called aerogels that can be used to construct lightweight, low-drag antennas for aircraft.

DEVELOPING SUSTAINABLE WATER PURIFICATION TECHNOLOGIES

A significant proportion of the world's population has little to no access to clean water, and the water consumed by industrial activities continues to grow. Researchers from the Nanotechnology Enabled Water Treatment (NEWT) Center, which is headquartered at Rice University, are developing cutting-edge purification technologies that can provide communities with access to clean and safe drinking water. They are also creating new wastewater treatment methods that allow the reuse of industrial effluent, to minimise freshwater withdrawals by industries. Instead of conventional methods that use large amounts of chemicals and energy, NEWT technologies are chemical free, and often utilise solar energy.

Responding to Water Shortages

Many people across the globe do not have access to clean water, and there remains a vital need to provide communities with potable water supplies. Seawater and other saline or compromised water sources are often readily available, but these supplies are typically unsuitable for consumption, given their high concentrations of salts, microbes, toxic metals, and other contaminants. Such water sources need to be purified before they can be used.

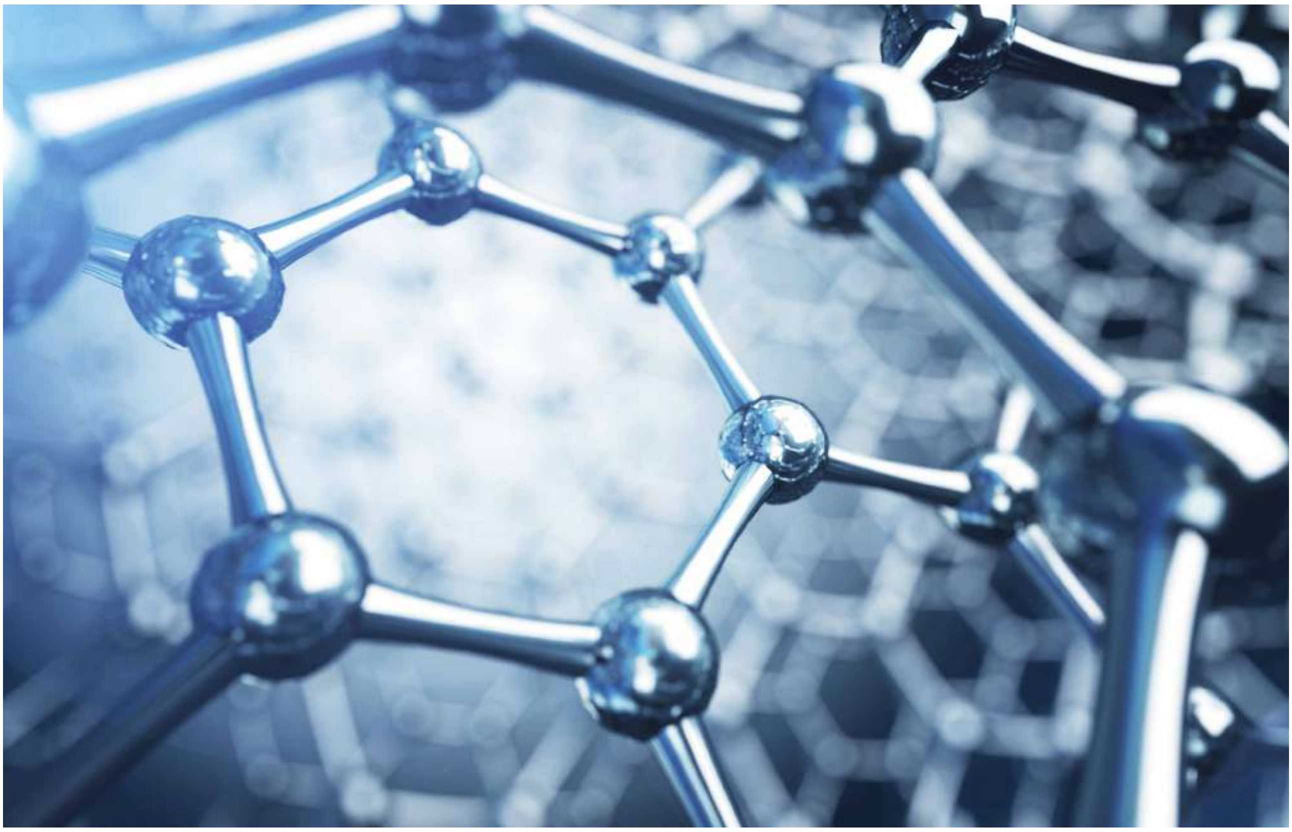
Multiple research teams from the 'Nanotechnology Enabled Water Treatment' (NEWT) Center are working to tackle these urgent problems. Funded by the US National Science Foundation, the Center is made up of researchers from Rice University, Arizona State University, Yale University, and the University of Texas at El Paso, with expertise spanning diverse disciplines, including environmental engineering, chemical engineering, materials science, chemistry and physics. NEWT's vision is to enable access to water of suitable quality almost anywhere in the world by developing next-generation, easy-to-deploy modular treatment systems enabled by nanotechnology.

Membrane Distillation

One purification method that NEWT researchers are working to improve is called 'membrane distillation'. In the process of membrane distillation, hot saltwater is passed over a membrane on one side, while cold, freshwater flows on the other side of the membrane. The membrane is porous, but keeps the saltwater and freshwater streams apart. The temperature difference across the membrane and between the two streams causes hot water from the saltwater side to vaporise through the membrane and join with the colder freshwater stream. The process does not require the use of chemicals and, overall, separates water from saltwater solutions.

The migration of water vapour from the saltwater side to the freshwater side occurs to a greater extent when the difference in temperature across the membrane is higher. When the temperature of the saltwater is high, the extent to which vaporisation occurs is similarly high. Likewise, when the freshwater temperature is low, the extent to which condensation occurs is also high.

These factors do, however, reveal an inherent limitation with membrane distillation. The act of vaporisation lowers the temperature of the hot, saltwater side and the process of condensation increases the temperature of the cold, freshwater side. The membrane also transfers some of the heat energy from the saltwater side to the freshwater side. These and other temperature-related factors subsequently reduce the difference in temperature across the membrane, therefore lowering the volume of water that can migrate across it. To maximise the migration of water



vapour, one would need to maintain a large temperature difference across the membrane.

Harnessing the Sun's Energy

Maintaining the temperature difference can be achieved by heating the membrane itself. Researchers from the NEWT Center found that by adding a layer that can absorb solar energy to the membrane surface on the saltwater side, and then directing sunlight to this layer, they were able to increase the quantity of water vapour transferred. The team's new technology, referred to as 'nanophotonics enabled solar membrane distillation' (NESMD), can thus be powered locally, using free, clean and widely available energy from the Sun.

In the team's NESMD technology, the layer on the membrane that absorbs sunlight is called 'carbon black' – a substance similar to activated charcoal. Sunlight is directed through an array of lenses to the carbon black layer, which absorbs nearly all frequencies of visible light, transferring the energy as heat to the membrane.

NESMD is relatively cheap to operate, since any potential purification plant would not need to heat the entire volume of saltwater. The NEWT researchers hope that their environmentally friendly purification process can be applied at different scales – from whole communities down to individual households, many of whom will not be connected to the national grid.

The team also investigated other energy-absorbing materials for NESMD. In one study, they applied 'silica', the main constituent of sand and glass, covered with gold to the surface of the membrane. The researchers found that the carbon black materials absorb more of the high-energy radiation in sunlight, comprising blue and violet light, whereas the silica-gold materials absorb more of the low energy radiation, corresponding to red and yellow light. Both NESMD membrane compositions performed more effectively than conventional membranes, maintaining the temperature difference needed to prolong vaporisation.

For applications that require large volumes of water 24 hours a day, such as industrial applications, NEWT researchers have also developed 'dual-power membranes'. These membranes harness energy directly from sunlight when it is available, and can then operate on electricity at night. One team of NEWT researchers developed a dual-power membrane comprising a nanolayer of boron nitride on a stainless-steel wire cloth, which demonstrates superior performance, making it suitable for industrial applications.

Another group of researchers fabricated a dense, non-porous 'pervaporation' membrane from a polymer called Nexar™. The team found that their membrane exhibited a salt separation performance superior to commercial pervaporation membranes, and equivalent to that of commercial membrane distillation membranes.

In another study, NEWT scientists used egg-shell waste to develop a highly efficient dual-power membrane. Specifically, they used the egg membrane, found just inside the shell, whose porous structure efficiently allows the selective movement of water into and out of the egg during incubation and hatching. In the manufacture of egg-containing products, these membranes are often discarded along with the shells. Therefore, combined with the use of renewable energy from the sun, the team's technology represents an even more environmentally-friendly and sustainable solution to water purification.

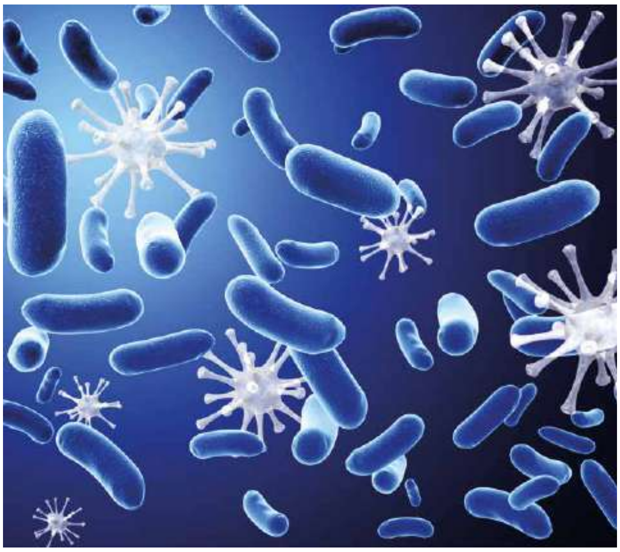
Selective Removal of Ions

In addition to their efforts to remove common salts from water, NEWT researchers have also been working on methods that remove contaminant ions that are far less abundant than common salts. For example, nitrate and chromate are negatively charged ions that cause a range of human health problems. Sulphate and calcium ions, although non-toxic at typical concentrations, can form solid deposits that cover surfaces and cause a range of problems in homes and industrial processes. Removal of these ions is challenging because highly abundant common salt ions interfere with the treatment processes.

Most techniques for removing calcium involve chemical treatments. Thus, NEWT researchers wanted to develop an alternative method that can selectively remove calcium ions from water using a process known as 'electrosorption'. During electrosorption, ions that have an opposite charge to that of an electrode are attracted to the electrode, removing these ions from water. Then, the charge on the electrode is reversed, releasing the ions into a saltwater stream that will be disposed of. The research team developed nanocoatings, which, when applied to the electrode surface, allow calcium to approach the electrode faster than the interfering common ions. This makes the electrode surface highly selective to calcium ions and provides a very effective method of calcium ion removal.

In several other studies, NEWT research teams developed electrodes that can remove negatively-charged ions, including sulphate. Some salts of sulphate ions are very insoluble in water, and over time they can contribute to water scaling. At higher concentrations, sulphate ions can even be converted into hydrogen sulphide by bacteria. Hydrogen sulphide is a toxic gas and its production is particularly problematic in the oil and gas industries, where sulphate and bacteria are abundant in the water used during crude oil extraction and processing. The researchers demonstrated effective and selective removal of sulphate ions from water using novel nano-electrode materials in the electrosorption process.

Using a similar approach, NEWT scientists also conducted research on the selective removal of a negatively charged ion called chromate. This highly toxic chemical can cause cancer, and is a widely occurring contaminant in groundwater. In their study, the researchers created an electrode made from a type of graphene called 'reduced graphene oxide', upon which they grew nanocrystals of a cobalt-containing compound. Applying a positive voltage to the conductive graphene material allowed it to attract the negatively-charged chromate ions, while the nanocrystals could then efficiently trap the ions in place. By then applying a negative voltage to the electrode, the researchers were able to release the chromate into a saltwater stream for disposal.



Deactivation of Microbes

The chemical-free deactivation of microbes in water is another important part of NEWT's research portfolio. Boiling large volumes of water to kill bacteria is considered inefficient. Instead, the team developed a method of successfully disinfecting water that uses gold nanorods or carbon black to channel solar energy into the water. This results in localised heating of the water, which subsequently kills nearby microbes.

Following a different approach, another team of NEWT researchers designed UV-light side-emitting optical fibres that can disinfect flowing water and prevent the growth of biofilms on surfaces, which would otherwise harbour pathogens such as Legionella. By depositing a layer of silica nanoparticles onto the surface of each optical fibre, the researchers could cause the germicidal UV light to become scattered from the side of the fibre like a glowstick. Upon testing their technology on *E. Coli* and other bacteria, the team was able to effectively kill over 99% of the bacteria in water samples and in slimy biofilms growing on surfaces.

Multidisciplinary Nanotechnology Research

Evidently, the work performed by the NEWT researchers is very comprehensive. Their collaborative and multidisciplinary efforts will prove vital to the health and wellbeing of communities and individuals across the world who do not have access to clean water, particularly as climate change and a growing human population continue to place greater stress on our global water supplies.

The NEWT Center

Nanotechnology-Enabled Water Treatment (NEWT) Center
Rice University
Houston, TX
USA

This research was carried out by academic members of the Nanotechnology Enabled Water Treatment Center, NEWT, a collaboration of research teams from across the US, with headquarters at Rice University. The principal investigators of the team are Professor Pedro Alvarez, Professor Qilin Li and Professor Naomi Halas from Rice University, Professor Menachem Elimelech from Yale University and Professor Paul Westerhoff from Arizona State University. In addition to their research partnerships with universities and industries across the world, the NEWT Center is also committed to providing high school students and teachers, as well as undergraduates and postgraduates, with hands-on research experiences.

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CLAY MATERIALS SHOW PROMISE AS FUEL GAS PURIFIERS

Finding new and improved methods for purifying fuel gases, to both improve their efficiency and reduce their environmental impact, is an active area of research. **Dr Matthew Lasich** at Mangosuthu University of Technology in South Africa has been utilising computational modelling to discover how clay-based materials can increase the efficiency of fuel gas derived from wood and also reduce the amount of hydrogen sulphide found in natural and landfill gas.

Purifying Fuel Gas

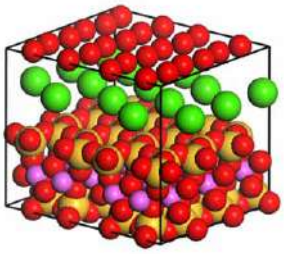
Natural gas and gas collected from landfills contain complex mixtures of combustible and non-combustible substances. Both are mostly made up of methane and other hydrocarbons with carbon dioxide and hydrogen sulphide being the other notable components.

Access to natural and landfill gas is limited for many rural communities. Synthetic gas, or more concisely 'syngas', is one of a few potential substitutes. Syngas can be produced locally from the partial combustion of organic matter with limited amounts of oxygen to produce a mixture composed primarily of carbon monoxide and hydrogen.

While the use of natural, landfill and synthetic gas is widespread, there remains room for improvement. The composition of syngas, for example, is rarely tuned to optimise its energy availability. Natural and landfill gases contain harmful levels of hydrogen sulphide, which has damaging impacts on both human health and the environment. In the presence of water, hydrogen sulphide can also crack processing plant pipes, increasing maintenance costs.

Dr Matthew Lasich of Mangosuthu University of Technology in South Africa applies computational techniques to design more sophisticated gas purification methods. The work described here focuses on Dr Lasich's computational simulations, which show how synthetic gases can be purified to optimise their energy output, in addition to how natural gas can be purified by removing hydrogen sulphide.

Such computational simulations provide highly targeted sets of results at much reduced costs compared with experimental results. Perhaps more importantly, such modelling techniques can be applied to chemical systems that are unsafe or simply inaccessible. 'We apply computer simulations to study systems in a more controlled manner than is possible in the laboratory,' explains Dr Lasich. 'In this way, we can gain insights that might be difficult to observe.'



Key to the success of Dr Lasich's purification methods is a clay known as 'bentonite'. Bentonite is readily available in many regions of South Africa and can effectively separate gaseous substances. The mechanism of action between bentonite and a gas is very similar to the process that occurs in the catalytic converter of commercial vehicles. As the gas passes over the surface of the material, some of the gas molecules stick to the surface, in a process known as 'adsorption', forming a relatively strong bond. In this example, bentonite is the solid material, and performs the role of an 'adsorbent'. The degree to which gases adsorb onto bentonite depends on the surrounding temperature and pressure, the nature of the gas and the chemical properties at the surface of bentonite.

Improving the Energy Output of Syngas

Wood gas is a form of syngas derived from timber, and is mostly made up of hydrogen and carbon monoxide. This renewable fuel can be prepared using small generators, which can provide energy to local communities that have limited access to other, more conventional forms of energy.

Dr Lasich's recent computational study simulates how wood gas can be refined to increase its energy output per kilogram of gas, by passing the crude gas over bentonite. The clay material can remove the non-combustible components of wood gas, such as carbon dioxide, resulting in higher proportions of combustible carbon monoxide, hydrogen and methane.

Dr Lasich applied a procedure known as 'pressure swing adsorption', where gases passed over an adsorbent are separated under pressure according to how well they can attach onto the surface. Dr Lasich simulated the adsorbent characteristics of bentonite at a temperature of 700°C and pressures of up to about 10 times atmospheric pressure. While these conditions would be considered modest by industrial standards, Dr Lasich wanted to establish methods that would be more suitable for domestic users who are unlikely to have access to industrial grade systems.

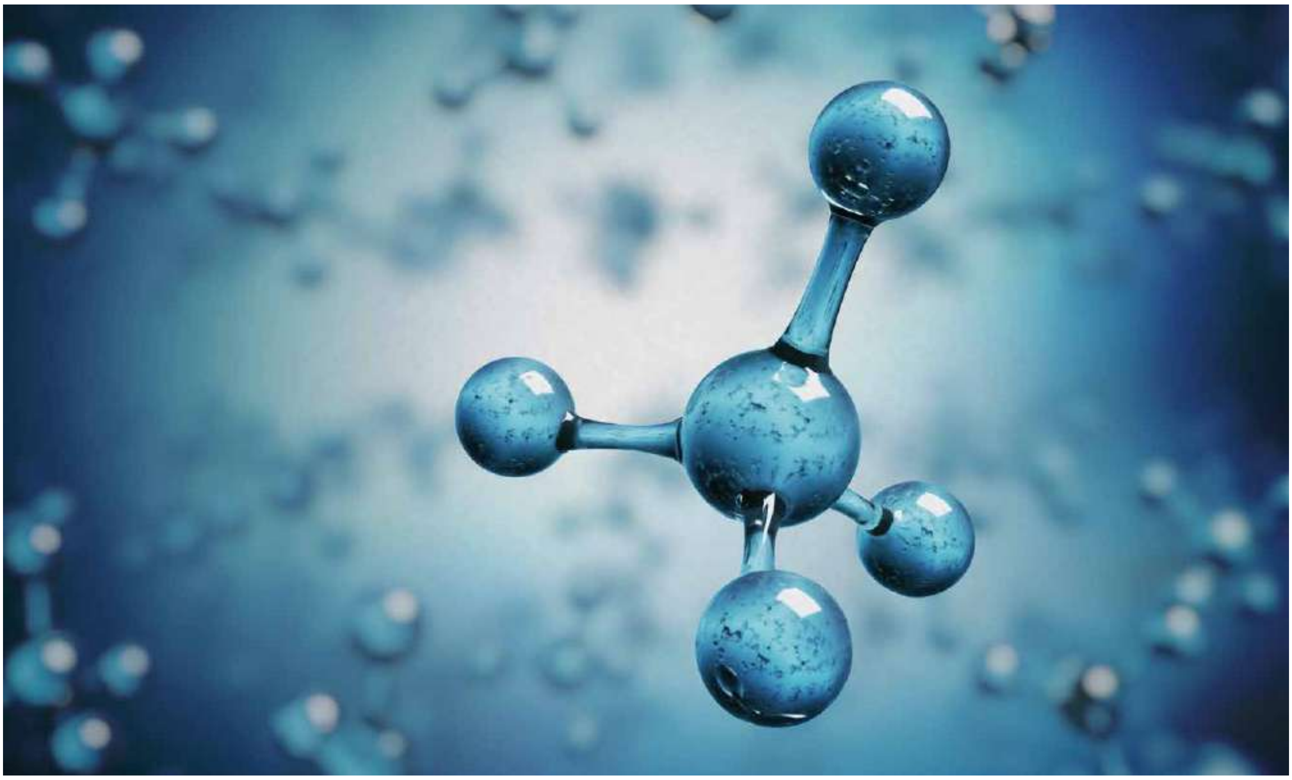
After performing multiple simulations, Dr Lasich found that as pressure increased, the extent to which each gaseous substance adsorbed to bentonite also increased, with hydrogen and oxygen adsorbing more readily than carbon monoxide and methane. This shows that the refined wood gas would contain higher proportions of methane and carbon monoxide, and lower proportions of hydrogen and oxygen. A statistical analysis of the results showed that the energy output per kilogram of wood gas increased by five percent. Over widespread use, a five percent improvement would be very significant.

'Our most important achievement has been demonstrating that a relatively common material – bentonite clay – can provide a boost to the energy content of renewable wood gas using a low energy process,' summarises Dr Lasich.

There are a couple of caveats to note. Dr Lasich explains that the pressure swing adsorption procedures needed to increase the energy content of wood gas may be compromised to some extent by the loss of gas during purification. In this case, he notes that a wood gas recycling system may be required. Furthermore, removing all the oxygen is not always desirable, since an oxygen supply is needed in the combustion of methane and carbon monoxide. In other words, more of the refined wood gas could pass through a combustion engine and be wasted because there was less oxygen available prior to combustion.

Removing Hydrogen Sulphide

Natural gas contains appreciable amounts of hydrogen sulphide, which is poisonous to human health and the natural environment. Therefore, finding new and efficient methods of removing hydrogen sulphide from natural gas is worthwhile. Other research teams have previously published work demonstrating the potential use of bentonite as an adsorbent of sulphur-containing compounds. Following similar lines of inquiry, Dr



Lasich conducted a computational study to find out how well bentonite can adsorb hydrogen sulphide from a natural gas-like mixture. In particular, he explored different bentonite-based materials to find one with a high affinity for hydrogen sulphide and a low affinity for other molecules found in natural gas.

One way in which researchers can modify materials is through a process known as 'doping'. With doping, materials are coated or impregnated with small quantities of a certain element – referred to as the 'dopant'. The inclusion of dopants in bentonite changes how the surface of the adsorbent responds to nearby gas molecules and subsequently, how readily gases are adsorbed.

Dr Lasich conducted a study to investigate the utility of bentonite doped with metal ions, applying conditions that mimic the typical composition of natural gas: carbon dioxide, methane, nitrogen, ethane and hydrogen sulphide. Dr Lasich performed simulations to find out how well the gas molecules adsorb to bentonite doped with either lithium, sodium or potassium atoms.

According to Dr Lasich's results, only methane, hydrogen sulphide and nitrogen adsorbed to the doped bentonite. Furthermore, he found that hydrogen sulphide adsorbs very strongly compared to methane or nitrogen. This result is encouraging because it shows that bentonite is far more selective to hydrogen sulphide compared to all other molecules present in a typical natural gas mixture.

Upon further investigating the results, Dr Lasich found that the extent of adsorption depends on the physical size of the dopant atoms and the nature of the forces of attraction between the adsorbed gas molecules and the surface of the doped bentonite. His research shows that potassium, the largest of the three elements used as dopants, yielded the strongest interaction, and that hydrogen sulphide, the heaviest gas adsorbed, also formed the strongest interactions. These data all support the idea that large molecules and atoms tend to form the strongest interactions.

Considering the overall results of the study, the dopant that possesses the greatest ability for removing hydrogen sulphide is potassium, followed by lithium and then sodium.

Future Technologies

Dr Lasich plans to further his research on many fronts. For example, he hopes to improve 'carbon capture' methods, where carbon dioxide is removed from flue gas before it is released into the atmosphere. As carbon dioxide is the primary driver of global climate change, this technology would have profound implications for climate change mitigation. There are also many other minerals to explore, some of which could perform equally well or better when compared to bentonite.

As the global demand for energy increases, more efforts will be required to identify efficient sources of energy that can be used by disadvantaged rural communities, with reduced impact on the environment. In this search for clean and equitable energy, the research contributions of Dr Lasich will no doubt prove invaluable.

Meet the researcher

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Dr Matthew Lasich received his PhD in Chemical Engineering in 2015 at the University of KwaZulu-Natal in South Africa, after which he continued his research with a two-year postdoctoral position. During his PhD studies, Dr Lasich also worked as a visiting researcher at the University of Paderborn in Germany. In 2017, he moved to Mangosuthu University of Technology in South Africa to take up his new role as a Lecturer of Chemical Engineering, and co-founding the Thermodynamics, Materials and Separations Research Group before being promoted to Senior Lecturer in 2020. Dr Lasich is an Affiliate Member of the South African Institution of Chemical Engineers, a Member of the Golden Key Honours Society and an Affiliate Member of the Institution of Chemical Engineers.

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FUNDING

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SMALL BUT MIGHTY: GAME-CHANGING NANOPORE RESEARCH

The far-reaching benefits of nanopore research encompass fields as diverse as physics, healthcare, big data processing and environmental studies. At the University of Illinois at Urbana-Champaign, **Dr Jean-Pierre Leburton** is conducting research focused on the use of nanopores in ultrathin solid-state molecular materials, such as graphene and 2D transition-metal dichalcogenides, for DNA sensing applications. This offers a low-cost and highly effective method of identifying biomolecules, and could have widespread medical applications, enabling rapid, early and effective disease diagnosis and prompting effective treatment, as well as providing invaluable technologies for assisting with DNA sequencing.

Nanopore-Based Biosensing

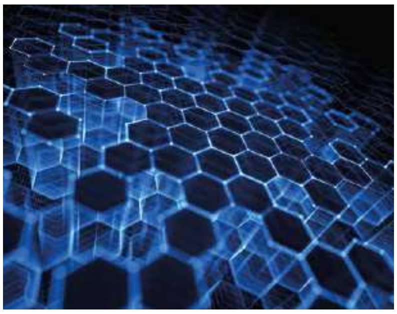
Nanopores are tiny holes with huge potential. They can be created in both biological materials, such as a lipid membrane, and 'solid-state' materials, including silicon nitride, graphene and transition-metal dichalcogenides (TMD) – and both types have a wealth of possible uses. One important application that has garnered attention in recent years is nanopore-based biosensing.

This technology involves a nanopore that connects two structures containing saline solution. A current made up of salt ions is passed through the nanopore, and when a biological molecule passes through, it causes alterations in the ionic conductivity, which can be measured as a change in current. These changes in current can then be used to identify molecules.

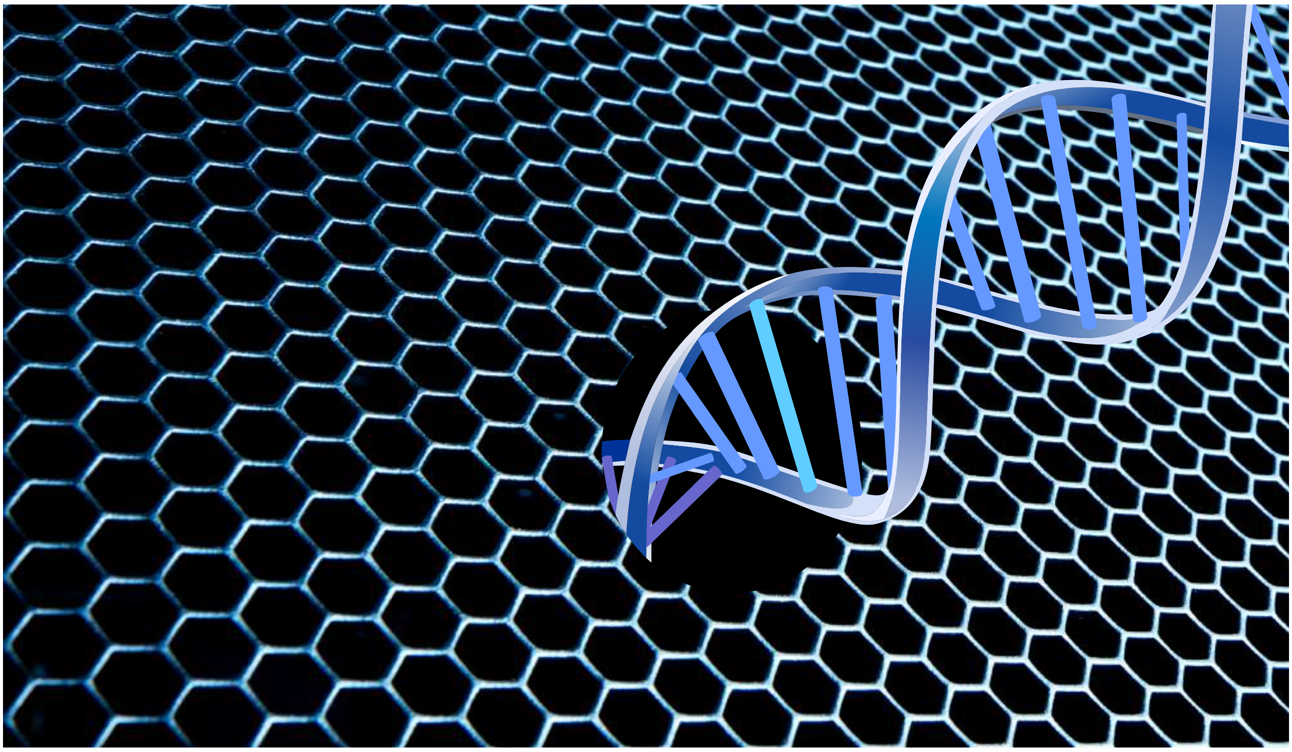
For example, each nucleotide on a DNA strand causes a specific change that can be used to identify that specific nucleotide, towards building a picture of the complete DNA strand. Thus, nanopore-based biosensing could represent a promising technology for DNA sequencing, which is used in a range of crucial applications – from assessing a patient's risk of genetic disease, to monitoring mutations in SARS-CoV-2, the virus that causes COVID-19.

Not only could nanopore-based biosensing be used for DNA sequencing, but it could also represent a low-cost method for detecting changes or damages in DNA strands that could indicate the development of a disease, such as cancer. This could be extremely beneficial in healthcare, allowing the early signs of a particular disease to be rapidly and accurately detected, and enabling clinicians to provide early treatment, leading to far better outcomes for patients.

Biological nanopores possess several significant limitations, including their set pore diameter and their sensitivity to experimental environments. Therefore, solid-state nanopores are a burgeoning area of research, as their pore dimensions can be tuned, and being more robust, they can be utilised across a range of different experimental conditions.



Graphene and TMD are particularly promising two dimensional (2D) solid-state nanomaterials, as they are ultrathin and boast favourable electrical and mechanical properties. These features make graphene and TMD nanopores well suited to DNA detection and sequencing. The use of graphene and TMD nanopores is one area of research conducted by Dr Jean-Pierre Leburton and his colleagues, who are based at the University of Illinois at Urbana-Champaign, USA.



Innovations with Cross-Disciplinary Impacts

Dr Leburton and his team are engaged in a range of interrelated projects involving 2D solid-state nanopores, quantum point contact transistors for DNA sensing and multipore systems. As well as pushing forward the envelope in physics, the team's impressive body of work could have important benefits for healthcare research, including the advancement of DNA sensing, which would have a profound impact on disease diagnosis and treatment.

The central idea of Dr Leburton's research is to shape 2D membranes into a ribbon around the nanopore, and take advantage of the material's semiconducting properties to flow an electronic current along the ribbon and detect the presence of DNA in the pore.

In a study entitled 'Graphene quantum point contact transistor for DNA sensing', Dr Leburton and his colleagues designed a device made from a 2D nanoscale semiconductor material that can be used to enhance DNA identification with nanopores. The team's highly-responsive graphene-based DNA sensing device is not only able to identify DNA, but can also control the molecules that pass through the nanopores. The researchers were able to demonstrate the device's ability to alter the electrical conductance of graphene nanopores, and to adjust their sensitivity to external charges to improve the accuracy of measurements.

In addition to being able to optimise detection sensitivity, the device also has the ability to control the motion and speed of the DNA strands that pass through the nanopore, which sets it apart from existing technologies. This innovation breaks boundaries by providing the ability to slow down the movement of DNA, allowing for accurate DNA sequencing.

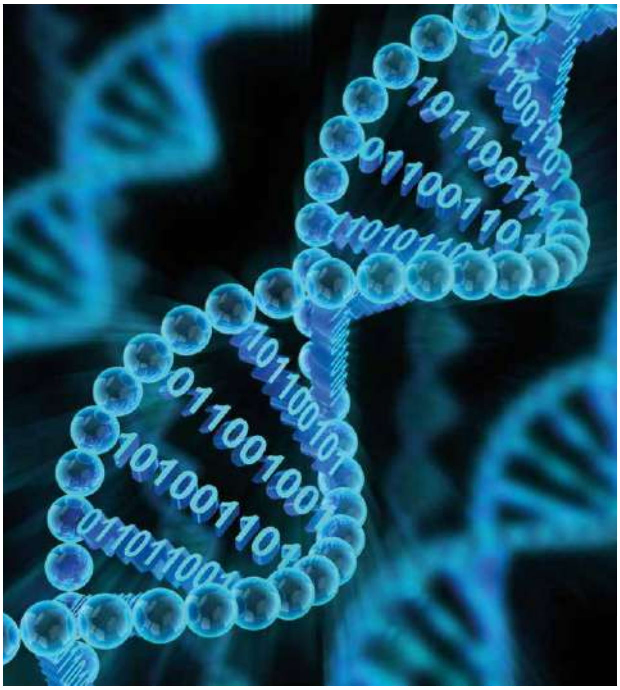
Ultimately, the rapid detection of molecules facilitated by the device could prove extremely useful in genome sequencing, in addition to early disease detection. In a subsequent study, Dr Leburton indicated that his paradigm of electronic detection offers the tremendous advantage of parallelism in biomolecule detection compared to the conventional 'ionic current blocking' approach, and could be easily and effectively integrated with semiconductor electronics for amplification and data processing, further enhancing its potential.

Detecting DNA Methylation

In a recent study, entitled 'Detection and mapping of DNA methylation with 2D material nanopores', Dr Leburton and his colleagues highlighted how they were able to detect and locate methylated DNA using nanopore sensors made of graphene or molybdenum di-sulphide (MoS_2).

Methylated DNA is a DNA molecule that contains a methyl group – a carbon atom bonded to three hydrogen atoms. Changes in DNA methylation can occur in the early stages of disease development, including cancers. Therefore, measuring these changes could allow clinicians to detect cancers and other diseases earlier, allowing them to provide much more effective treatment.

The reason that Dr Leburton and his colleagues decided to use graphene and MoS_2 when fabricating their nanopore membranes is because of their excellent physical and electrical properties. Hence, these materials allow the team to build solid-state nanopores that



overcome the limitations typically encountered with biological nanopores.

In their sensing technique, Dr Leburton and his team labelled DNA methylation sites with a protein called MBD1. The researchers then allowed methylated DNA strands to pass through the nanopores in their graphene or MoS_2 membranes. By monitoring changes in electrical current passing along the membrane, they were able to locate the methyl groups at different positions on the strands.

This innovative work indicates the possibility of using solid-state nanopore membranes to efficiently locate the sites of methylation along a strand of DNA. In addition to detecting diseases through changes in DNA methylation, these nanopore membranes could also be used in other areas, including DNA barcoding, which can be used to identify different species in the environment. Identifying the species present in a given ecosystem is invaluable for monitoring biodiversity, and allows for the design of more effective conservation strategies.

DNA Damage Detection for Disease Diagnosis

In another study, Dr Leburton and his collaborators used nanopores to detect and map DNA damages. Again, they made use of graphene and MoS_2 nanopore membranes, and were able to sense minute changes in the structure of DNA passing through the nanopore by measuring the current.

This is important research, given that damages or breaks (also called nicks) on double-stranded DNA can lead to a range of diseases, including cancers. Rather counterintuitively, chemotherapy and radiation therapy used in the treatment of cancer can also cause DNA damages, potentially leading to the development of further tumours. In both of these cases, the ability to detect DNA damages early on is vital for improving patient outcomes.

Using computational modelling techniques, Dr Leburton and the team were able to illustrate the ability of their device to detect structural changes in DNA strands, and identify the precise location of these changes along each strand. They also explained the interactions that can occur between different types of DNA nicks.

The researchers believe that this research could help enhance our understanding of nicks on DNA and their impact on cell activities. Additionally, there is potential for this research to contribute to the regulation of chemotherapeutic drugs and radiation dosage in the treatment of cancer. Outside of this, the work could contribute to further applications such as DNA data storage for computation.

Versatile Devices with Various Applications

In a later study entitled ‘Classification of Epigenetic Biomarkers with Atomically Thin Nanopores’, Dr Leburton and his team combined the use of molecular and device simulations with statistical signal processing algorithms to present a versatile and generally applicable biosensor technology.

The technology again uses a 2D solid-state nanopore membrane for the detection of several different types of biomolecules, in real time, based on their unique electrical current alterations. Because of its versatility, the technology can be adapted and applied to detect a range of different biomolecules and changes in DNA.

In this work, the team was able to successfully establish the impressive detection resolution of the device and its ability to conduct measurements of DNA strands through multiple different channels simultaneously.

Dr Leburton and his colleagues’ interrelated investigations make up an impressive body of research that has the potential to be powerfully impactful in myriad fields, including big data collection and processing, physics, electronics, healthcare and environmental studies. Their work provides a tangible example of seamless crossover between disciplines, with an expert in physics, with particular knowledge in electrical and computer engineering, breaking boundaries in seemingly disparate fields.

Not only has he presented promising new technologies that could facilitate low-cost and highly effective DNA sequencing, which is a crucial process for getting to the heart of DNA and understanding the make-up of the human body, his devices could save lives by enabling diseases to be detected early on, leading to optimal treatment. Fittingly for an electrical engineering scientist, Dr Leburton is making waves, not just in physics but far beyond.

Meet the researcher

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Professor Jean-Pierre Leburton received his PhD from the University of Liege, Belgium, in 1978. He joined the University of Illinois, USA, in 1981, having previously worked as a research scientist at the Siemens A.G. Research Laboratory in Munich, Germany. He held the Hitachi LTD Chair on Quantum Materials at the University of Tokyo, Japan, in 1992 and was a Visiting Professor in the Federal Polytechnic Institute in Lausanne, Switzerland in 2000. He is currently the Gregory Stillman Professor of Electrical and Computer Engineering at the University of Illinois at Urbana-Champaign and Adjunct Professor at the University of Illinois in Chicago. His research interests are non-linear transport in quantum wires and carbon nanotubes, spintronics and molecular and bio-nanoelectronics, and he is author and co-author of more than 300 research papers in international journals, and of several patents in device electronics. Professor Leburton is the recipient of numerous high-level awards, including the 2004 ISCS Quantum Device Award, the Gold medal for scientific achievement by the Alumnus Association of the University of Liège, Belgium (2004), the CCMR Serendipity Award, Seoul Korea (2019), and the 2021 IEEE Nanotechnology Council Pioneer Award. He is also an associated member of the Royal Academy of Science of Belgium.

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ILLINOIS

THE THINNEST OF MATERIALS MAY HOLD A CURE FOR OSTEOARTHRITIS

Since the turn of the century, a myriad of exciting applications for graphene have emerged. Amongst the most exciting might be its use as a scaffold for promoting tissue growth in the treatment of various medical conditions, including osteoarthritis. Researchers at Boise State University in the USA and Carl von Ossietzky University of Oldenburg in Germany are gaining a greater understanding of the interactions between graphene and cells, towards the development of implantable graphene-based devices that can rebuild damaged tissue.

Crippling Osteoarthritis

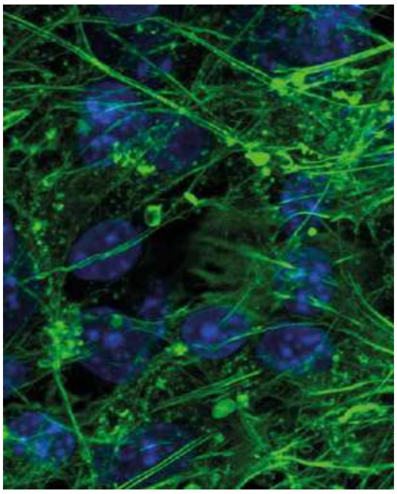
Osteoarthritis is a debilitating musculoskeletal disorder of the bones, muscles and connective tissues that results from the breakdown of cartilage tissue in joints. The resulting pain that accompanies osteoarthritis can be crippling – reducing the quality of life for those afflicted with the disease.

Affecting almost 250 million people worldwide, osteoarthritis is the most common form of arthritis, and can result in significant disability. In the US, the condition affects 50% of the population over the age of 65. Given that between 2015 and 2050, the proportion of the world's population over 65 years of age will almost double, the World Health Organization has categorised osteoarthritis as a priority disease in urgent need of new therapies. Currently, there is no cure for osteoarthritis; instead, most therapies simply alleviate symptoms.

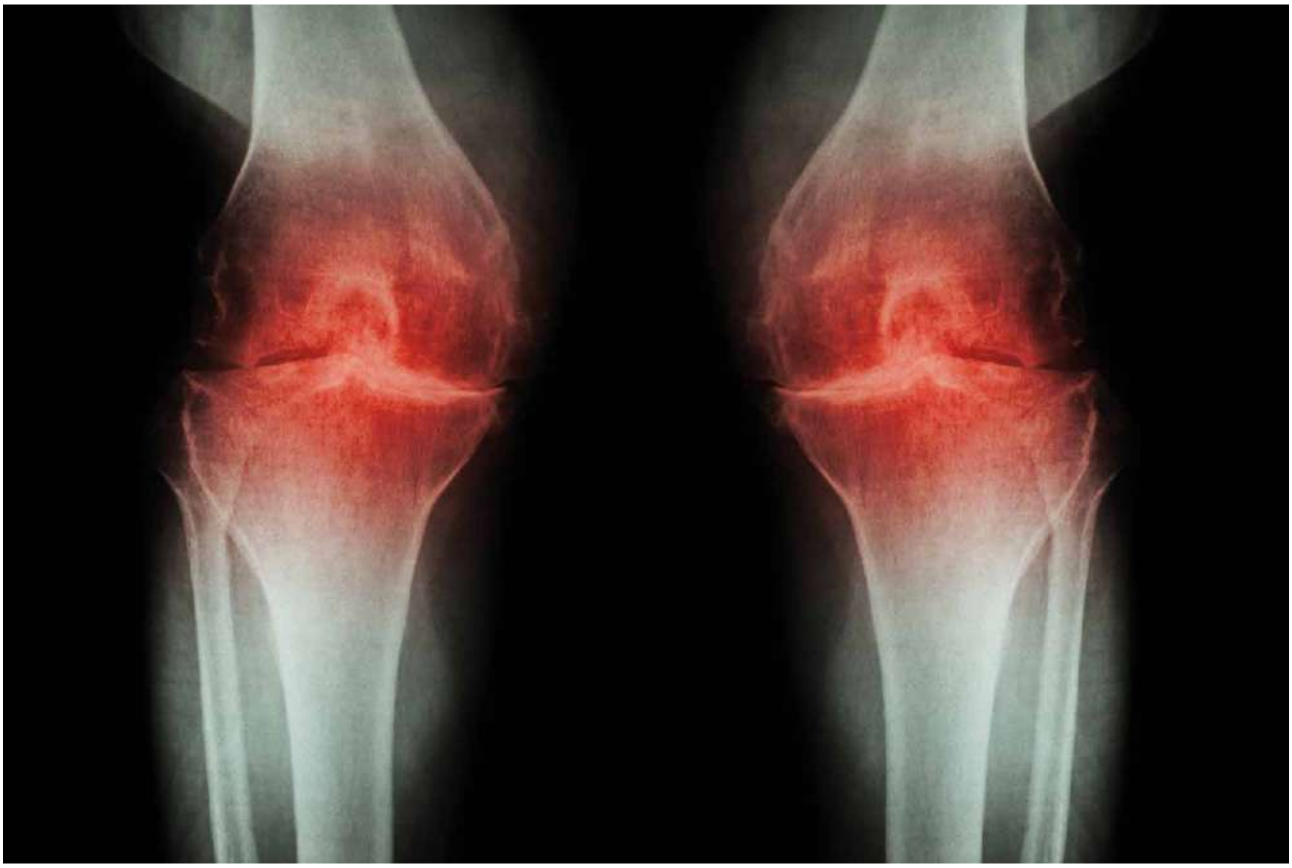
Tissue Engineering

Applying principles from engineering and life sciences, tissue engineering involves the development of biological substitutes that can repair damaged tissue. This exciting field often involves the use of materials called 'bioscaffolds', which can be seeded with cells and implanted into the body to regenerate an area of damaged or lost tissue. Stem cells are special cells that have the ability to develop into many different types of tissue, such as cartilage. Combining stem cells and bioscaffolds represents a promising method to replace the cartilage lost due to osteoarthritis.

A well designed bioscaffold can encourage stem cells to develop, or 'differentiate', into the type of tissue required for the desired application. In the case of osteoarthritis treatment, a bioscaffold should provide a conducive environment to promote the development of cartilage-producing cells, and ultimately, functional musculoskeletal tissue.



There are various different environmental factors that determine the type of tissue that stem cells will develop into. Therefore, scientists are trying to understand the effects of these chemical, physical and mechanical factors on cells, so that they can be tuned to create an ideal environment that encourages the formation of a particular tissue type.



The Potential of Graphene

Graphene is a single layer of carbon atoms arranged in a two-dimensional hexagonal crystal structure, which has exceptional strength and conductive properties. These characteristics have led to its use in many different fields including electronics and energy, but its application in tissue engineering has yet to be fully exploited.

With the potential to communicate electrically and mechanically with adhered stem cells, graphene represents a unique bioscaffold material. Under the right conditions, graphene has been shown to encourage stem cells to differentiate into cartilage tissue. Therefore, it could play a vital role in regenerating damaged or lost cartilage tissue in osteoarthritis patients.

Dr David Estrada and Dr Julia Oxford at Boise State University, USA, and Dr Solov'yov at Carl von Ossietzky University in Oldenburg, Germany are studying the influence of this material on stem cells under a broad range of conditions, towards the development of optimised bioscaffolds for regenerating damaged tissue, including cartilage.

Uncovering the fundamental interactions between graphene and stem cell biology requires interdisciplinary knowledge and expertise, which is why these three researchers have combined forces. With Dr Solov'yov's interest in biological processes, Dr Estrada's extensive experience in graphene research and Dr Oxford's track record in advancing stem cell biology, the team is perfectly equipped to make great advances in this area.

Graphene Foam

Recently, the researchers have become particularly interested in a porous, three-dimensional form of graphene known as graphene foam. Its flexibility and conductive properties make it suitable for helping nerve cells transmit information, while its three-dimensional porous nature means that many cells can be seeded throughout the material's structure.

The team has been investigating whether it is possible to adhere a patient's own stem cells to a graphene foam scaffold, and then insert this material into the body to repair and regenerate cartilage tissue. Graphene foam's exceptional flexibility and strength make it ideal for this application, because cartilage in joints must regularly dissipate high-impact forces.

Before the research team's investigations, little had been reported about the mechanical properties of graphene foam with adhered cells under dynamic compressive forces. Likewise, the use of graphene foam as a three-dimensional scaffold needed examination, so the researchers began by assessing stem cell attachment, and subsequent cell differentiation under different conditions. After first demonstrating that graphene foam could be used to grow muscle tissue, they built bioscaffolds by mixing graphene foam with animal cells and tested their mechanical properties.

After measuring the elastic and viscous characteristics of these bioscaffolds under deformation, the researchers were able to determine the cellular contribution to the mechanical strength and elastic properties of the composites, as well as concluding that cartilage-producing cells were viable on graphene foam.

Combining the Micro with the Nano

Another aspect of three-dimensional graphene foam scaffolds is their potential to combine micro-scale material and nano-scale molecular properties. In particular, the team evaluated the impact of these combinations on cell attachment and cell morphology.

The researchers achieved this by coating graphene foam with a protein called fibronectin before growing stem cells within the scaffold. They found that the fibronectin coating increased the elastic strength of the scaffold, predominantly through interactions between the graphene and the protein, which also alters the cellular response to graphene foam. The team found that their modified scaffold provided an environment conducive to creating early-stage cartilage formation.

Selecting appropriate molecular modifications for scaffold materials can be key for ultimately growing a particular tissue type, such as cartilage, as this is regulated by a combination of the molecular and material properties of the underlying scaffold. In other words, the nature of the proteins used to modify scaffolds must be considered carefully.

Improving Fundamental Understanding

The research to date has been encouraging, but a more fundamental understanding of the chemical and physical interactions between graphene and stem cells that promote tissue development is still needed, in order to optimise a potential graphene foam scaffold for osteoarthritis patients.

Towards this aim, Dr Oxford, Dr Estrada and Solov'yov are embarking on a major project funded by the US National Science Foundation, entitled 'Graphene as a Bioscaffold for Musculoskeletal Tissue Engineering'. Through this project, the team aims to modulate the electrical, thermal and mechanical properties of graphene foam in just the right way to guide and differentiate stem cells into musculoskeletal tissue that will rebuild cartilage.

First of all, the researchers plan to explore the effects of graphene's electrical voltage on the growth of stem cells, and their differentiation into musculoskeletal tissue. By heating graphene to different temperatures, they also plan to study how temperature influences stem cell behaviour. The third aspect of graphene that they plan to investigate is its mechanical stiffness, which can be modulated during the manufacturing process. Once these studies have been conducted, the team hopes to achieve a complete dataset that will reveal the effects of graphene's physical properties on the behaviour and differentiation of stem cells.

The researchers are also planning to investigate different methods of fabricating graphene, to obtain variations in the material's structure. Preliminary data have shown that structural changes significantly impact graphene's performance as a bioscaffold in terms of cell growth and differentiation. The team plans to utilise various fabrication methods, including inkjet printing, chemical vapor deposition, and sublimation of silicon from silicon carbide wafers, to create a range of different graphene films with varying structures and properties. They aim to pay particular attention to tuning the surface roughness of the material, as this property is known to affect cell behaviour.

As the abovementioned preliminary experiments will utilise two-dimensional graphene, the next part of the team's project will extend their results to three-dimensional graphene foam, where softness, porosity and pore shape are related factors that are known to play key roles in helping cells to adhere to bioscaffolds. Like their work with two-dimensional graphene, they aim to modulate the various characteristics of graphene foam to identify an optimum set of properties that will encourage the growth of stem cells and their differentiation into cartilage tissue.

Disruptive Devices

Until now, symptomatic relief – or in extreme cases, complete joint replacement – has been the only viable therapeutic option for osteoarthritis sufferers. Repairing damaged cartilage has always been challenging in regenerative medicine, due in part, to the limited ability for cartilage to heal. Implantable graphene-based biomedical devices may hold the key to revolutionising tissue engineering as a viable therapy for those suffering from osteoarthritis. There can be little doubt that Ds Estrada, Dr Oxford and Dr Solov'yov sit at the vanguard of this future breakthrough.

Meet the researchers

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Having gained a PhD in 2013 from University of Illinois at Urbana-Champaign, Professor David Estrada subsequently went on to hold several Associate Professorships within Boise State University, including at the Micron School of Materials Science and Engineering and Center for Advanced Energy Studies. Currently, he is also Advanced Manufacturing Deputy Director of Academic Research at Idaho National Laboratory. Professor Estrada's research output has realised the filing of more than 6 patent applications on topics ranging from nanoparticle inks to printed graphene-based biosensors.

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Professor Julia Thom Oxford gained her PhD in Biochemistry and Biophysics at Washington State University in 1986. She is currently Distinguished Professor in the Department of Biological Sciences of Boise State University, where she holds the Stueckle Endowed Chair, as well as being Director of the Center of Biomedical Research Excellence in Matrix Biology and Director of the Biomolecular Research Center. Over the course of her successful research career, Professor Oxford has been awarded in excess of $40 million in grant funding. In addition to her tissue engineering research, she is also passionate about cultivating the next generation of STEM professionals, supervising numerous student research projects and teaching an array of different biology and chemistry courses.

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Professor Solov'yov graduated with a PhD in Physics from Johann Wolfgang Goethe University, Germany, in 2008. After conducting postdoctoral research at University of Illinois at Urbana-Champaign in the US, he worked as an Associate Professor at the University of Southern Denmark between 2014 and 2019. He currently works as Professor of Physics at Carl von Ossietzky University in Germany, where his research interests cover a broad range of areas relating to biomolecules and smart inorganic materials. He has published over 120 research articles, and is currently an Academic Editor for the journal *Scientific Reports*, which is published by the Nature Publishing Group.

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National Science Foundation #0923535 Mass Spectrometry
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PEROVSKITE-BASED SENSORS: DETECTING ENERGETIC PHOTONS WITH EXTREME SENSITIVITY

Organo-metallic perovskite crystals are widely known for their ability to boost the performance of solar cells, with efficiencies reaching 25% and beyond. This is because photons of light can mobilise electrons in these materials with very high efficiency. **Professor László Forró** and his team at Ecole Polytechnique Fédérale de Lausanne have realised that this same ability could be harnessed in the development of high-performance sensors that detect photons of various energies. By integrating perovskite with graphene or carbon nanotubes, the team's detectors show outstanding sensitivity, with the ability to detect single photons. Their technologies are leading to new applications ranging from more sensitive medical diagnostics, to safer nuclear reactors.

Perovskites

Solar cells have made their way to the forefront of public discussion in recent years. With its ability to convert the energy contained in photons of sunlight into useable electrical currents, the technology promises to play an increasingly important role in renewable energy generation in the coming years. However, even the most advanced solar cells available today continue to face shortcomings relating to their efficiency. Although physical processes limit the efficiency of solar cells to 33.7% – with some energy inevitably being converted into unusable heat – the light-to-electricity conversion efficiencies of solar cells have remained particularly low, until recently.

Today, rapid improvements are being made to solar cell efficiencies, thanks to a special family of minerals named 'perovskites'. Featuring particular arrangements of atoms in orderly crystal lattices, these materials are both easy and inexpensive to manufacture, and are known to strongly absorb light across a broad range of frequencies contained within sunlight. As a result, they have enabled researchers to increase the efficiencies of some commercially available solar cells by over 25% in the past decade – promising a bright future for the industry. For Professor László Forró at the Swiss Federal Institute of Technology Lausanne, these exciting advances are only the beginning of perovskite's full potential.

Growing Sensitive Nanowires

While perovskite is already a highly advanced material, Professor Forró and his colleagues proposed in their earlier research that its efficiency could be raised even further if it were manufactured in the form of wires just a few nanometres in width. At first, they manufactured these so-called nanowires using a 'slip-coating' method, whereby a perovskite solution is confined between two surfaces which slide in opposite directions.

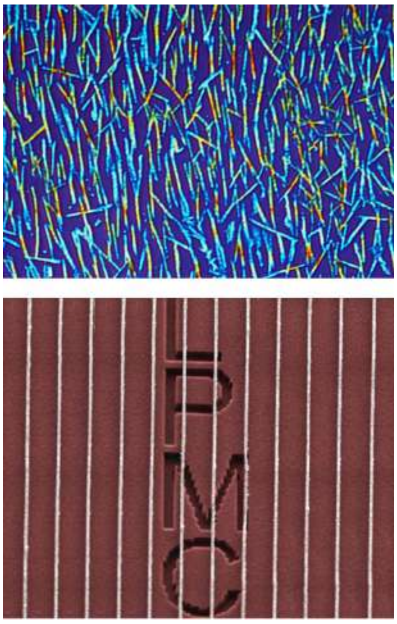

Figure 1: Nanowires grown by slip-coating (top) and in lithographic channels (bottom). Typical lateral dimensions are in the 10–500 nm range.

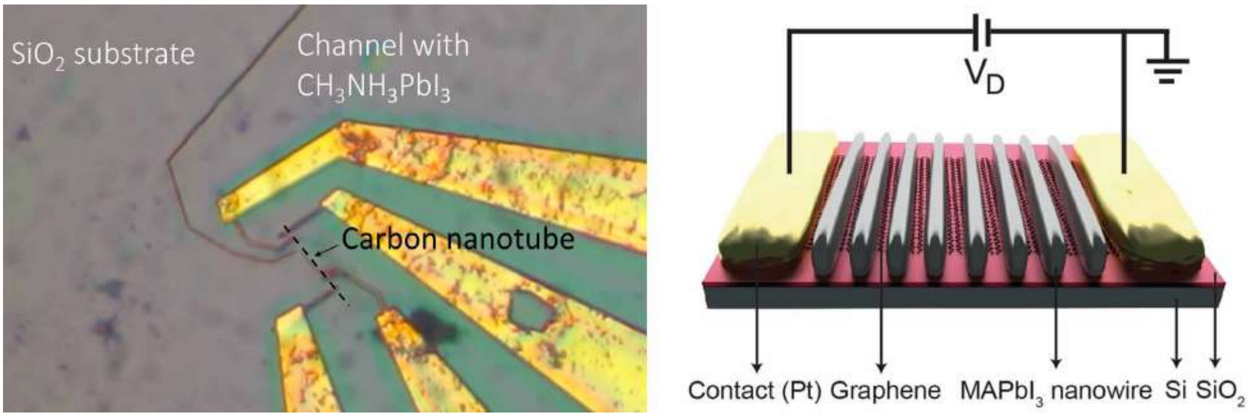

Figure 2: Photon detector comprising single carbon nanotubes and perovskite nanowires (left). Supersensitive photon detector based on graphene and perovskite nanowires (right).

As the liquid evaporated, the crystal grew out of groups of bonded atoms named 'nucleation centres'. The result was a network of solid wires, which spread out in patterns resembling the seeds of a dandelion (Figure 1; top). The material used by the researchers was a 'lead halide' perovskite – where each unit of the crystal lattice features an atom of lead, and three atoms of a halogen element, such as bromine. Lead halide perovskites are widely known for their excellent ability to convert light into electrical current, meaning each of the team's nanowires could function as a microscopic, highly efficient solar cell.

Following on from their initial studies, Professor Forró and his team members, Pavao Andričević, Endre Horváth, Márton Kollár, Bálint Náfrádi, Gábor Náfrádi and Massimo Spina, showed how nanowire fabrication could be improved further. They did so by etching a series of nano-sized channels into layers of silicon, and then depositing a lead halide solution inside them. Since the liquid could move to fill the channels through the process of capillary action, this gave the researchers far more control over the lengths, widths, and orientations of their nanowires (Figure 1; bottom). This technology already promised to improve the capabilities of perovskite solar cells – but the team's nanowires would soon be surpassed by even more advanced structures.

Boosting Performance with Carbon Nanotubes and Graphene

As research into perovskites was gathering pace, another material that was increasingly grabbing the attention of physicists was graphene. Featuring atom-thick layers of carbon arranged in a honeycomb pattern, the structure of graphene makes it an excellent electrical conductor. By introducing other materials to the carbon honeycomb, its electrical properties can be improved even further. In addition, graphene can be 'rolled' into thin cylinders, creating structures named carbon nanotubes – which possess their own unique electrical properties.

Professor Forró's team showed how lead halide perovskite nanowires could be grown directly on the surfaces of carbon nanotubes or graphene (Figure 2). As photons of light interact with the perovskite, the electrons they contained jumped into higher energy levels, leaving behind positively-charged 'holes', which behave like particles in themselves. Afterwards, these holes and electrons could be rapidly transferred to the carbon nanotubes or graphene – amplifying the electrical signal produced by the perovskite.

Working together, the perovskite material with nanotubes or graphene can convert the energy contained in photons into electrical current with extremely high efficiency. Their combined properties make them around ten-million times more responsive to light – producing detectable currents from a single photon. In addition, the setup could operate over a wide region of the electromagnetic spectrum: from ultraviolet to red light. Immediately, the benefits of these materials to detector technologies were clear.

In a similar study, the team grew perovskite onto the surfaces of vertically-aligned 'forests' of carbon nanotubes (Figure 3). 'The perovskite engulfs the carbon nanotubes, providing an excellent interface between these two materials,' explains Professor Forró.

His team now hopes to investigate whether their carbon nanotube forests could be used to create high-performing solar cells. 'For photodetectors this technology works perfectly, and it remains to be seen whether it could be expanded to solar panels,' says Professor Forró.

Harvesting Energy from X-rays

X-rays carry far more energy in their photons than visible light, which could in theory produce stronger electrical currents if successfully absorbed by perovskite materials. Unfortunately, however, these photons cannot be easily harvested using existing solar cells. After prolonged exposure to x-rays, the crystal structures of these materials will instead become

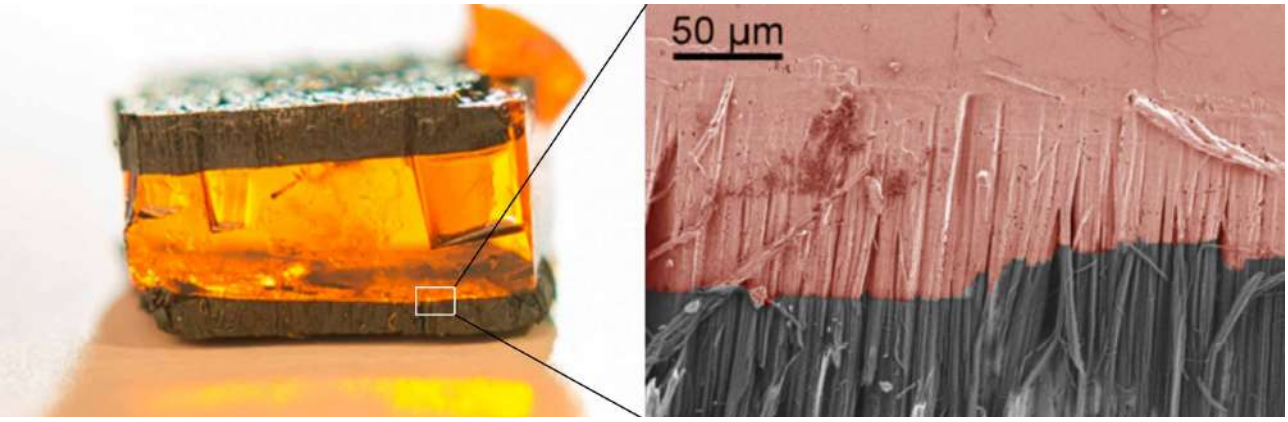

Figure 3: Perovskite crystal with carbon nanotube 'forest' electrodes at both sides (left). Magnification of the interface, showing that the perovskite material (coloured) engulfs the vertically aligned forest of carbon nanotubes, creating a perfect contact (right).

damaged, diminishing their ability to convert further incoming photons. So far, this has meant that x-rays needed to be prevented from reaching solar cells, restricting access to a large fraction of the energy radiated by the Sun. Through their research, Professor Forró and his colleagues aimed to alleviate this issue.

This time, the team assessed the properties of a lead halide containing iodine – the heaviest of the four stable halogen elements. Not only does this perovskite possess a high light-to-electricity conversion efficiency – the heavy atomic nuclei it contains can also readily absorb x-ray photons, without sustaining significant damage. Furthermore, the material remains stable over long periods of time, even when exposed to high doses of x-ray radiation.

These properties were clearly promising, but the material alone cannot generate useful electrical currents. Through their latest research, the team has developed a new approach to achieve this goal.

Aerosol-jet Printing

In this study, the researchers used a novel 3D-printing technique named 'aerosol-jet' printing. In this method, a solution containing perovskite in the form of tiny droplets is focused onto specific places on a surface using a jet of nitrogen gas. After being fired from a fine nozzle, the solvent within these droplets will mostly evaporate during flight, and perovskite crystals grow, before being deposited onto the surface of a material called a substrate. This technique enables researchers to deposit materials in highly intricate patterns, such as networks of spirals and pillars (Figure 4; top), onto a wide variety of different substrates. In their study, Professor Forró's team used aerosol-jet printing to deposit their perovskite material in a specific pattern on a graphene substrate.

To maximise the performance of the perovskite, the team printed it out in a grid-like pattern of straight, interlocking lines, featuring tall pillars of material where the lines met. Like with the carbon nanotubes used in their previous studies, the holes produced when electrons were excited by x-rays could then rapidly transfer to the graphene substrate, amplifying the perovskite's electrical signal. Through their experiments, Professor Forró and his colleagues demonstrated an x-ray sensitivity over 10,000 times greater than current state-of-the-art devices. One particularly important application for this technology lies in medical diagnostics.

Safer X-ray Doses

X-rays have long been widely used in medicine, owing to their ability to pass straight through many lower-density materials, including biological tissues, without being absorbed. Crucially, they enable doctors to view higher-density regions inside the body, particularly bone, without the need for invasive operations.

Today, x-rays are used in diagnostic techniques including radiography, fluoroscopy, and CT scans. Unfortunately, however, these processes can expose patients to high amounts of ionising radiation, inducing DNA damage and increasing their risk of developing cancer.

Through access to technologies that are more sensitive to x-rays, doctors would be able to obtain the information they need with far smaller x-ray doses, greatly reducing this risk. Using an aerosol-jet printed perovskite pattern with a highly sensitive detector, x-rays could simply be detected by photocurrent measurements, without the need for a complex electronic set-up.

By encapsulating perovskite layers within a specialised polymer, the researchers demonstrated an advanced detector (Figure 4; bottom), which produced reliable electrical signals from far lower x-ray intensities than those currently used in medicine. At the same time, the device remained stable for over nine months, with no degradation in performance. The

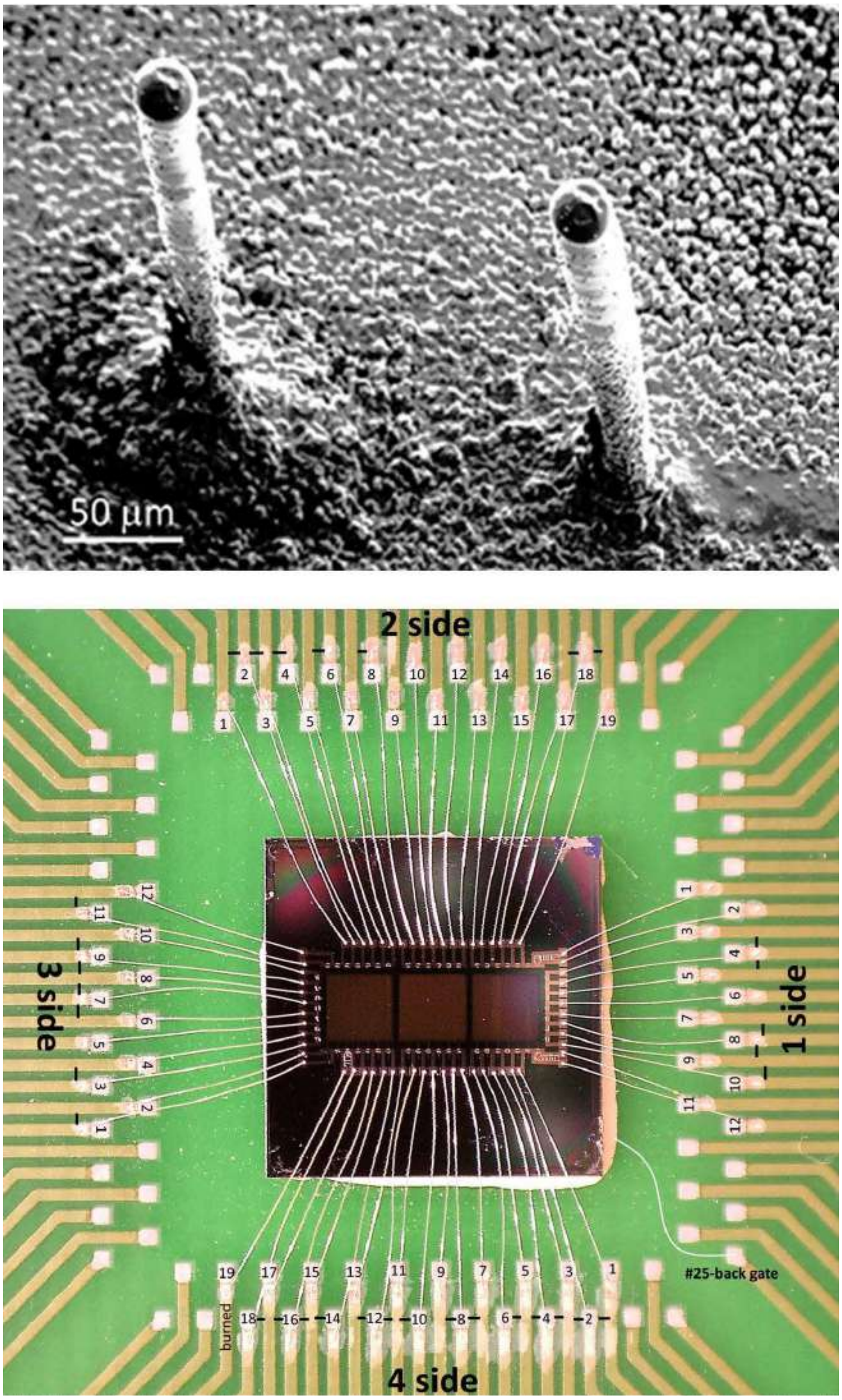

Figure 4: Pillars of perovskite deposited by aerosol jet printing for detecting x-rays (top). Chip for the image plate of the x-ray detector (bottom).

clear success of the team's approach could now open up new routes towards safer x-ray diagnostics, without incurring significant costs for healthcare organisations. This achievement was another victory for the team, but their work was still not done yet.

Kilogram-scale Crystals

Occupying the highest range of energies of all frequencies in the electromagnetic spectrum, gamma rays are released during the decay of highly radioactive atomic nuclei. They can be highly damaging if they come into contact with many materials, particularly biological tissues – creating a crucial need to tightly monitor gamma ray photons wherever they are produced. However, with such high energies, gamma rays are very rarely absorbed even within higher-density materials, passing straight through most crystals, making them incredibly difficult to detect.

In their latest research, Professor Forró's team overcame this issue through a new technique for fabricating perovskites on scales of kilograms. To overcome limitations in the sizes of the crystals – which are typically just millimetres across, the researchers aligned many smaller, cube-shaped crystals side by side. Then, they immersed them in a solution, fusing them seamlessly together.

The result was a single block of perovskite some 3.8 kilograms in mass (Figure 5) – which was by no means an upper limit, with even heavier crystals possible through the fusing of further smaller crystals. Within this highly sensitive block, enough heavy atomic nuclei were present to absorb a fair proportion of incoming gamma ray photons, producing a reliable electrical signal.

Safer Nuclear Reactors

Unlike many previous studies into the capture of gamma rays, Professor Forró and his colleagues are not solely focused on detecting them. Rather, they propose that just like visible light and x-rays, the large amounts of energy they contain could be harvested for practical use. This idea is particularly relevant in nuclear power generation.

With its high energy yield, and complete lack of carbon emissions, many researchers believe that an increased rollout of nuclear power alongside renewable sources will be key to tackling climate change. All the same, due to several catastrophes being triggered by nuclear power plant malfunctions in previous decades, there is still a strong reluctance among governments and the public alike to take these steps.

Although the chances of such malfunctions are now minuscule with present-day technologies, Professor Forró's team proposes that their safety could be improved even further with the ability to harvest the energy of gamma

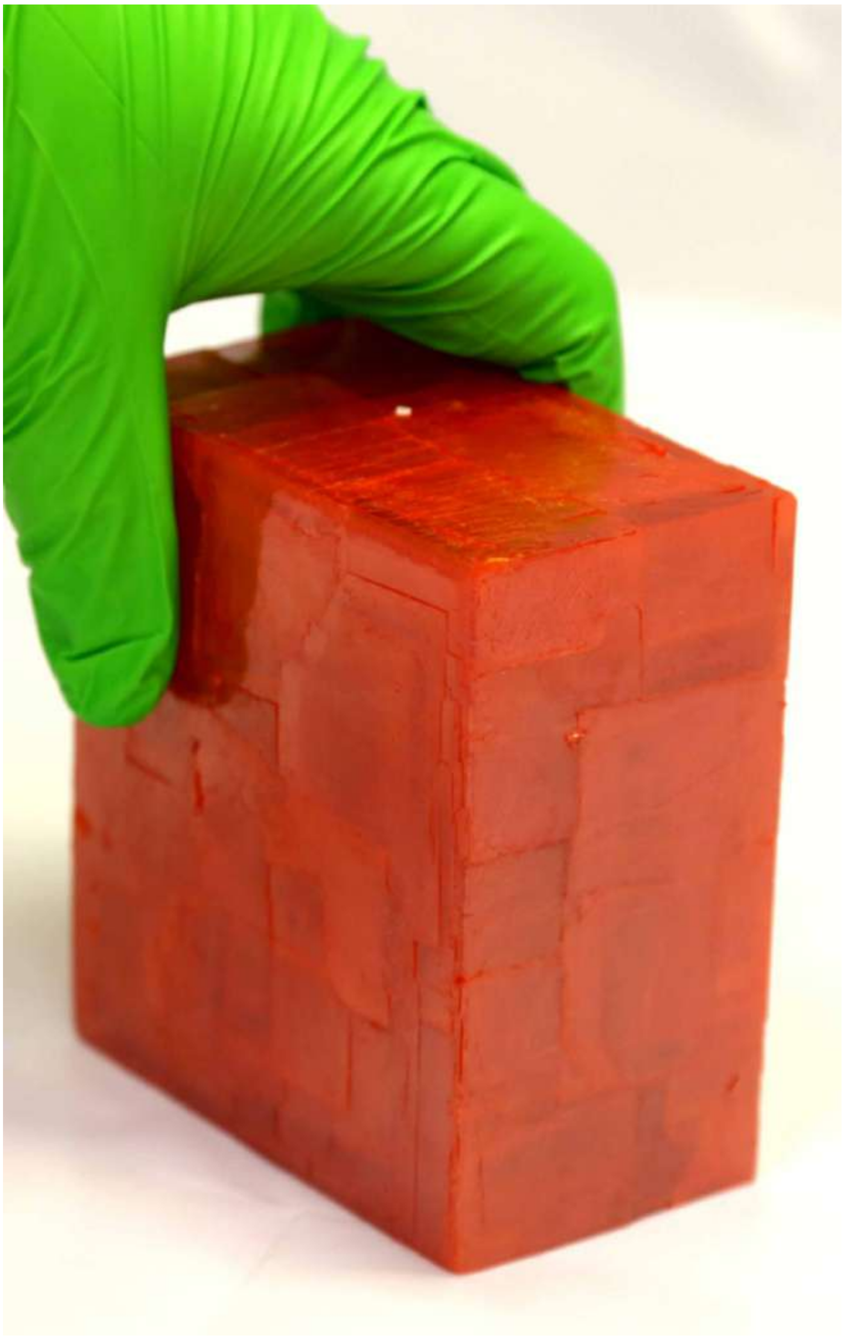

Figure 5: 3.8-kilogram perovskite crystal for gamma ray detection.

rays directly. For example, they propose that the 2011 Fukushima disaster could have been largely prevented, had just 1% of the reactor's remnant gamma radiation been converted into electricity, helping to power the reactor's cooling system. Such conversions could be easily achieved using the team's massive perovskite crystal. By utilising the electrical signals produced as gamma ray photons interact with such a material, their radiation could finally become useful, instead of solely damaging.

Powering Interplanetary Spacecraft

One final promising application of the team's techniques relates to spacecraft undergoing interplanetary voyages. While on Earth's surface, the atmosphere largely protects us from intense x-rays and gamma rays produced by the Sun, any vehicle travelling through outer space will be completely unshielded from this radiation. This is a particular problem for solar cells, which can be crucial power sources for spacecraft undergoing missions spanning many years. Without adequate protection, these devices can steadily diminish in performance over time.

To address the issue, Professor Forró and his colleagues propose that lead halide perovskites can be used to convert high-energy x-ray and gamma ray photons into electrical power in outer space – where sunlight is faint, but cosmic radiation is abundant. Since they absorb these photons very efficiently, they can also protect the delicate parts of the spacecraft. 'It is kind of a miracle, that these perovskite materials withstand high energy radiation, without being damaged,' says Professor Forró.

Through further improvements, their high-durability over long periods of time could make them suitable for use in spacecraft electronics. If integrated onto solar cells, these materials could enable unmanned probes to travel to distant regions of the Solar System in far better condition.

A New Region for Energy Harvesting and Detection

With such a wide array of important applications, Professor Forró's team hopes that through the growth of perovskites on carbon nanotubes, their deposition on graphene substrates through aerosol-jet printing, and the production of massive perovskite blocks, we could soon see widespread use both in research, and in our everyday lives.

For now, the researchers will continue to improve the capabilities of their materials and techniques even further, with the ultimate aim of making them widely available. They also hope to expand their applications into other areas, such as neutron detection. If their goals are achieved, these technologies could lead to the widespread ability to detect and harness photons in the highest-energy regions of the electromagnetic spectrum.

Meet the researcher

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László Forró obtained his BS in physics at Eötvös Loránd University, Budapest, and his MS at Université Paris XI. He then received his PhD from the University of Zagreb in 1985. He was full professor at the Ecole Polytechnique Fédérale de Lausanne, holding the chair of Nanostructures and Novel Electronic Materials. This autumn, he will move to University of Notre Dame (USA), where he will create and direct the Stavropoulos Center for Complex Quantum Matter. Through his work, Professor Forró develops experiment-driven partnerships, with a focus on correlated matter, the design of new nanostructured materials and biological physics. This vision has led him to founding and organising a bi-annual conference in Dubrovnik (http://dubrovnik.epfl.ch/) with the theme: From Solid State to Biophysics. Throughout his career, he has achieved many honours and awards, including the Spiridon Brusina Award of the Croatian Society of Natural Sciences and the Serbian Material Science Society Award. He is also a Doctor Honoris Causa of the University of Szeged and the Technical University of Budapest, and a Member of the Hungarian Academy of Sciences, the Croatian Academy of Sciences, and the Serbian Academy of Sciences.

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A NEW SOLUTION FOR DIRECT LASER WRITING

Direct Laser Writing is a remarkably useful way to deposit intricately patterned materials onto surfaces. So far, however, the range of materials that can be used in the technique has been severely restricted. Now, **Dr Hiroaki Nishiyama** and his team at Yamagata University in Japan introduce an entirely new approach based on the unique properties of nanoparticles when suspended in a silver-based solution. When illuminated with ultra-short laser pulses, the setup can create highly stable patterns with sophisticated nanoscale structures – substantially broadening the range of materials available for use in the technique.

Direct Laser Writing

Direct Laser Writing is a highly versatile technique. It offers a rapid yet simple method for fabricating microscale and even nanoscale devices, without any need for complex setups. It first involves coating a substrate with a specific light-sensitive material, and then illuminating it with laser light at a specific wavelength. Under the right conditions, the atoms of the light-sensitive material become deposited onto the substrate at the point of the laser's focus. By moving this focus across the substrate in specific patterns, researchers can build up a wide variety of desirable structures.

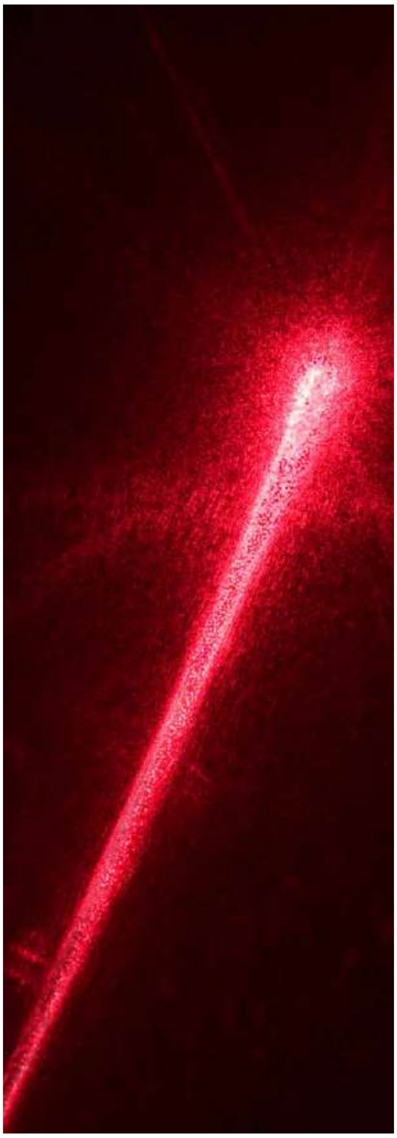
In previous studies, Direct Laser Writing has been applied for fabricating intricate and useful devices in fields as wide-ranging as optics, electronics, fluid dynamics, medicine, and many others.

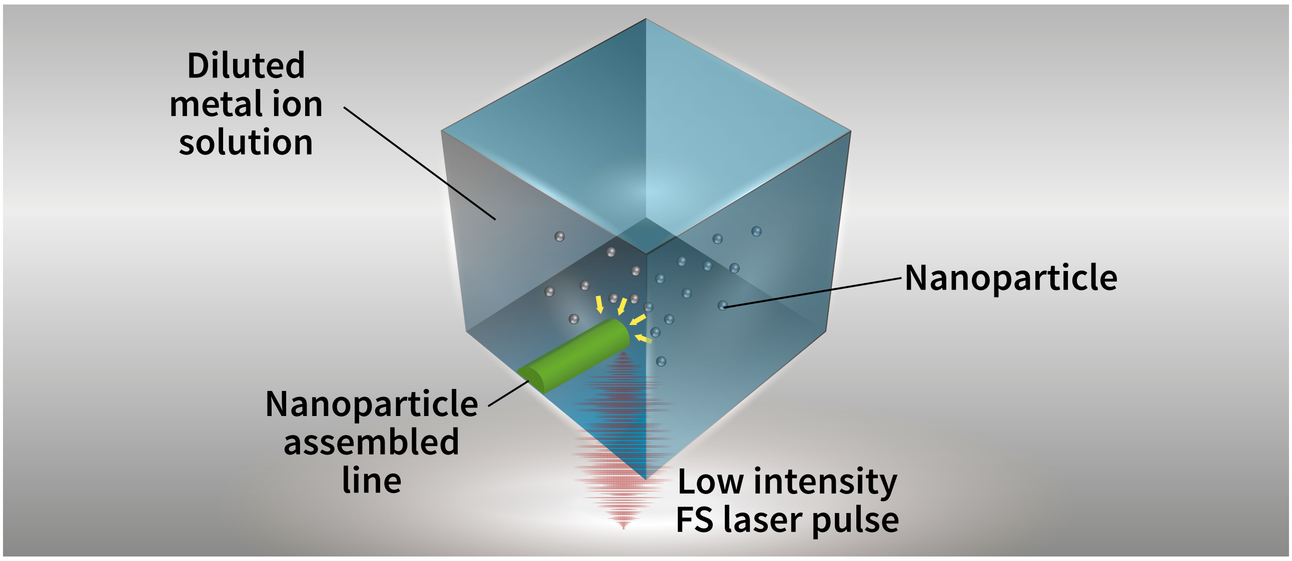
So far, Direct Laser Writing has been achieved using light-sensitive coating materials including those comprising metal nanoparticles, carbon-based materials, and several specific polymers. In one method, silver nanoparticles are added to a specialised resin, which is applied to a substrate. On exposure to light, the nanoparticles aggregate to form microstructures, while the resin decomposes due to the laser-generated heat. Beyond these useful capabilities, however, Direct Laser Writing faces a clear limitation.

Insensitivity to Light

So far, all of the substrate coating materials used in Direct Laser Writing have the specific property of being highly sensitive to light. Unfortunately, the optical responses of many other materials – including many that would be highly desirable in microstructures and nanostructures, are not nearly as strong. This means that they remain virtually unchanged when illuminated by lasers under similar conditions, making them unsuitable for use in Direct Laser Writing.

These shortcomings have severely restricted the range of applications made possible with the technique. As a result, different coating materials will not necessarily display the absorption properties or chemical reactions appropriate for creating the patterns desired by researchers. Overcoming this problem would require appropriate reactions to occur in a far broader range of materials.





Stringent Limitations

In one example, these types of reaction can be achieved using specific laser wavelengths, which happen to be strongly absorbed by certain light-sensitive resins. In previous studies, this effect has been studied using resins that form rigid polymer chains by absorbing two photons at the same time – resulting in sturdy microscopic structures. In one particularly interesting study, researchers constructed a tiny polymer bull, with clearly definable features including horns, legs, and a tail.

However, this technique faces its own limitation. Since most materials are not photosensitive, it is difficult for researchers to give them further functionalities such as semiconducting properties. Ultimately, efforts to expand the application of Direct Laser Writing in this way are hindered by the need for an adequate overlap between appropriate wavelengths of laser light, and suitable levels of light absorption in desirable materials. In the case of highly absorbent materials, laser irradiation can cause surface damages, while in transparent materials, photochemical or thermal reactions won't occur. So far, a lack of clear solutions to this issue has meant that a strategy to overcome the strict limitations in the current selection of useable materials has remained elusive.

Inserting Nanoparticle Solutions

In their recent research, Dr Hiroaki Nishiyama and his colleagues at Yamagata University in Japan have introduced a more sophisticated approach. Their method first involves dispersing nanoparticles of the material required to make a pattern in a diluted silver nitrate solution. Then, they insert the solution onto the surface of the substrate where patterns would be deposited, and illuminate it with laser pulses – each lasting less than one trillionth of a second.

By moving the focus of the laser across the substrate's surface, reactions in the solution enable the team to successfully build up intricately structured patterns, at speeds of up to 0.9 millimetres per second.

In their study, they used three solutions overall: containing nanoparticles of titanium dioxide, silicon dioxide, and iron oxide – each of which has a different sensitivity to light. Using the technique, they drew miniature images including precise spiral patterns, and even wrote out the chemical symbols for silicon (Si), titanium (Ti), and iron (Fe), using each respective element.

'Silicon dioxide is highly transparent, iron oxide has a high absorption, and titanium dioxide is halfway between them; our approach enables us to form micropatterns regardless of absorption strength,' explains Dr Nishiyama.

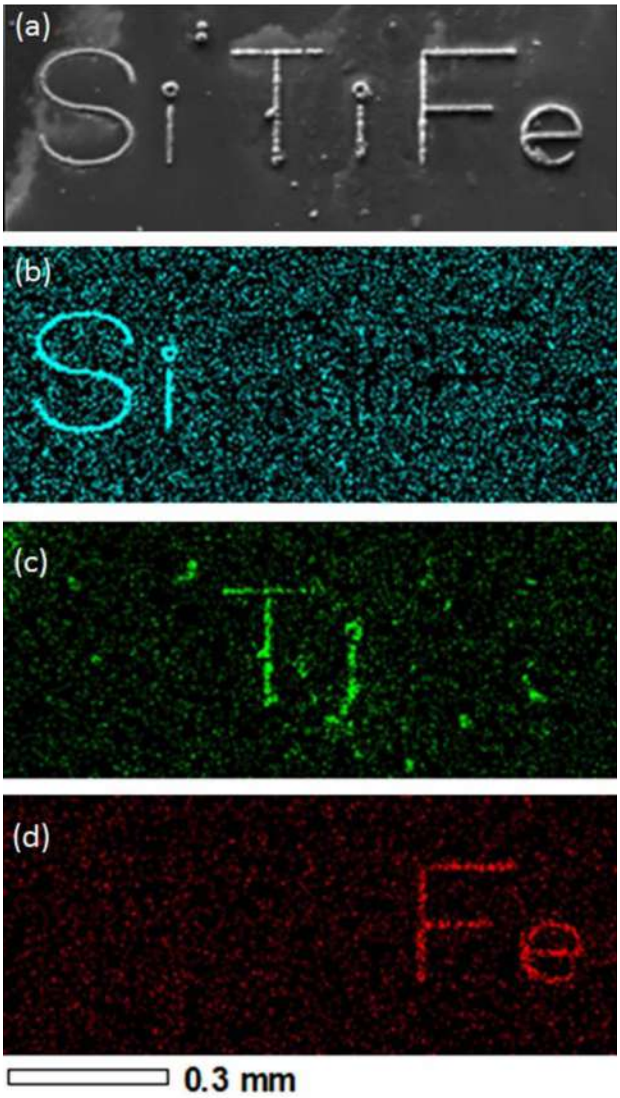
Key to the success of this approach were the intricate arrangements of atoms that formed inside the precipitated lines. To study them, Dr Nishiyama's team transmitted beams of electrons through their semi-circular cross sections. Using a technique named 'Transmission Electron Microscopy' (TEM), they revealed a highly sophisticated structure.

Imaging Cross-sections

Within the TEM images, the researchers identified three distinct regions: an empty void at the centre of the cross-section; a thick clad layer on the outside; and an intermediate layer separating them.

Notably, the clad layer was made up of closely-packed nanoparticles of either silicon dioxide, titanium dioxide, or iron oxide, with other elements only sparsely present. In contrast, the intermediate layer contained characteristic spots of pure silver, but these were surrounded by an abundance of silicon, titanium or iron atoms, along with oxygen. This was a clear example of a 'hierarchical' structure – where the collective properties of many smaller structures create advanced properties in larger-scale, more complex structures.

‘Silicon dioxide is highly transparent, iron oxide has a high absorption, and titanium dioxide is halfway between them; our approach enables us to form micropatterns regardless of absorption strength.’



SEM image (a) demonstrating the application of the laser writing technique, and elemental maps showing the chemical symbols Si (b), Ti (c), and Fe (d).

In this case, the structure generated by the team’s Direct Laser Writing technique was highly stable: the micropatterns adhered to their substrates so rigidly that they could not be cleaved away. Dr Nishiyama’s team attributed this resilience to the robust silver core.

In terms of the laser writing process itself, the researchers also identified two key advantages compared with previous approaches. Firstly, the success of the technique doesn’t necessarily depend on the optical properties of the nanoparticles in the solution. This means that precipitation can occur over a far broader range of laser wavelengths, at low enough intensities so as not to induce any damage on the material or substrate. Secondly, the densities of nanoparticles in the clad layer run continuously along the path of travel of the laser’s focus. Crucially, this means that the resulting patterns can work effectively as either electrically conducting or insulating paths.

‘In addition, we can obtain the patterns with other functions such as semiconducting, magnetic, biocompatible material by using various kinds of nanoparticles,’ says Dr Nishiyama.

Exploring Formation Mechanisms

Having identified these structures and their advantages, Dr Nishiyama and his colleagues next examined the potential mechanisms that could have given rise to them. Since they took place over such short timescales, these processes were difficult to study directly – but several aspects of the structures gave the researchers key clues as to how they could have formed. Firstly, they predicted that the silver-based core built up at the focus of the laser, due to the interactions of the material with the laser’s photons and the heat it generates.

Afterwards, the team proposed that the high temperature of the core formed a hemispherical bubble in the solution surrounding the laser focus, creating a gas-liquid interface at its surface. Crucially, temperatures were far lower at this interface than at the laser’s point of focus. Because of this extreme temperature difference, strong convective flows attracted the nanoparticles to the interface, instead of reacting to the laser focus – causing them to amalgamate into a continuous, semi-circular clad layer.

Finally, since the nanoparticles have migrated away from the laser focus, an empty void is left at the centre of the bubble. The end result is the continuous, three-layered, highly stable structure, which the researchers observed using TEM.

A Diverse Range of Applications

The team’s results demonstrate for the first time that the micropatterns produced by Direct Laser Writing do not need to be limited to a narrow range of light-sensitive materials. By dispersing different types of nanoparticles in a silver-based solution, stable hierarchical structures can be produced from a diverse array of useful materials – including nanoparticles of silicon dioxide, titanium dioxide, and iron oxide.

Dr Nishiyama and his colleagues now envisage many different applications for their new technique. These may include ‘supercapacitors’, which can store up to 100 times more energy per unit volume than regular capacitors, and superhydrophobic surfaces, which can strongly repel water. In addition, it could be used to fabricate bio-scaffolds, which allow medical researchers to build artificial biological tissues.

With such a diverse array of potential uses, the researchers now hope that their findings will soon gain widespread traction in many different fields of research, and will now aim to improve their techniques even further.

Meet the researcher

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Dr Nishiyama completed his PhD in Laser Materials Processing at Osaka University in 2005. He then joined the university's materials processing group as an assistant professor, before becoming an associate professor of the nanostructured photonics group at Hokkaido University in 2010. Since 2013, he has been an associate professor in graduate school of science and engineering at Yamagata University. Dr Nishiyama's main research interests lie in ultrafast laser processing and nanostructured photonics. He is particularly interested in how laser-induced microbubbles can be used to manipulate functional nanomaterials, and how these interactions can be exploited in technological applications.

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Yamagata University

INTRIGUING MOLECULAR DISCOVERIES IN DISPLAY MATERIALS

It is a widely-accepted scientific fact that the motions of molecules increase as their temperature rises. However, **Dr Masahito Oh-e** at the National Tsing Hua University in Taiwan has recently made a counterintuitive discovery in an organic semiconductor called 'CADN'. Within a thin film of this material, his team has found that the motion of one part of the CADN molecule increases, while another part becomes more ordered as the temperature increases and approaches the material's phase transition. This research is scientifically intriguing, but also has profound implications for improving display technologies based on organic semiconductor materials.

Indispensable Display Technology

Human society has become increasingly dependent upon display technologies, which are an indispensable part of our smartphones, televisions, tablets and computer monitors. During the COVID-19 pandemic, such technologies have played an even more prominent role in our daily lives, allowing us to work, socialise, learn and attend cultural events, all from the safety of our homes.

Thankfully, these technologies have improved dramatically in recent years, in part due to the variety of materials that can be used to produce displays. Liquid crystals are one such group of materials, which have properties between those of a liquid and those of a solid crystal. These materials form the basis of liquid crystal displays (LCDs), which are commonly used in all kinds of devices.

Dr Masahito Oh-e at the National Tsing Hua University in Taiwan is one of the inventors of in-plane switching LCDs. This technology involves arranging and switching the orientation of molecules within liquid crystals, in order to achieve vibrant colour from all viewing angles. Dr Oh-e also contributed to developing ultra-broad-angle LCD screens, which are now an industry standard, being used in numerous common devices including iPhones. His vast experience in this area has allowed him to deeply investigate the properties of these materials, to find ways of making them even more efficient and high-performing.

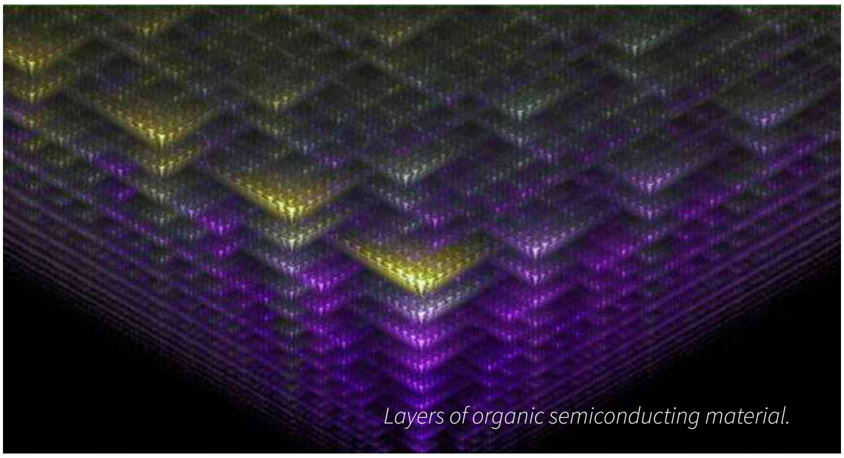
Exploring Molecular Orientation

Dr Oh-e is particularly interested in studying the orientation of molecules within liquid crystals. LCD technology relies on a layer of molecules in a liquid crystal state, which are sandwiched between two substrates with electrodes. These molecules manipulate the light that passes through them, which is then controlled in a way that produces an image on a screen.

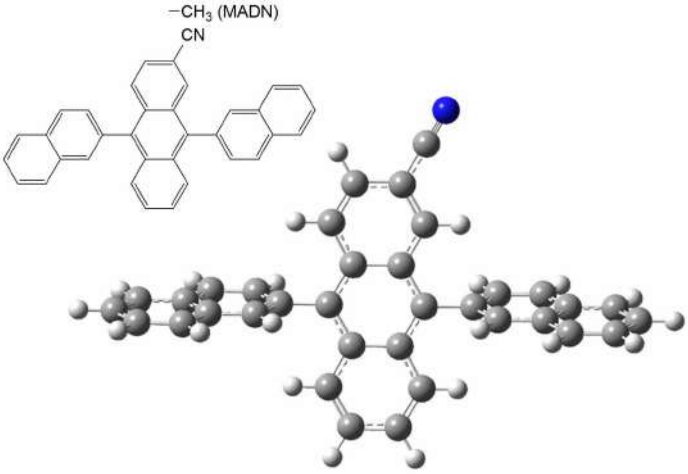
Energy efficiency, and the quality of image produced, are both influenced by the way in which molecules arrange themselves. Therefore, it is important to understand how these molecules arrange themselves and what affects their orientation.

OLEDs: An Exciting Alternative

Although liquid crystals remain the most commonly used material in current display technologies, organic light-emitting-diodes (OLEDs) are another technology that can produce vibrant, flexible and inexpensive displays. OLEDs are composed of films of an organic semiconductor – special



Layers of organic semiconducting material.



The cross-shaped CADN molecule.

materials comprising mainly carbon and hydrogen atoms, whose behaviour lies somewhere in between that of an electrical conductor and that of an insulator.

When an electrical current is passed through an OLED, it emits light of a certain colour. By making up a matrix of these components, scientists have developed high-quality displays that produce vibrant images. OLED technology has been making its way into many of our devices over the years, including televisions, smartphones, tablets and laptops.

Because of their low cost and flexibility, it's easy to see why research into organic semiconductors is so important. Therefore, scientists across the globe are studying their properties in detail, to identify ways that they can be optimised for various device applications. Alongside their research into liquid crystals, Dr Oh-e and his team have also been studying molecular orientation in organic semiconductors for over a decade.

Much like with liquid crystals, the properties of organic semiconductor films can be heavily influenced by the way in which their constituent molecules are oriented. Differences in molecular orientation can have an impact on the behaviour of these films, and the properties of the resulting electronic device. For instance, molecular orientation in OLED films can affect device lifespan and energy efficiency, so it is important that scientists understand what controls orientation, and how it can be tuned. However, these films can be made up of molecules with complex shapes, making their orientation difficult to control.

A Cross-Shaped Semiconductor Molecule

Dr Oh-e and his team employ a uniquely shaped organic molecule called CADN in order to investigate molecular orientation and alignment in semiconductor films. CADN is a cross-shaped molecule, with different electronic properties across its different branches. Its unique shape makes it a good candidate for studying orientation, as it is relatively easy to determine which way it is facing.

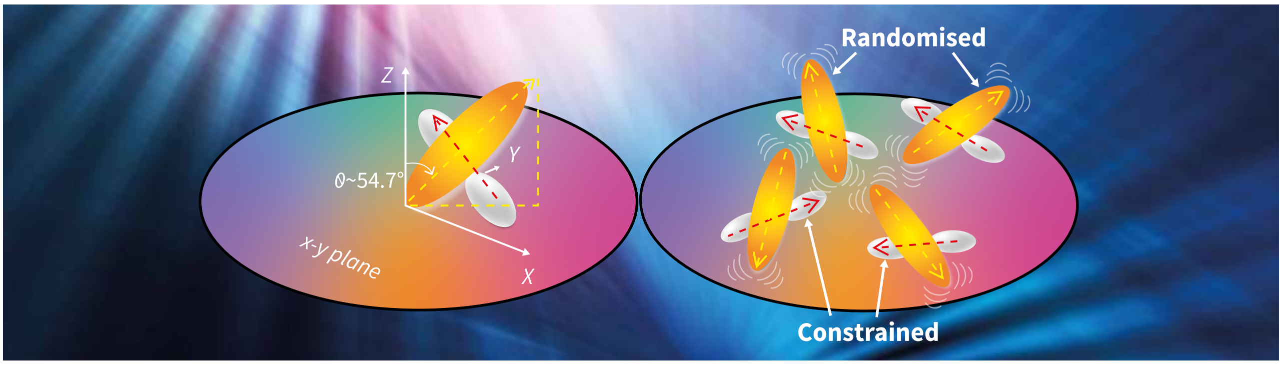
In a recent study, the team first experimented by preparing films of CADN, using a technique called vacuum vapor deposition, which is practically adopted in the manufacturing process of OLEDs. Vapour deposition involves preparing a surface made from a silicon wafer and applying a thin coating of the organic material in question, while under a vacuum. The benefit of this technique is that it allows for the creation of evenly coated films with a defined thickness, while creating a stable non-crystalline state.

Once the team had produced CADN films with a thickness of 100 nanometres (just one ten-thousandth of a millimetre), they set to work analysing them. Using a technique called variable-angle spectroscopic ellipsometry, Dr Oh-e and his team were able to monitor how the molecules were orienting themselves with respect to the surface.

The team took measurements as they varied the temperature from room temperature up the material's phase transition temperature, beyond which the material becomes a so-called 'supercooled liquid'. This means that the film was still below its melting point but was able to behave more like a liquid.

An Interesting Discovery

Upon analysing the data they had collected, the team found that the molecules were aligned to one another throughout the film. As cyano groups in the molecules pull electrons towards



Orientation of a CADN molecule at room temperature (left), and changes in the molecular orientation of CADN with increasing temperature (right).

them, causing each molecule to be electrically polarised, the team measured a large polarisation effect in the bulk material.

The cross-shaped CADN molecule can be perceived as consisting of two intersecting bars. Dr Oh-e and his colleagues found that one bar of the molecule preferentially aligned parallel to the surface of the silicon wafer, while the other bar was oriented close to the so-called 'magic angle' (about 54.7°) from the surface. As the temperature rose, the motion of the latter bar increased, causing its orientation to become even more random. This was unsurprising, as when the temperature of a material increases, the motions of its constituent molecules also increase.

However, the team was surprised to discover that the bar that was preferentially aligned parallel to the surface behaved in an unusual manner when the temperature increased. Although the rising temperature first caused the orientation of this bar to become disordered, as the temperature continued to rise and approached the phase transition, its parallel alignment to the silicon surface became even more orderly.

This discovery is highly counterintuitive, as one would expect that the increased heat energy would cause all parts of the molecule to move more freely, leading to random orientations. This surprising finding was very carefully observed while measuring the sample and analysing the data. Interestingly, such behaviour has not been observed in other organic semiconductor materials.

'We observed that part of the molecule becomes more randomised while another becomes more constrained as the temperature increases,' says Dr Oh-e. 'This observation of molecular orientation is significantly striking and interesting.'

This observation was supported through the use of another technique, called second-harmonic generation analysis. Using this method, the team was able to gather even more data on how the orientation of the CADN molecules changes while the temperature increases, based on the different properties of each bar of the cross-shaped molecule. The data collected here consistently supported the previous conclusions, coming together to make a strong case for their observation.

The Bigger Picture

Through this study, the team gained important insights into the behaviour of molecules that comprise organic semiconducting films, wherein one part of a molecule is disordered while another becomes well-ordered with increasing temperature. 'To have a solid picture, we need further efforts to collect more data including other molecules by independently probing two different moieties of a molecule,' says Dr Oh-e.

They have also provided insights into how molecular alignment of CADN films can be manipulated, through simply heating the material to near its phase transition temperature. This was not the first time either; a previous study by Dr Oh-e used a similar molecule to CADN, known as 'MADN'. The results of the two studies were consistent with one another, further supporting the case for how these uniquely shaped molecules prefer to orient themselves with respect to the silicon surface they are attached to.

This information is vital to understand when it comes to designing and fabricating organic semiconductors for any application. It is known that molecular alignment in a thin film semiconductor can affect its conductivity, ability to produce and absorb light, and efficiency. In Dr Oh-e's MADN study, he showed that when one bar of each molecule was well aligned with the silicon surface, the conductivity of the film was improved. This is also likely the case with CADN, as this molecule is very similar in structure to MADN.

On top of this, understanding how to control molecular orientation in organic semiconductors and liquid crystals alike opens a whole world of potential applications, as it means that they will be more customisable than ever before.

Dr Oh-e and his team have conducted research that will change the way that we look at both liquid crystals and organic semiconductors, and will hopefully go on to improve the quality and variety of applications that we use them for.

Meet the researcher

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Dr Masahito Oh-e earned his master's degree from the Tokyo Institute of Technology, after which he worked as a research scientist at the Hitachi Research Laboratory of Hitachi, Ltd. He then went on to gain his PhD from the Tokyo Institute of Technology in 1998, before becoming a visiting research fellow at the University of California, Berkeley. Continuing to work with Hitachi, Dr Oh-e worked with the Japanese government on several projects involving nano-structured liquid crystals between 2002 and 2008, before being offered a position as the department director and chief technical research fellow of the Sharp Labs of Tokyo. As of 2016, he has worked as a professor at the Institute of Photonics Technologies at the National Tsing Hua University, Taiwan. Here, his research focuses on fundamentally exploring multidisciplinary photonics and materials science, and addressing current technical challenges including optoelectronic applications.

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NTHU

FINE-TUNING POLYMERS AS FLEXIBLE ANTENNA SUBSTRATES FOR AIRCRAFT

The pursuit to design more lightweight aircraft that can travel over greater distances never ceases. One area that has received much attention is the development of lighter and more aerodynamic antennas. Researchers at the NASA Glenn Research Center are at the forefront of this effort. The research team, which includes **Jessica Cashman**, **Baochau Nguyen**, **Haiquan Guo**, **Marcos Pantoja**, **Kevin Cavicchi**, and **Mary Ann Meador**, is designing flexible polymer materials that can be used to construct lightweight, low-drag antennas that lie along the surface of an aircraft.

Surface Conforming Antennas

Many unmanned aircraft communicate using large dish antennas. These antennas can be unnecessarily heavy and bulky, and project far above the surface of the vehicle, creating added drag, effectively adding extra weight. A certain type of antenna, known as a phased array antenna, can address these drawbacks. Phased array antennas are clusters of antennas that direct signals electronically without physically moving and can be installed conformally along the curved surface of a wing or fuselage.

The development of phased array antennas has been on-going. They are made up of an array of antenna elements separated by a low electrical loss material, known as a substrate. The antenna substrate needs to be readily installable at any given location of the vehicle where the surface is almost always curved. In addition, the substrate should possess electrical characteristics that do not impede signal transmission. Researchers at the NASA Glenn Research Center in the US, are developing materials that can be fabricated as flexible substrates suitable for building antennas.

The research team focuses on developing and evaluating polyimide aerogels, which have both the mechanical and electrical properties needed to build suitable antennas. Aerogels are unique in that they have one of the lowest dielectric constants of any structural material, meaning that they do not interfere with the antenna's ability to transmit signals, allowing for the maximum amount of data to be transferred. These materials also have very small pores, meaning that they can be viewed by the antenna elements as a solid substrate.

Polyimides are polymers, that is, they are made up of many (poly) repeating carbon-containing units (mers) connected to form a backbone. The chemical structure of the backbone influences the stiffness of the polymer, as well as other properties. Polyimides are typically rigid backbone polymers, since the mers contain less flexible ring structures.

Preparing Polymer Substrates

The preparation of polyimide aerogels involves several stages. First, the polymer precursors (monomers) are dissolved in a solvent and immediately react to form linear chains. Then a crosslinker is added, which reacts with the chains forms a network structure. This solution is poured into moulds before the network formation is complete. As network formation goes to completion, a gel is formed where the solvent remains trapped within the polymer network. Consequently, when

Reprinted with permission from Pantoja, M.; Boynton, N.; Cavicchi, K.; Dosa, B.; Cashman, J. L.; Meador, M. A. B. Increased Flexibility in Polyimide Aerogels Using Aliphatic Spacers in the Polymer Backbone, ACS Appl. Mater. Interfaces 2019, 11, 9. Copyright 2019 American Chemical Society.

the solvent is removed, it leaves behind pores in the material where pockets of solvent had been. The resulting aerogel material possesses an extremely nano-porous structure.

Polymer aerogels can be viewed as a complex network of overlapping and interlocking molecular chains. The density of a polymer aerogel can be controlled by the amount of molecules in solution, but is also influenced by how much shrinkage occurs during processing. The denser the aerogel, the more it will resist physical deformation and the stiffer the material will be. However, the less dense the aerogel is, the less it will interfere with the antenna.

NASA's polymer aerogel team can fine-tune how the chains pack together by changing the structures and ratios of the repeating groups of molecules along the polymer backbone. To develop the best possible antenna substrate, the researchers have been optimising the mechanical properties such as the flexibility, pore size, and water resistance of polyimide aerogels, by incorporating flexible links alternating with units of rigid polyimide. They aim to achieve an aerogel material with the lowest possible density, and thus dielectric constant, combined with an optimum flexibility.

Effects of Flexible Linking Group Length

The research team began their studies by incorporating a flexible linking group into the backbone of the polyimide polymer and investigating how the length of the linking group affects the physical properties of the polyimide aerogel. Polyimide is a rigid polymer and adding the flexible linking groups to the backbone is what makes the polymer more flexible. They also explored the proportions of reagents needed to alter the backbone, and how these ratios ultimately affected the aerogel's physical properties.

Specifically, they investigated how the number of methylene groups used to vary the length of the flexible linking group can affect the characteristics of the material. Since methylene groups form a linear chain, they allow the chain to fold easily. An analogy to this is a beaded necklace. The rigid polyimide units are like the beads and the flexible chains of methylene groups are like the thread between the beads. The team compared different sizes of the flexible linking groups with four, six and ten methylene groups.

Their results revealed that the length of the flexible linker positively influenced some of the material properties, while also proving problematic for others. The following summarises the results gleaned from the study.

The team found that the flexibility of the aerogel increased when at least 25% of the flexible linker was added, but the length of the methylene chains did not have much of an influence on flexibility. In addition, using greater than 25% flexible linkers caused more shrinkage, leading to higher density aerogels. Interestingly, they were able to demonstrate how a two-millimetre-thick aerogel substrate could be bent so that the folds were about two inches apart.

The researchers also investigated whether their aerogel materials would absorb water, which would short the antenna elements. Fortunately, they showed that aerogels made up of longer methylene chains absorb very little water. From this result and the above mechanical properties, the team concluded that 25% of longer flexible linking group resulted in the optimum material.

In a more recent study, the researchers performed a similar analysis with polymer compositions containing 12 methylene groups. They achieved similar flexibility using this spacer, but the material's resistance to water was even better.

Studying Bulkier Backbones

Continuing the overall theme of their previous work, the team then investigated the utility of a different chemical group when altering the backbone. In this study, they compared the effect of neopentyl groups with their work involving methylene groups. Neopentyl is flexible because it consists of a three-carbon chain between two ether groups. However, the middle carbon contains two methyl groups, which makes it more moisture resistant.

The researchers investigated how different proportions of reagents needed to incorporate neopentyl groups into the polymer chains affect the structure of the polymer, and ultimately, the mechanical properties of the aerogel. They also compared some of the key results between their methylene and neopentyl studies.

When the solvent is removed from a wet gel to form an aerogel, the structure shrinks. Minimising shrinkage of the aerogel is desired in order to maintain a low density and dielectric constant. The researchers found that aerogels shrank the most when they had added a large amount of neopentyl-containing monomer during the synthesis.

They were also able to derive other trends when higher proportions of neopentyl-containing monomer were introduced. For example, more sophisticated experimental methods that approximate the surface area of the dried aerogel revealed that the surface area of the porous aerogel decreased. This relates quite well with the shrinkage of the aerogel. As the aerogel shrinks, the pores collapse, and the available surface area decreases.

They also analysed the ability of the aerogel to absorb water and found that adding 50% of neopentyl-containing monomer resulted in minimal water uptake. If the proportion was reduced or increased from the optimal point, then the aerogel would absorb more water.

As shown in their methylene study, the researchers demonstrated how a two-millimetre-thick film of the neopentyl-based aerogel could be bent to within a couple of inches. Overall, the researchers concluded that adding 50% of neopentyl containing monomer would yield an aerogel with optimal flexibility, combined with a low dielectric constant.

The work carried out by NASA's polymer aerogel team was intricate and challenging. Nonetheless, understanding the relationships between atomic-level attributes and large-scale mechanical properties proved invaluable in their search for the most suitable conformal antenna substrates. In fact, in all three of the studies described here, the team achieved desirable flexibility in each optimised material, making them ideal for use in the manufacture of lightweight, high-performing antennas for more efficient unmanned aircraft.

Meet the Team

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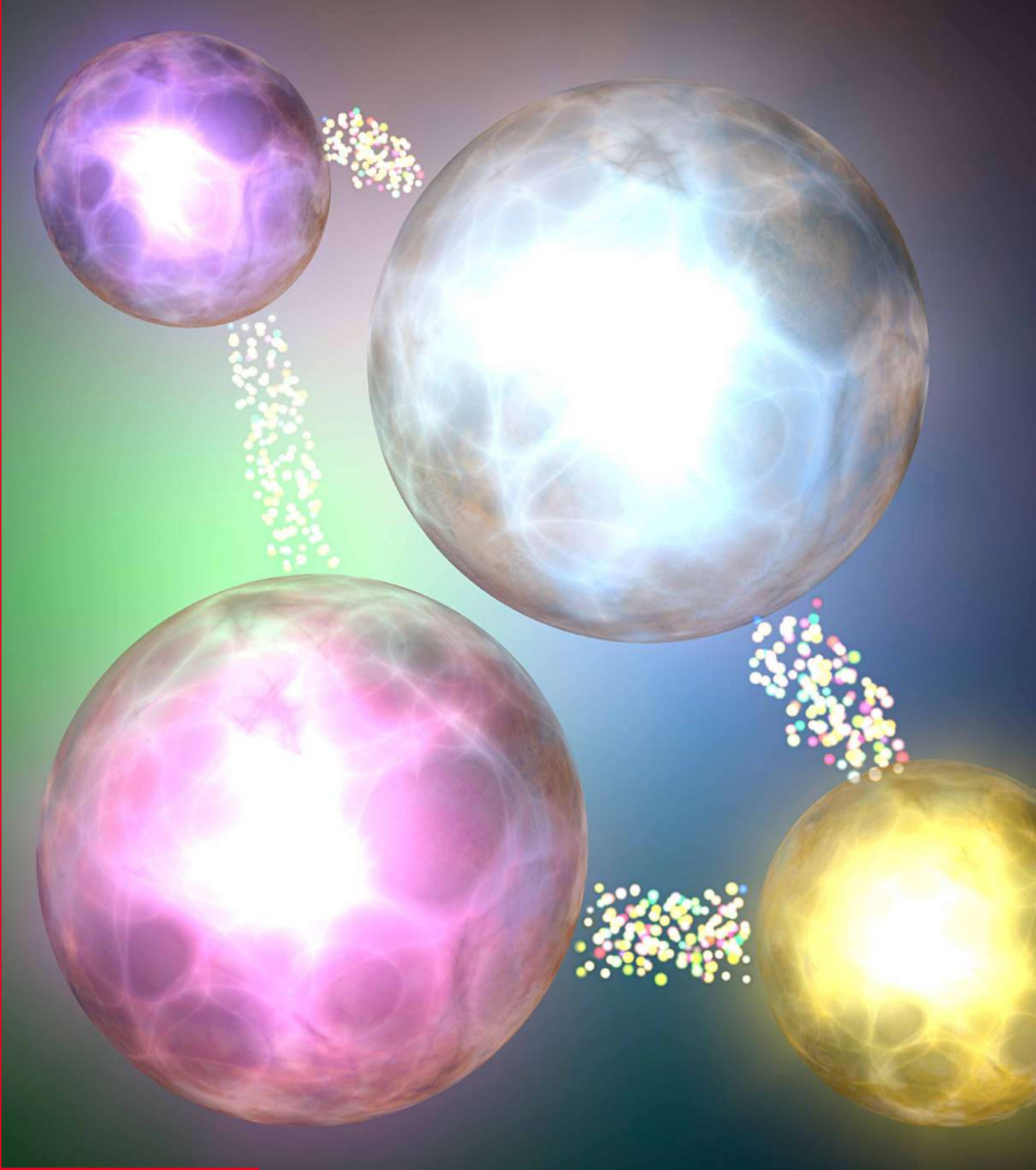
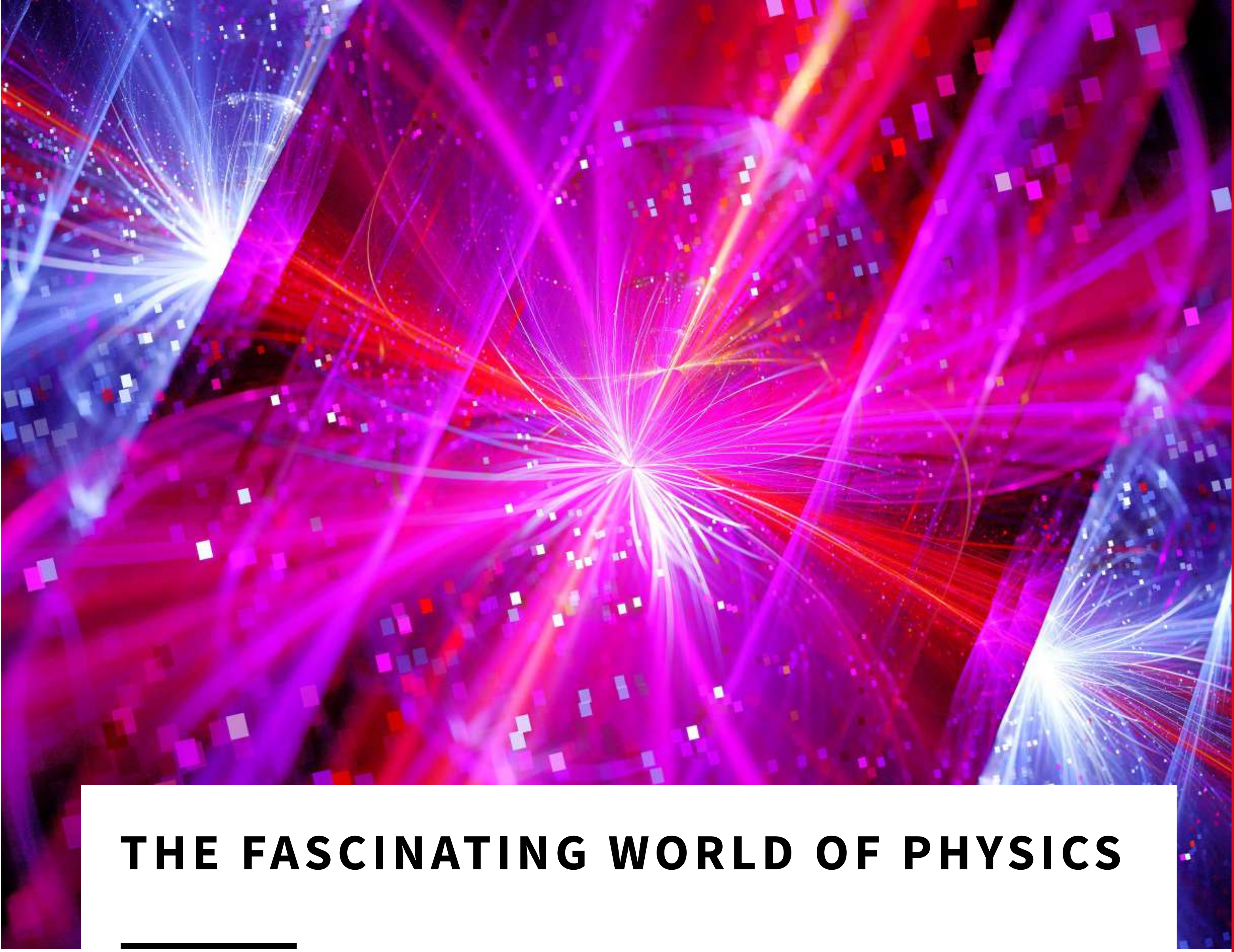
PHYSICS





THE FASCINATING WORLD OF PHYSICS

In the third section of this exciting edition, we delve deeper into the nature of matter, and the forces that have given rise to the weird and wonderful universe we inhabit today. Here, we highlight the latest discoveries and innovations in the world of physics, from understanding how the universe evolved, to the creation of gigantic atoms the size of a grain of sand.

First, we explore how matter behaved in the extreme environment of the early universe, just a small fraction of a second after the Big Bang. Because of the colossal temperatures at this time, fundamental particles that are now tightly bound into groups were free to wander individually. Using the latest particle accelerator facilities, researchers today can recreate fluids of these particles, named 'Quark Gluon Plasmas'. Here, we introduce the work of Dr Rene Bellwied at the University of Houston, who uses the results from these experiments to explore the fascinating dynamics of Quark Gluon Plasmas, and the products that emerge in their aftermath. His team's findings are now shedding new light on the enigmatic nature of matter itself.

Next, we investigate theoretical particles called magnetic monopoles. Representing isolated magnetic charges, these particles have so far remained elusive to physicists who have tried to detect them experimentally. Through their extensive research, scientists at Terra Quantum AG, the University of Perugia, and SwissScientific Technologies show that magnetic monopoles must be real, and their discoveries also set the stage for exciting technological advances.

From here, we move on to the exciting world of Rydberg atoms, which have a single outer electron that has been excited to an extremely high energy state. Because of its extreme energy, this electron can venture far from the nucleus of the atom, while still remaining bound to it. Typically, atoms measure picometres across (billionths of a millimetre), but Rydberg atoms can have diameters of larger than the width of a human hair.

In the final article of this section, Dr Barry Dunning and Dr Thomas Killian give us a crash course in the weird and wonderful physics of Rydberg atoms, and their very unusual physical and chemical properties. They also discuss how the extreme properties of Rydberg atoms now enable emerging technological applications in sensing and quantum computation.

UNDERSTANDING THE NATURE OF MATTER THROUGH QUARK GLUON PLASMAS

In the extreme environment of the primordial universe, fundamental particles that are now tightly bound into larger groups were, for the briefest moment, free to wander individually. Using the latest particle accelerator facilities, researchers today can recreate fluids of these particles, named 'Quark Gluon Plasmas', through high-energy collisions between heavy ions. In his research, **Dr Rene Bellwied** at the University of Houston uses results from these experiments to explore the fascinating dynamics of the plasmas, and the products that emerge in their aftermath. His team's findings are now shedding new light on the enigmatic nature of matter itself.

Quarks

Quarks are a fundamental part of much of the matter in the universe that we can observe. Although these particles can come in six possible 'flavours', most fall into just two such categories: these are the 'up' and 'down' quarks, which make up the protons and neutrons that surround and compose us.

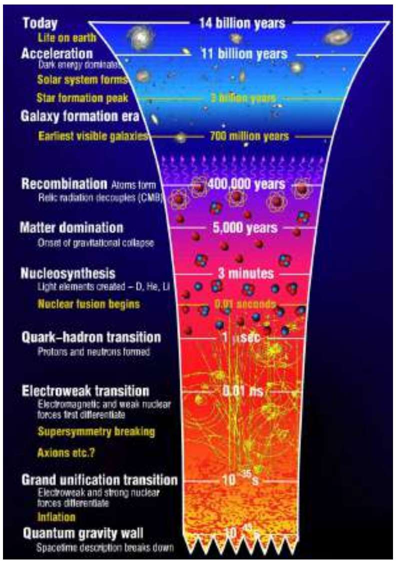
For an absolutely vast majority of the universe's history, virtually all quarks in the universe as far as we know have been bound to one or more additional quarks, and can never exist on their own. In protons and neutrons, for example, they exist in groups of three, which are held together by massless particles named 'gluons'.

Over the past few decades, physicists have discovered a growing number of more exotic particles – composed of different types and combinations of quarks; and yet the rule that quarks must always be confined within larger particles continued to hold.

Nonetheless, this wasn't always the case: for the briefest moment following the Big Bang, temperatures were so colossally high that the rule could be temporarily broken. For roughly one trillionth of a nanosecond, quarks and gluons existed as individual particles within an enigmatic, ultra-hot fluid. Today, physicists call this elusive substance a 'Quark Gluon Plasma'.

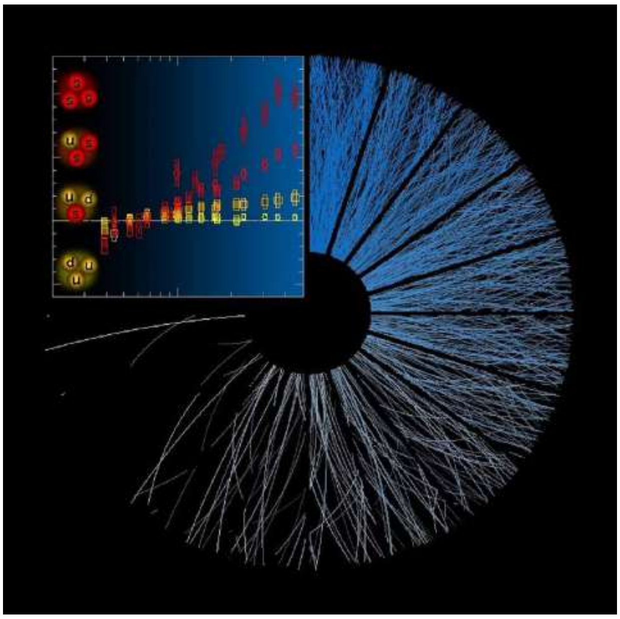
Recreating the Early Universe

The brief era where Quark Gluon Plasmas dominated the universe may now be in the distant past – but thanks to the latest generation of particle accelerators, researchers can now recreate this primordial environment in controlled lab conditions. At its core, the concept behind their experimental process is fairly simple: they must release as much energy as possible, within the smallest possible space. To do this, researchers can accelerate subatomic particles to an appreciable fraction of the speed of light, smash them together, and observe the particles that emerge in the aftermath.



Evolution of the universe as a function of time.

To maximise the energy – and thereby the temperatures and densities of these collisions – physicists use ions of heavy, stable elements such as lead, which carry far more momentum than smaller particles when travelling at the same speed. Over the past two decades, their efforts have yielded promising results. 'Through experiments at the Relativistic



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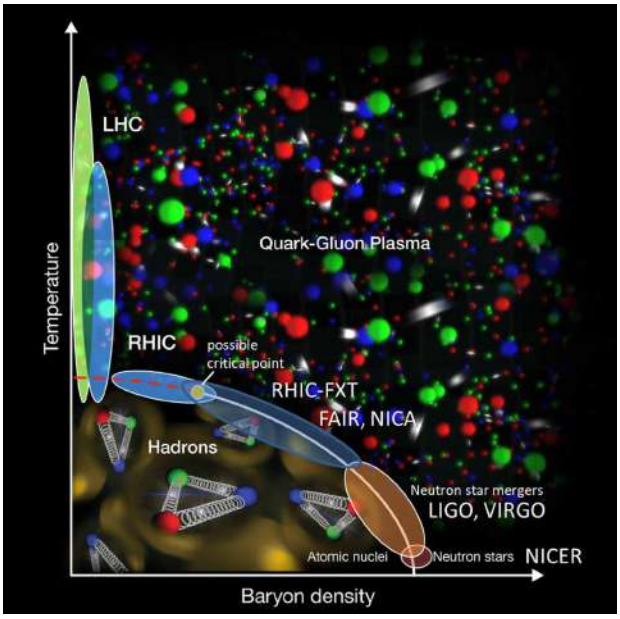


Phase diagram of nuclear matter and the facilities that can measure the phase transition.

Heavy Ion Collider at Brookhaven National Laboratory on Long Island, and the Large Hadron Collider at CERN, Geneva, we have established that the matter at these high temperatures and densities can transition into a Quark Gluon Plasma,' says Dr Rene Bellwied of the University of Houston.

Just like in the early universe, the fluid doesn't stick around for long. As Quark Gluon Plasmas created in the aftermath of high-energy collisions cool down, they will rapidly 're-confine' – with independent quarks and gluons grouping together to form new particles. Most often, this will result in new protons and neutrons – yet as Dr Bellwied and his colleagues have discovered, the re-confinement process can be highly varied. With the right approach, researchers can use their analysis of re-confinement to gain a deeper understanding of the nature of matter itself.

New Experimental Opportunities

The ability to generate Quark Gluon Plasmas on demand has opened up a wide array of opportunities for particle physics experiments in recent years. As Dr Bellwied explains, two lines of research in this area are particularly important. 'Firstly, we characterise the new short-lived state of matter and its properties to learn about the fundamentals of free quarks and gluons,' he says. 'Secondly, we attempt to understand the formation of matter and new forms of matter through studying the transition back out of the Quark Gluon Plasma.'

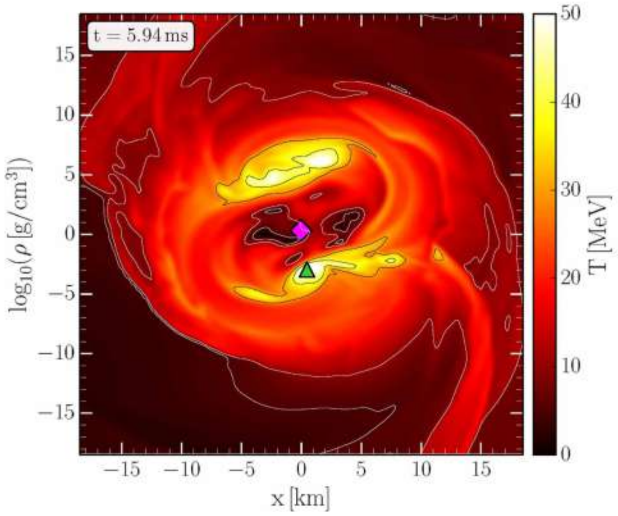
This first aspect of Quark Gluon Plasma research can perhaps yield the most immediate benefits to our understanding of particle physics. As fundamental particles, quarks and gluons are both key elements of the Standard Model, which describes the nature of all matter in the universe according to our current understanding. With the ability to study the physical properties of individual particles, free from the influence of others, researchers could improve the predictions of the Standard Model, and perhaps even expose some of its limitations.

In his research, Dr Bellwied focuses more closely on the second aspect he describes. By studying the Quark Gluon Plasma re-confinement process and the products of its aftermath in more detail, his team's findings are providing new insights into aspects of the nature of matter that cannot be proved through more conventional experiments. Three specific areas of his research are particularly intriguing, including particles containing 'strange' quarks, the enigmatic contents of ultra-dense neutron stars, and the mysterious influence of quantum mechanics on plasma dynamics.

Enhancing Strangeness

Compared with up and down quarks, strange quarks are both far heavier, and far less stable – with any known form of matter containing the particles decaying just brief moments after their formation. Dr Bellwied and his colleagues have now discovered that during Quark Gluon Plasma re-confinement, comparatively high numbers of these quarks are created: a phenomenon known as 'strangeness enhancement'.

'My group established a significant enhancement in the production of strange particle, which contain strange quarks in addition to the common up and down quarks,' Dr Bellwied illustrates. 'These particles appear following high-speed heavy ion collisions, and can be generally considered a signature for plasma formation.' Initially, the researchers achieved these results using collisions between heavy ions alone. Yet through subsequent research, they discovered that similar mechanisms could appear following collisions between two protons, provided the collision energy is high enough.



Energy profile of a neutron star merger. Particles 2, 1, 44.

In parallel with these experiments, Dr Bellwied has worked with his colleague Dr Claudia Ratti, also at the University of Houston, to develop a theoretical framework for strangeness enhancement. Their theories explained how the characteristics of the re-confinement process can vary with the Quark Gluon Plasma's temperature – revealing that strange particles will result from hotter plasmas than those that generate protons and neutrons. In subsequent research, these ideas would be key to determining how matter behaves in some of the most extreme conditions found in the known universe today.

Glimpsing the Interiors of Neutron Stars

When stars between 10 and 25 times the mass of our Sun reach the end of their lives, they will explode in dramatic supernovae, leaving behind dark, rapidly spinning cores named 'neutron stars'. Although they measure just tens of kilometres across, neutron stars have similar masses to the Sun, making them unimaginably dense. On its surface, a neutron star appears to be composed mostly of vast numbers of highly compacted neutrons, resembling a giant atomic nucleus. However, what lies beneath the surface has largely remained a mystery so far.

Currently, the most promising techniques for studying these interiors lie in the detection of gravitational waves. These ripples in spacetime are created as colliding neutron stars spiral into each other, and eventually merge together. 'We have now shown that high-speed collisions at lower energies generate the same energy density as those measured in neutron star mergers, as detected by gravitational waves,' Dr Bellwied explains. 'The makeup of the neutron star interior should generate a unique signature in the emitted wave.'

Some theorists now suggest that the extreme masses of neutron stars could be due to an abundance of stable strange quarks hidden deep in their interiors. In future research, the signatures generated by Dr Bellwied's team could lead to experimental proof of this theory. If correct, it would suggest that hot Quark Gluon Plasmas are generated when massive stars collapse. Furthermore, this line of research may even lead to new insights into the formation of yet more enigmatic black holes.

The Influence of Entanglement

Through his latest research, Dr Bellwied has begun to explore how the dynamics of Quark Gluon Plasmas are influenced by the phenomenon of quantum entanglement. The effect describes systems of one or more particles whose fates are intrinsically bound to each other – so that if their states are measured at the same time, the outcomes of all observations will directly correspond to each other, no matter how far apart in space the particles are separated.

In a system of quantum particles as deeply complex as a Quark Gluon Plasma, quantum entanglement creates an intricate web of interactions between constituent quarks and gluons – strongly influencing their dynamics. Until now, however, this influence has not been widely considered. 'I have started to look at the effects of quantum entanglement on the initial state of the plasma formation, and how it might affect the production and emission of the final state particles,' says Dr Bellwied. 'This is the first time that we have applied quantum mechanical principles to the evolution of deconfined matter.'

Dr Bellwied hopes that these results will lead to new insights both into the behaviours of unconfined quarks and gluons, and the nature of the matter produced following re-confinement. In turn, the findings could benefit his team's other fields of research: including strangeness enhancement, neutron star composition, and even the fundamental properties of quarks and gluons.

Expanding the Scope for Exploration

The research of Dr Bellwied and his colleagues has already yielded important advances in our understanding of Quark Gluon Plasma and its re-confinement. However, there is still an expansive scope for future research. In the coming years, the Relativistic Heavy Ion Collider and Large Hadron Collider will be joined by two other cutting-edge particle accelerators: the Facility for Antiproton and Ion Research (FAIR) in Germany; and the Nuclotron-based Ion Collider Facility (NICA) in Russia. Even further into the future, Brookhaven National Laboratory is planning to expand its collider facilities with an Electron-Ion Collider (EIC), and Dr Bellwied's team has recently been asked to join a collaboration to prepare the next generation detector and physics program for the EIC.

Through the more extensive collision measurements enabled by these additions, physicists may soon gain an even more advanced understanding of the dynamics that shaped our universe in its very first moments.

Meet the researcher

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Dr Rene Bellwied completed his PhD in Chemistry and Physics at Johannes Gutenberg University in Germany in 1989. After a Feodor Lynen Fellowship at Stony Brook University in New York, he moved to Detroit, where he worked as a Professor for 18 years at Wayne State University. In 2010, he became a Professor at the Physics Department at the University of Houston. His main research interests lie in experimental nuclear physics, and he has contributed to research into relativistic heavy ion physics at both CERN and Brookhaven National Laboratory for more than 30 years. Dr Bellwied has received much recognition for his ground-breaking research, including a Distinguished MD Anderson Endowed Chair and the 2020 University of Houston Research Excellence Award.

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SUPERINSULATORS: THE HIDEOUT OF MAGNETIC MONOPOLES

Magnetic monopoles have long been dismissed as impossible by many physicists, but their existence has nonetheless been theorised for many decades. Through their extensive research, scientists at Terra Quantum AG, the University of Perugia, and SwissScientific Technologies, show that the end could soon be in sight for this conflict. The team's investigations into superconducting materials not only show that magnetic monopoles must be real – their discoveries also set the stage for exciting technological advances.

Single or Matched?

The concept of single electrical charge is ubiquitous in physics. Whether they are protons, electrons, or quarks, particles carrying either positive or negative charges are crucial to understanding many fundamental aspects of our universe.

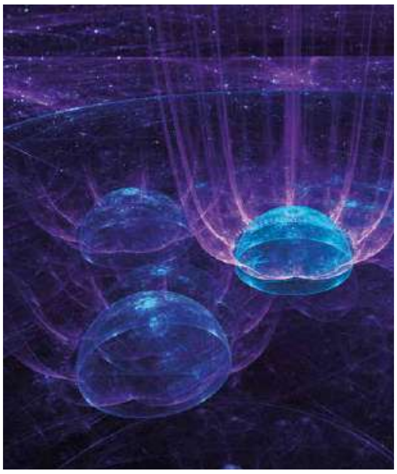
Meanwhile, however, magnetism appears to operate under a different set of rules. Instead of being single, magnetic charges come in inseparable pairs – like the north and south poles in a bar magnet – which are connected by looping field lines. If such a magnet were broken in half, their two poles would not simply separate. Instead, they would each re-form an opposing pole – creating two new bar magnets.

This principle is at the centre of the theory that isolated magnetic charges, named 'magnetic monopoles', cannot possibly exist. The idea was even expressed in the foundational equations of electromagnetism, first set out by James Clerk Maxwell in the 1860s – and stood unopposed for many decades afterwards.

However, this situation didn't last. In the 1930s, Paul Dirac expressed doubt in the idea of a fundamental difference between the properties of electrical and magnetic charges, whose resulting fields are otherwise treated in similar ways in Maxwell's equations. Through ground-breaking theoretical calculations, he showed for the first time how magnetic monopoles could exist after all.

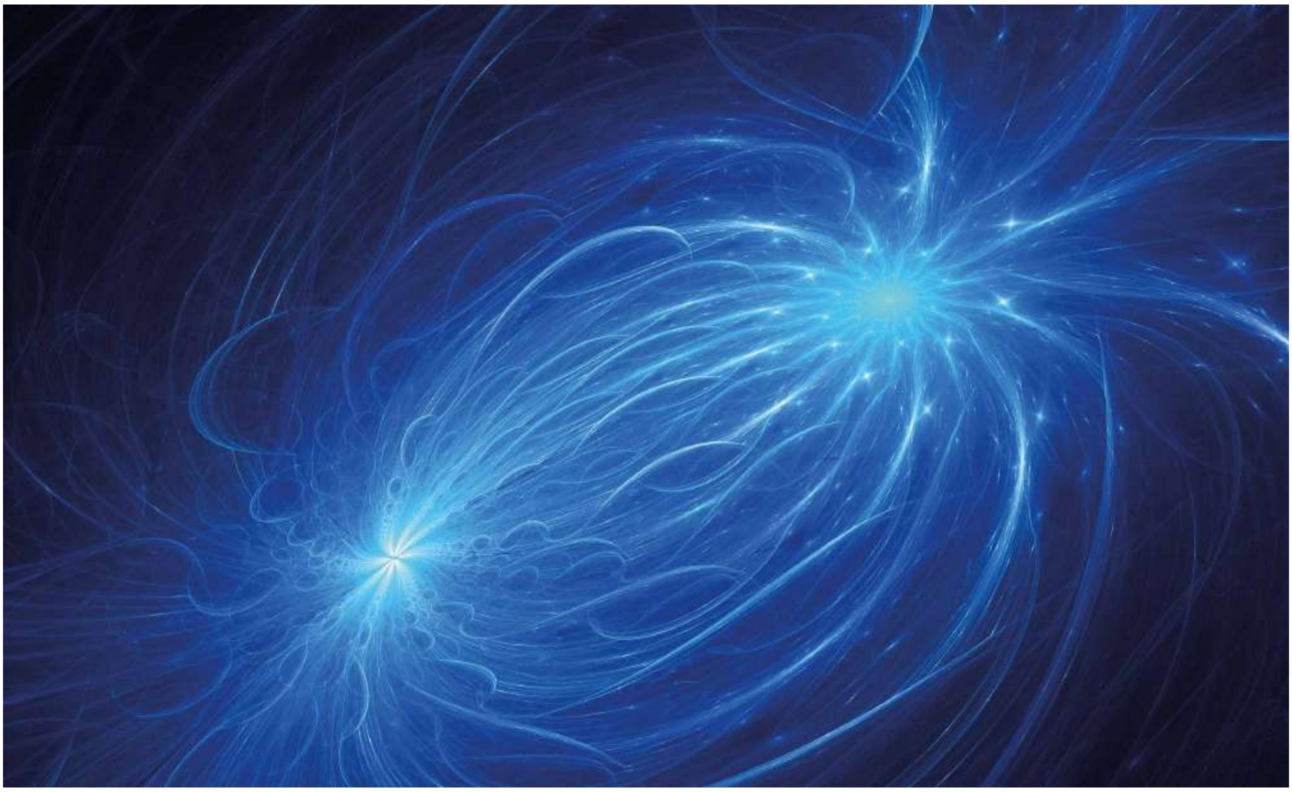
Dirac's Case for Monopoles

Dirac's ideas did not appear intuitive at first, but lead to a perfectly consistent quantum theory of electromagnetism, including both electric and magnetic charges. Magnetic charges cannot exist, because they lead to unacceptable singularities. However, if the product of the magnetic and electric charges is an integer multiplied by 'the Planck constant', these singularities become unobservable. The Planck constant is an important value in physics demonstrating that quantum mechanics underlies our world.



Crucially, Dirac's idea removes the inexplicable asymmetry between the properties of both charges within Maxwell's equations. Furthermore, if combined with other fundamental forces – namely the strong and weak nuclear interactions – a theory emerges for the formation of magnetic monopoles shortly after the Big Bang, when temperatures across the universe were vastly hotter than they are today.

Despite the robust reasoning and elegant outcomes of Dirac's theory, researchers have still found no experimental evidence for such fundamental magnetic monopoles to date, even after many decades of searching. So far, several studies have



offered tantalising glimpses of the effects predicted by his ideas, but hard evidence for them still remains elusive.

Now, through extensive research, Dr Maria Cristina Diamantini at the University of Perugia, Dr Valerii Vinokur at Terra Quantum, and Dr Carlo Trugenberger at SwissScientific Technologies, predict that this long-standing deadlock could soon be about to change, by pointing out that magnetic monopoles should be searched for in materials in the laboratory rather than in the cosmos.

Advances in Superconductivity

The team's theories originate from an effect that appears at first to be unconnected to the search for magnetic monopoles. First discovered as far back as 1911, superconductivity is a phenomenon that allows electrical currents to flow through some materials with zero resistance. It arises in certain materials at ultra-cold temperatures, where pairs of oppositely-spinning electrons couple together through the effect of exchange by lattice vibrations called 'phonons'. The result is a 'Cooper pair' of electrons, which can flow through the material without dissipating any of their energy in the form of heat.

Superconductivity is a key example of a quantum effect that can be observed on macroscopic scales. It contrasts with the common misconception that quantum laws can only apply to small groups of particles, or over minuscule distances. The effect has now been known and studied for well over a century, but several of its aspects remain a mystery to physicists. Superconductors can be homogenous materials or synthetic arrangements of superconducting granules, called 'Josephson junction arrays'. In Josephson junction arrays, Cooper pairs exhibit quantum tunnelling between adjacent superconducting granules, mediating an electric current with no energy loss.

Superinsulators: The Hidden Face of Superconductors

In 1996, theoretical studies of regular Josephson junction arrays led Dr Diamantini and Dr Trugenberger to a new discovery: under certain conditions, the superconducting properties can switch around entirely, and a Josephson junction array can fall into a new state, which they called a 'superinsulator'. At ultra-low temperature, they predicted that these materials have an infinite electrical resistance, making it impossible for Cooper pairs to flow through them. As a result, superinsulators are 'twin mirror images' of superconductors in terms of their physical properties.

In their study, Dr Diamantini, Dr Trugenberger and a colleague demonstrated that superinsulating states could emerge close to the point of transition between superconducting and insulating states within Josephson junction arrays. Further to the insulating side, Cooper pairs would less readily tunnel between different granules, but would not be stopped entirely. At just the right point, however, they predicted that the material's conductivity would drop straight to zero.

Such an idea implied the need for a duality between the properties of electrical and magnetic charges: a principle that itself relied on the existence of magnetic monopoles. The team's discovery was so unexpected at first that it didn't receive much attention following its initial discovery. As a result, their findings remained largely unvisited for over a decade.

Rediscovery and New Understanding

In 2008, exploring superconductor-insulator transitions in a seemingly unrelated physical system, strongly disordered thin films, Dr Vinokur and his research team discovered that upon cooling, the conductivity of an insulating film suddenly drops to zero at a certain temperature – decreasing its magnitude over a million times. This drop is the opposite to superconducting behaviour: when taken across the superconductor-insulator transition onto the superconducting side, the same film displayed a drop to zero electric resistance at superconducting transition temperature. Having followed in Kamerlingh Onnes footprints, Dr Vinokur's team also independently termed this newly discovered state with zero conductivity a 'superinsulator'. Dr Vinokur and his colleagues conjectured that close to the superconductor-insulator transition, the films self-organise into arrays of superconducting droplets coupled by Josephson tunnelling. Indeed, they demonstrated that near this transition, these disordered films behave exactly as regular Josephson junction arrays, as if there was no disorder whatsoever.

Dr Vinokur's team has built a solid understanding of the origin of a superinsulator on the foundational concept of quantum mechanics: the Heisenberg uncertainty principle. This principle states that it is impossible to measure two conjugated variables of a quantum system (for example, the position and the momentum of a particle) with absolute precision. The more accurately we know one of these variables, the less accurately we can measure the other.

Josephson junction arrays host two conjugated entities: Cooper pairs, representing electric charges, and superconducting vortices that impersonate magnetic charges. In superconductors, Cooper pairs form quantum fluid called a 'Bose condensate' that manifests quantum properties on macroscopic scales.

The basic experimental fact about superconductors is that the number of 'magnetic charges' is always known and fixed. This means that the number of Cooper pairs in the Bose condensate is fully uncertain and they move without scattering (otherwise one could have counted them), and hence, without resistance.

By reversing the uncertainty principle, Dr Vinokur and his colleagues ruled that fixing electric charges implies that magnetic vortices arbitrarily fluctuate around and become indistinguishable, forming a Bose condensate of magnetic charges. According to fundamental law of superconductivity, the 'Josephson effect', moving vortices create finite voltage. And finite voltage in the absence of current implies infinite resistance, hence formation of a superinsulator.

Characteristics of Quantum Fluids

Using the Heisenberg uncertainty principle brought about an understanding that is now supported by experiments, whereby the effect of infinite resistance at finite temperatures observed by Dr Vinokur's team at the insulating side of the superconductor-insulator transition stems from formation of the Bose condensate of magnetic charges.

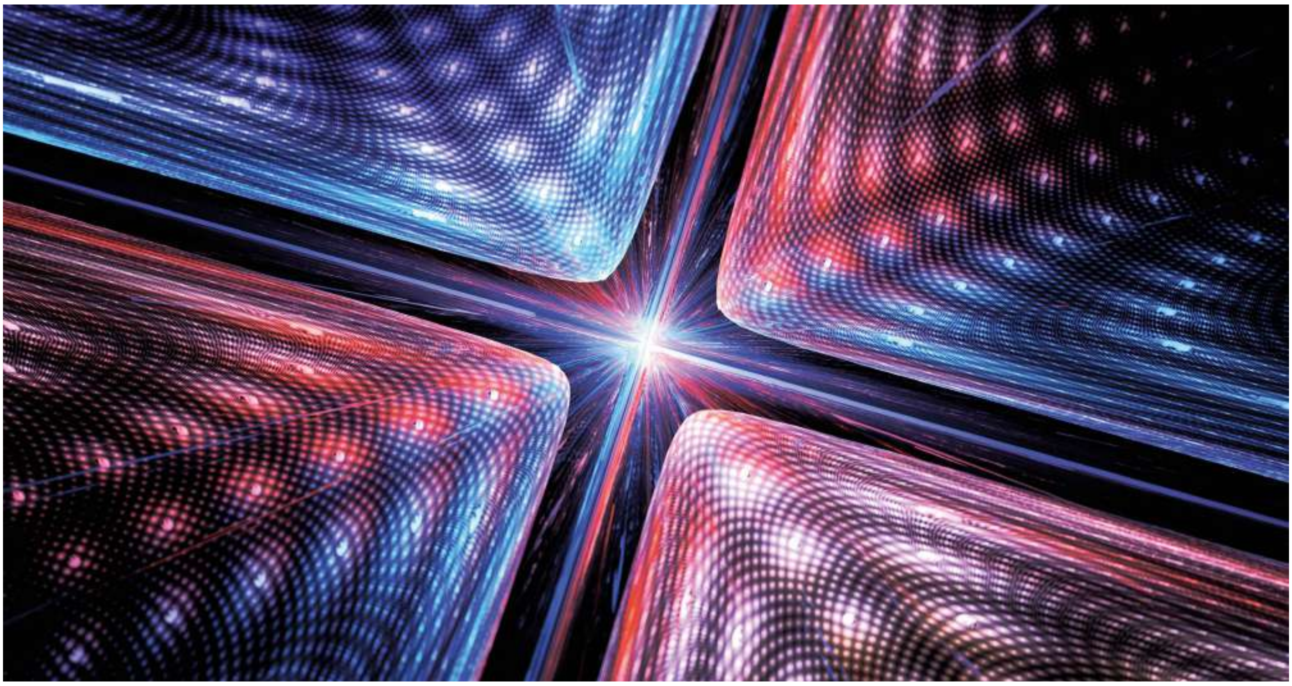
This Bose condensate is a mirror twin of the Bose condensate of paired electrons that is characteristic for the superconducting state. Therefore, duality between electrical and magnetic charges emerged again – now as a consequence of the most fundamental concept of quantum mechanics – and was strongly evidenced by experiment.

Squeezed Magnetic Filaments

The second fundamental effect characteristic to superconductivity to stem from Bose condensates of paired electrons emerges when superconductors are penetrated by magnetic fields. According to Maxwell's laws of electromagnetism and the hydrodynamics of charged superfluid liquids, this causes superfluid paired electrical charges within a material to move in circular paths around the magnetic field lines.

In turn, the magnetic fields created by these circularly moving charges will squeeze the external magnetic field lines into extremely thin filaments. These circling currents are known as 'Abrikosov vortices', and are a key demonstration that homogeneous superconductivity and homogeneous magnetic fields cannot coexist. Superconductors that allow for the penetration of a magnetic field in the form of Abrikosov vortices are called 'type II superconductors'.

Josephson junction arrays host a slightly different kind of magnetic vortices, which can exercise quantum tunnelling in



the grainy Josephson junction arrays observed in Dr Vinokur's experiments. This behaviour mirrors the Cooper pairs' tunnelling between superconducting granules and supports the picture of duality between the properties of electrical and magnetic charges. According to Drs Diamantini and Trugenberger's earlier theories, perfectly mirrored processes should also play out on the superinsulating side of the transition – demanding the presence of magnetic monopoles.

Until then, such effects had gone almost entirely unexplored – but this was about to change through the combined research of Dr Vinokur, Dr Diamantini, Dr Trugenberger, and their colleagues.

Parallels in Superinsulators

After more than a decade of repeating and improving on this initial experiment, the team has now gathered indisputable proof of this effect. Through their observations, they have discovered a necessity for magnetic monopoles to exist on the superinsulating side of Josephson junction array transitions.

Moreover, these singular charges must behave just like quantum particles – forming Bose condensates at ultra-low temperatures, which flow in circular paths around any electric fields that penetrate the material. In the same way that superconductors expel magnetic fields, this process squeezes electric fields into thin filaments, which tightly bind positive and negative charges together. In turn, any free flow of current is completely eliminated, resulting in an infinite resistance in the material.

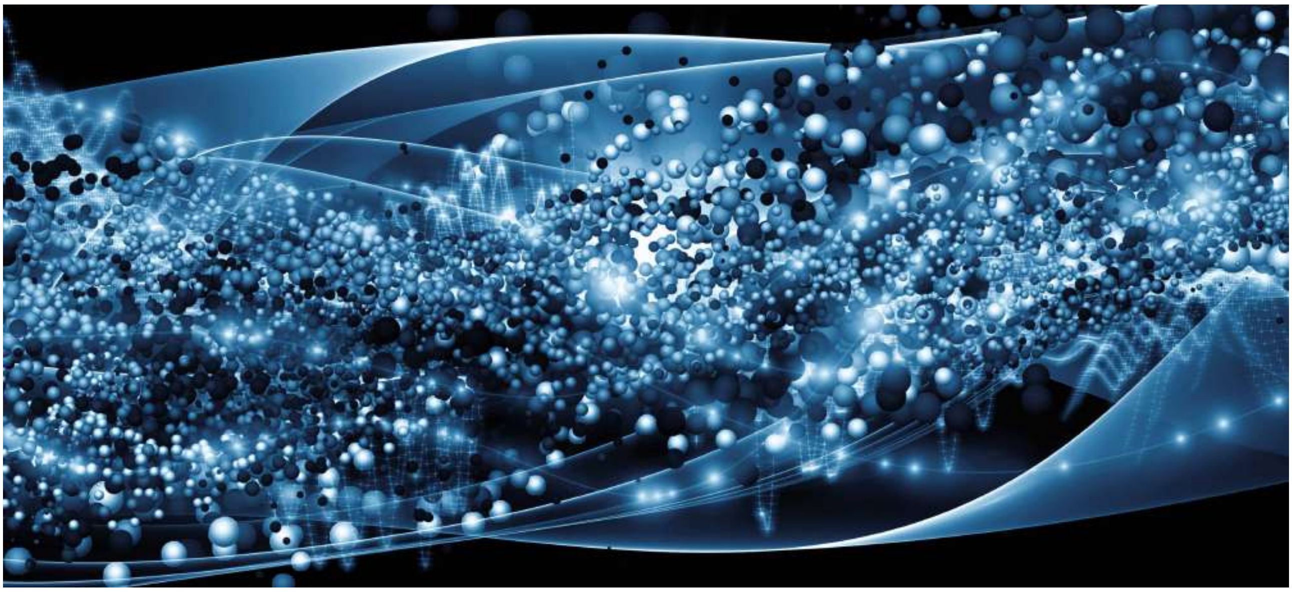
Clearly, this behaviour perfectly mirrors that of the magnetic filaments that form on the other side of the transition – fully realising the duality between electrical and magnetic charges first put forward by Dirac. In addition, the electric filaments display a remarkable similarity with pions – bound states of quarks. These fundamental particles are described by the Standard Model of particle physics, and form the basis of hadrons: a family of particles including protons, neutrons, pions and a diverse range of other, more exotic particles.

Pion-like Strings

Because of the strong nuclear force, a quark can never be observed outside of a hadron. If a physicist ever attempts to isolate a quark, other quarks will be generated spontaneously to ensure the laws of physics are not broken. As a result, the mechanisms used by quarks to bind together into hadrons can only be studied indirectly through high-energy collisions, and are still poorly understood. Such a property is notably comparable with the impossibility of separating the magnetic charges in a bar magnet – and according to the researchers, this is no coincidence.

Previous studies have given rise to theories involving a property named 'colour'. They suggest that quarks interact via the strong force by exchanging three possible colours – whose exact physical nature is still far from clear. In their research, Dr Diamantini, Dr Vinokur and Dr Trugenberger noted remarkably similar roles in the electric filaments observed in their superinsulators.

In particular, the Cooper pairs bound by the filaments have the same electrical properties of particles named 'pions': hadrons containing one of either an up or a down quark, and one of either of their antimatter counterparts. Moreover, this behaviour can be modelled using just one colour – avoiding the need to make any assumptions about unknown aspects of fundamental physics. Such a clear analogy could soon shed new light on a difficult problem in particle physics.



Generalising the Picture

Up until this point, Drs Vinokur, Diamantini, and Trugenberger had only studied the properties of superconductor-insulator transitions in 2D. To gain a full picture of the physics involved, they would need to extend their predictions to a more generalised, 3D case. From their earlier descriptions of electric filament confinement as a mechanism for superinsulation, alongside previous theories of the quantum fields that underly the universe's fundamental particles, the team has now made this step in their latest research.

Through these studies, they have found that magnetic monopoles can display even more exotic behaviours in 3D materials. In particular, they discovered clear evidence for electrical charges being carried on top of magnetic monopoles: particles named 'dyons' by theoretical physicists. Furthermore, these particles can also settle into Bose condensates when cooled, giving rise to even further intriguing properties.

These observations have now improved physicists' understanding of the once mysterious effect of high-temperature superconductivity, which enables current to flow with zero resistance at above ultra-cold temperatures. The researchers have now clearly shown that this behaviour can arise from the interplay between Cooper pairs and dyon condensates – once again, showcasing the key role of magnetic monopoles.

A New Mechanism for Attraction

Through this improved understanding, Drs Diamantini, Trugenberger and Vinokur were next able to shed new light on the mechanism that allows electrons to become paired in the first place, through interactions within their host materials. Previously, this mechanism was thought to be particle-like vibrations named 'phonons', which travel through solid atomic lattices. However, this would no longer work in high-temperature superconductors, where pairing mechanisms would need to be far stronger.

Instead, the researchers have suggested an entirely different route to Cooper pair formation, based on the attraction provided by magnetic monopoles. Unlike phonons, monopole-based mechanisms would allow electrons to become paired even when higher temperatures introduce more vibrations to atomic lattices – which would otherwise drown out the information carried by individual phonons.

This insight could soon be exploited by engineers to design new materials specially tailored to display superconductivity at room temperatures: now one of the most widely pursued goals in materials physics.

Unifying Two Charges

For nearly a century since Dirac's initial theories, the very idea of a symmetry between singular magnetic and electrical charges has been either heavily doubted, or dismissed entirely by many physicists. Yet through their ground-breaking discoveries of the crucial roles played by magnetic monopoles in providing a full picture of the duality of superconducting materials, Drs Vinokur, Diamantini, and Trugenberger are rapidly transforming this picture.

Not only do the team's ideas hold the potential to unify the physics of magnetic charges with those of electrical charges – the technological implications would also be profound. Through new ways to produce high-temperature and even room-temperature superconductors, researchers could soon produce technologies ranging from extremely high-performance sensors, to electrical circuits in which no energy is lost to heat. In turn, such discoveries could pave the way to tackling some of the newest and most exciting technological challenges emerging today.

Meet the researchers

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Dr Maria Cristina Diamantini completed her PhD in theoretical physics at the University of Perugia in 1995. She then held positions at both CERN and the University of Oxford with a fellowship of the Swiss National Science Foundation, while becoming a Humboldt fellow at the Free University in Berlin. She now teaches Theoretical Physics and Statistical Mechanics at the University of Perugia, and is part of the Noise in Physical Systems Laboratory in Perugia and of Italy's National Institute for Nuclear Physics (INFN, Perugia's section). Dr Diamantini has now been part of a wide variety of exciting research projects across Europe.

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Dr Carlo Trugenberger obtained his PhD in theoretical physics at ETH Zurich in 1988, and then pursued an international academic career, eventually becoming an associate professor of physics at the University of Geneva. He then went on to found two artificial intelligence companies – one of which he continues to manage today. Dr Trugenberger's research interests lie in both theoretical condensed matter physics and quantum gravity, and he continues to be an active part of both research communities.

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Professor Dr Valerii Vinokur completed his PhD in theoretical condensed matter physics at the Institute for Solid State Physics of the Academy of Sciences of USSR in Chernogolovka in 1979, where he worked until 1990. In 1990, he assumed an appointment at Argonne National Laboratory, USA. In 2021, he retired from his position of Senior Scientist and Argonne Distinguished Fellow, to join Terra Quantum AG as its Chief Technology Officer in the US. Professor Vinokur is a Foreign Member of the National Norwegian Academy of Science and Letters and Fellow of the American Physical Society. He has won numerous awards for his groundbreaking research, including the International John Bardeen Prize in 2003, the Alexander von Humboldt Research Award in both 2003 and 2013, and the Fritz London Memorial Prize in 2020.

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RYDBERG ATOMS: GIANTS OF THE ATOMIC WORLD

Article written by Dr F. Barry Dunning and Dr Thomas C. Killian

The creation of giant atoms whose size is comparable to that of a grain of sand might sound like the stuff of science fiction, but in fact such species exist in nature and can now be created in the laboratory using advanced laser systems. Such exotic atoms, in which one electron is placed in a highly-energetic state, are termed Rydberg atoms, after the Swedish spectroscopist J. R. Rydberg who first characterised their properties. As might be expected, such extreme atoms possess very unusual physical and chemical properties. Their study has provided many new insights into the properties of Rydberg atoms themselves, their interactions with other atoms and molecules, and phenomena that arise from their collective interactions. The extreme properties of Rydberg atoms now enable emerging technological applications in sensing and quantum computation.

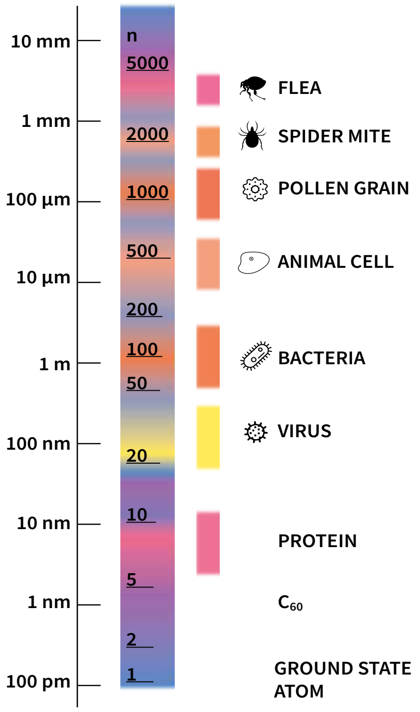
Energetic Electrons

Atoms comprise a compact, positively-charged nucleus, surrounded by one or more negatively-charged electrons, which are bound to the nucleus by electrostatic forces. The size of the atom is determined by the volume occupied by the electrons. Under normal conditions, the electrons are held close to the nucleus, and a billion atoms placed side-by-side would extend only a few centimetres.

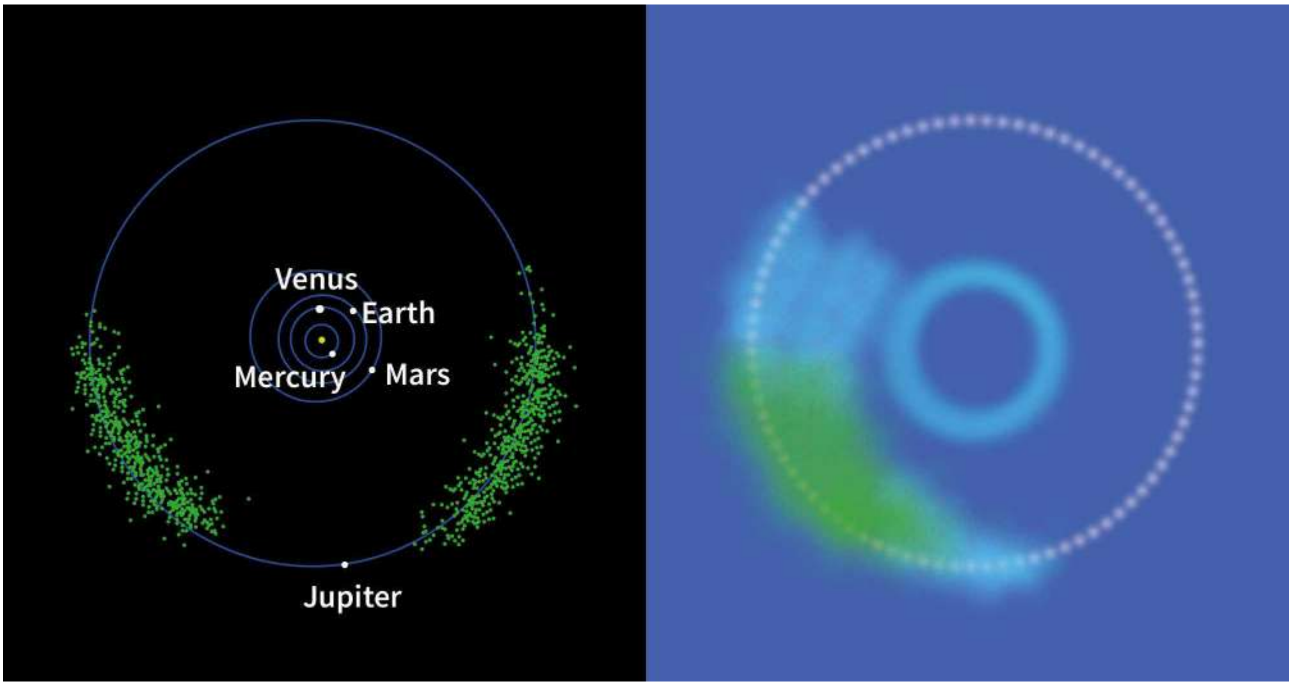
If an electron in the atom is given additional energy, it can jump into one of a series of allowed 'excited states', whose energies and orbital motions are defined by the principal quantum number, *n*. As the energy transfer and *n* increase, the electron is able to travel farther from the nucleus – the distance scaling as n^2. Indeed, if the energy transfer is sufficient, the electron can escape, causing the atom to become ionised.

The largest atoms observed to date have n values of over 1200 and diameters greater than the width of a human hair. However, since the majority of the atomic volume is only occupied by a single electron, these so-called Rydberg atoms are transparent and not visible to the naked eye.

As *n* increases, the extra energy required to remove the electron from the atom, termed its binding energy, decreases rapidly, scaling as $1/n^2$. As a result, high-n atoms are not only very large but are also very fragile. Even a perfect vacuum can be a hostile environment for such atoms, because they can be destroyed by interactions with thermal radiation emitted by the walls of their enclosure at room temperature. However, their natural lifetimes are long. Whereas the lifetimes of low-lying excited states are typically measured in nanoseconds, those of very-high-*n* states can be milliseconds or longer, allowing plenty of time for their study.



Growth of Rydberg atom size with principal quantum number n.



The image on the left shows Jupiter's Trojan asteroids in their orbit, and the image on the right shows the electron probability density distribution in a Rydberg atom that mimics their behaviour.

Controlling Electron Motion

In very-high-*n* Rydberg atoms, the excited electron is so far from the rest of the atom (the 'core ion'), that the electrostatic attraction it experiences from the nucleus is very weak, and its motion can be strongly perturbed or even dominated by weak external electric (and magnetic) fields.

Because the orbital period of the excited electron can approach a few tens of nanoseconds, the electron motion can be controlled with remarkable precision by applying external forces, or 'kicks', in the form of short-duration electric field pulses. Applying a carefully-tailored series of such pulses can be used to engineer the electron orbit and create 'designer' atoms.

This approach has been employed, for example, to localise the electron in a near-circular orbit about the nucleus, creating an atom that mimics the original Bohr model of the hydrogen atom, which pictured an electron in a classical circular orbit about the nucleus. Whereas this model has now been supplanted by more modern quantum theories, it still provides a convenient basis for discussing many Rydberg atom properties.

Similar control techniques have been used to create a model of the solar system within an atom by placing the electron in an orbit that mirrors the behaviour of Jupiter's Trojan asteroids. These asteroids, named after figures in the Trojan Wars, orbit the sun at a similar radius some 60 degrees ahead of, and behind, the planet. In the future it appears possible to create a 'planetary atom' with two highly-excited orbiting electrons.

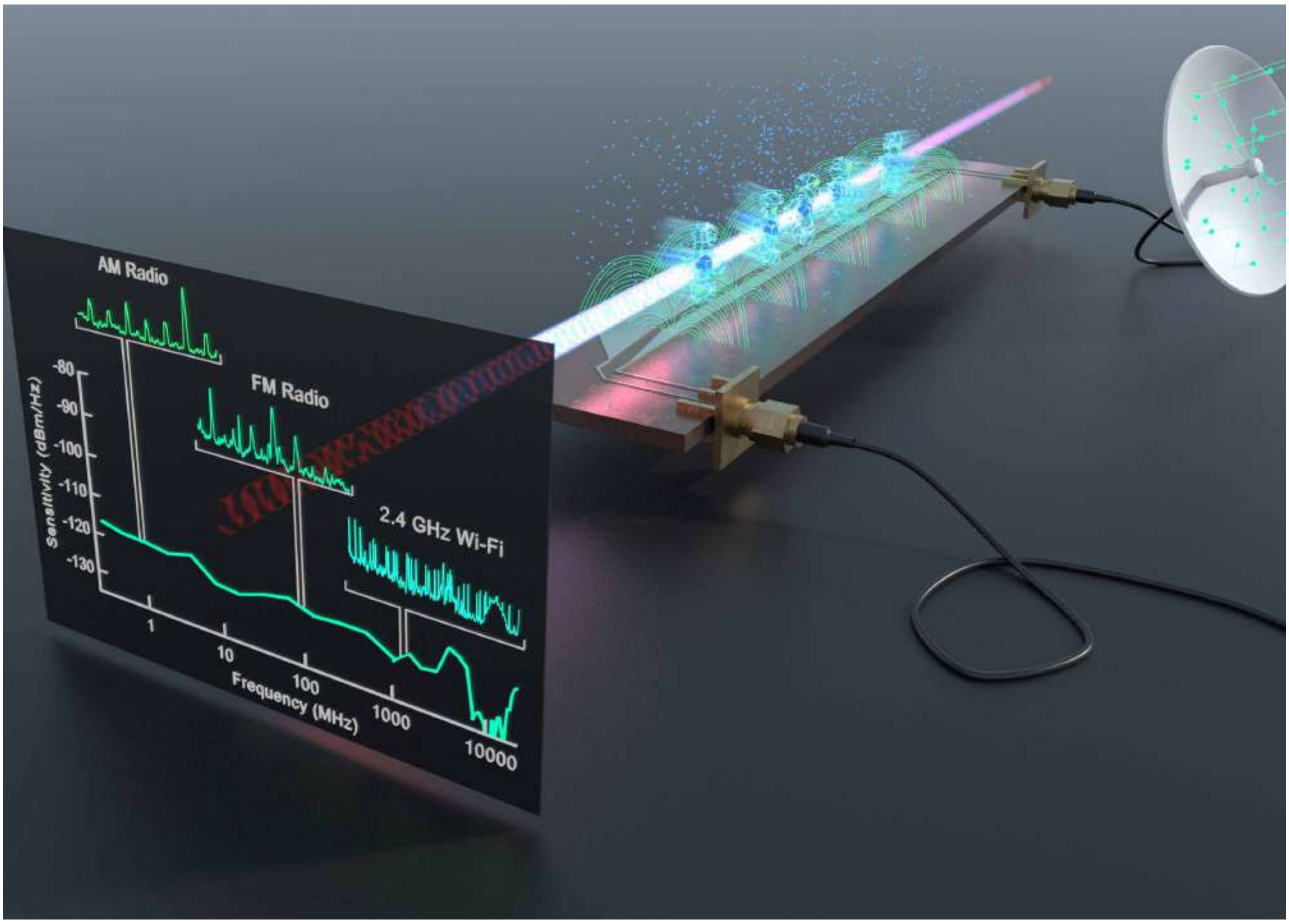
Sensing Applications

Their sensitivity to external electric fields makes Rydberg atoms natural electric field sensors, especially for oscillating fields extending from radio-frequencies to the far infrared. Central to such applications is an effect termed electromagnetically-induced transparency, which involves a collection of atoms through which is directed a 'probe' laser beam tuned to a frequency that the atoms would normally strongly absorb, and a superposed 'control' laser beam tuned to a Rydberg state.

Under appropriate conditions, the presence of the control beam can result in the transmission of the probe beam through the otherwise opaque medium. Given that Rydberg atoms are extremely sensitive to external electric fields, such fields can cause marked changes in the probe beam transmission.

These changes have been exploited to detect radio-frequency fields over a wide frequency range that encompasses AM, FM, bluetooth, and Wi-Fi signals. Because atomic properties are intrinsically stable and are well characterised, the measurement technique is self-calibrating, permitting accurate measurements of absolute field strengths with widespread applications in, for example, communications, radar, and healthcare.

The ability to control the propagation of light through the medium afforded by electromagnetically-induced transparency has also been exploited to slow the speed of light in the medium and create 'slow light' with group velocities as low as a few kilometres per second.



A Rydberg receiver and spectrum analyser above a microwave circuit can detect a wide range of radio signals, including AM, FM, Wi-Fi and Bluetooth. CREDIT: US Army

Collisions and Molecule Formation

Because of their large physical size, in collisions with other atoms or molecules, Rydberg atoms behave not as a single atom, but rather as a pair of independent particles, namely the orbiting electron and the core ion. This behaviour is very different from that of atoms in the ground state or low-lying excited states, and results in a broad range of possible reactions, many unique to Rydberg atoms.

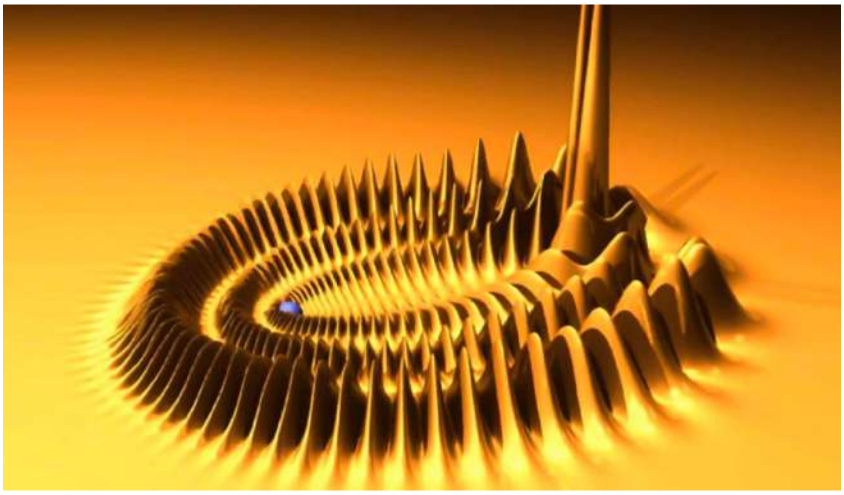
In collisions that are dominated by electron-target interactions, the electron behaves like a free particle, except that its average kinetic energy is determined by *n* and is very low. Indeed, Rydberg atoms provide a remarkable microscale laboratory in which to study a broad range of electron collision processes at effective collision temperatures under 1 Kelvin (–272°C), well below those accessible using any alternate techniques.

One novel outcome of collisions with targets that attach low-energy electrons to form negative ions is the creation of molecules that comprise an electrostatically-bound positive-negative ion pair that orbit at large separations. These giant neutral molecules, termed 'heavy Rydberg' molecules, possess many of the characteristics of Rydberg atoms, except that the electron is replaced by a much heavier negative ion.

A different giant molecular species is formed in Rydberg collisions with molecules that have large permanent electric dipole moments. The Rydberg electron is captured by the target molecule, becoming weakly bound in its dipole field and creating a 'dipole-bound' negative ion. The electron orbits at a large radius near the positive end of the dipole and much of its behaviour again parallels that of a Rydberg electron.

The scattering of the Rydberg electron from a neighbouring ground-state atom creates a novel chemical bond and allows the creation of ultralong-range Rydberg molecules with an internuclear separation comparable to the size of the Rydberg atom itself. The bond is very weak and such molecules are not stable at room temperature. Nevertheless, with the advent of laser cooling and trapping techniques, it is possible to create atomic gases with temperatures of 1 microkelvin or less, which permits the creation and study of such molecular species in the laboratory.

Initial work produced rubidium dimer molecules consisting of one Rydberg atom and one bound ground-state atom. Several different Rydberg dimer species have now been produced and their rich vibrational structure examined. So-called trilobite Rydberg dimers have also been realised that possess giant (permanent) electric dipole moments.



Theoretical electron density pattern of a weakly bound Rydberg molecule, resembling a trilobite. CREDIT: Chris Greene, Purdue University.

Since the size of a Rydberg molecule is determined by the size of the parent Rydberg atom, their formation depends on having atom pairs with the appropriate initial separation. Measurements of dimer formation as a function of n therefore provide a valuable probe of spatial correlations in quantum gases, allowing effects such as particle bunching in a gas of bosons and antibunching in a gas of fermions due to Pauli exclusion to be seen. The formation of more complex molecules with a Rydberg atom bound to two or three ground-state atoms has also been observed.

Rydberg Atoms in Dense Gases

Measurements have been extended to Bose-Einstein condensates, in which the atom densities are so high that a Rydberg electron orbit can enclose tens to even hundreds of ground-state atoms. Those atoms within the Rydberg orbit form weak bonds and create a molecule composed of many 'atoms within an atom', the atoms being corralled by the orbiting electron which serves the role of a shepherd.

The many atoms contained within the molecule constitute a novel form of 'quantum matter' and their interactions can lead to novel collective responses including the formation of 'quasi-particles' similar to those that play important roles in determining the properties of many materials. Indeed, Rydberg molecules provide a valuable window into many of the important phenomena that emerge from many-body interactions in condensed-matter settings.

Quantum Research

Rydberg atoms interact strongly with each other even at large separations. The strength of their interactions is millions of times larger than those between ground-state atoms and is tuneable through the choice of the Rydberg states excited and their physical separations.

Rydberg-Rydberg interactions form the basis of many ongoing studies of quantum simulation and of quantum logic devices. Central to this work is the phenomenon of 'dipole-blockade', in which resonant excitation of one atom to a Rydberg state can shift the energy of neighbouring atoms within some critical 'blockade' radius preventing their subsequent excitation.

The use of focused laser beams, termed 'optical tweezers', to trap and hold atoms now permits atoms to be positioned with remarkable precision. This has enabled the realisation of fast and robust quantum gates using pairs of atoms positioned within the blockade radius. Such gates utilise conditional logic where the excitation of the second atom is governed by excitation of the first one. Quantum gates, or 'qbits', are critical to the operation of a quantum computer.

Tweezer arrays, as well as 'optical lattices' formed by intersecting laser beams, provide the opportunity to assemble one-, two-, and even three-dimensional ordered arrays of Rydberg atoms with precise control of their separations and geometry. Such arrays can be engineered to mimic the arrangement of atoms within a solid. They therefore provide a powerful quantum simulator with which to probe the physical processes that underpin quantum effects that give rise to high temperature superconductivity and magnetism.

Furthermore, by varying the atomic arrangements and interactions, a wide variety of 'artificial' structures not normally found in nature can be simulated and their properties explored. The effects of defects introduced by removing one, or more, atoms from the array at selected points can also be examined. Such studies promise an improved understanding of the behaviour of many condensed matter systems and will enable the design of new materials with enhanced electronic and magnetic properties.

A Future of Discovery

As is evident from the above examples, to study Rydberg atoms is to wander in a land of giants with exciting research opportunities appearing around every corner. They form a valuable bridge between the microscopic world described by quantum mechanics and the macroscopic world governed by Newton's laws, and illuminate the transition from one realm to the other as the length scale increases.

New experimental capabilities continue to drive new avenues of research that exploit their novel characteristics, and going forward it is certain that they will remain the focus of much activity and provide many exciting discoveries.

Meet the researchers

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Dr F. Barry Dunning is the Sam and Helen Worden Professor of Physics at Rice University in Houston, Texas. He received his BSc and PhD degrees from University College, London and moved to Rice University immediately on completion of an ICI Postdoctoral Fellowship. His research interests lie in experimental atomic, molecular, and optical physics. Dr Dunning was an early pioneer in the study of Rydberg atoms and his interest in such atoms and their applications continues to this day.

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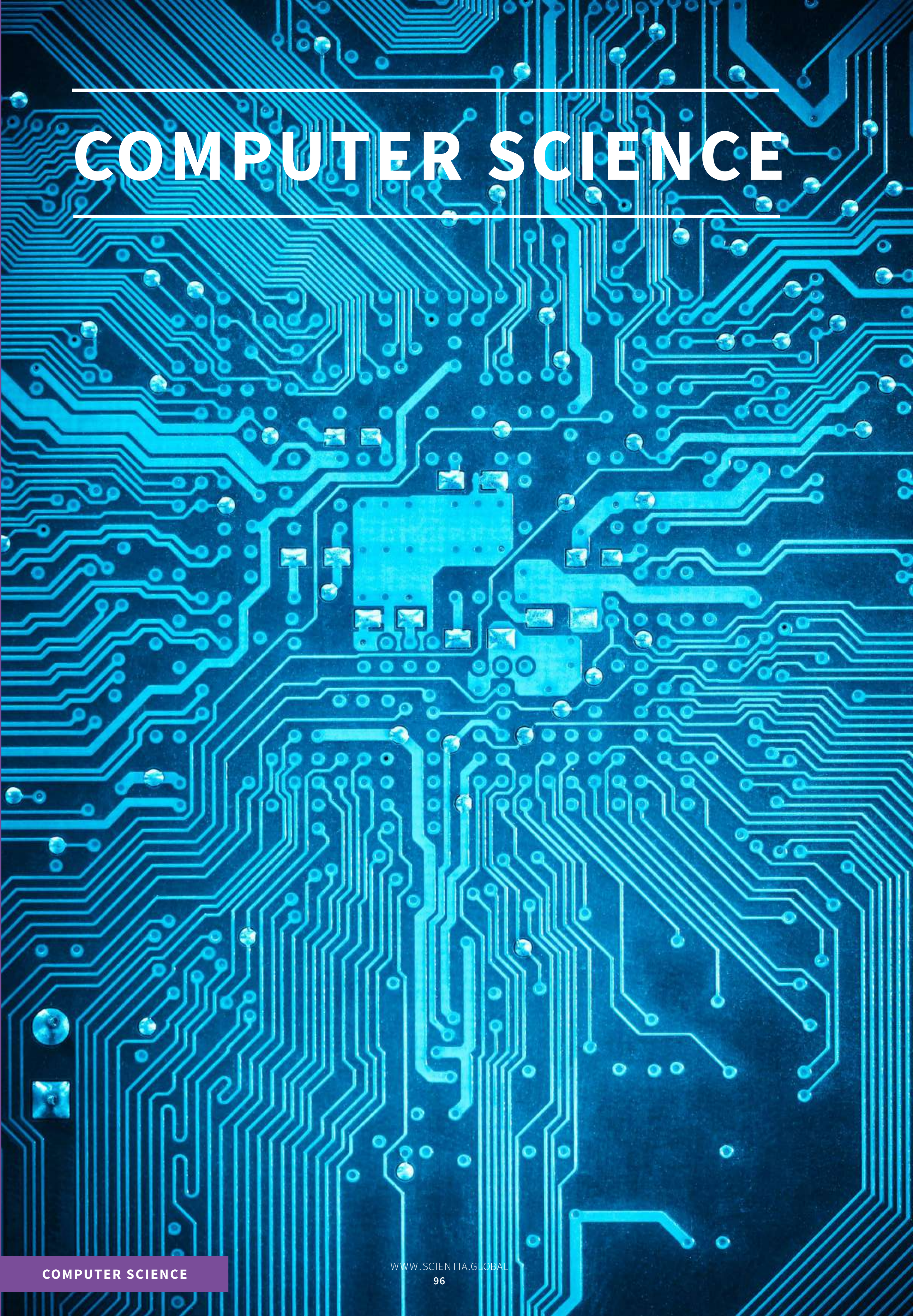
COMPUTER SCIENCE



REVOLUTIONARY ADVANCES IN COMPUTING

The 21st century has witnessed phenomenal advances in computing technology. Computing is now such an ingrained part of modern society, that it's difficult to imagine life without it. From healthcare to education, and from our jobs to our social lives, digital technology pervades almost every aspect of modern life.

During the COVID-19 pandemic, advances in computer science have allowed for countless lives to be saved. Through rapidly processing vast quantities of data, computer models have been widely used to monitor and predict the spread of the virus, speed up diagnosis, identify at-risk groups and rapidly screen thousands of potential drug treatments. Digital technology has also helped to curb viral transmission by enabling us to work, learn, shop and socialise without leaving our homes, which would have been impossible just two decades ago.

To celebrate these great achievements, this section of the edition features researchers who are spearheading the latest innovations in computer science.

We open this section with a focus on quantum computers, which are predicted to revolutionise modern computing technology with their extreme processing power and remarkable capabilities. Over the past few years, the capabilities of quantum computers have reached the stage where they can be used to pursue scientific research with widespread technological impact. However, the software that such computers employ is highly specialised, meaning that it is inaccessible to most researchers in non-quantum fields.

Through their research, Dr Rosa Di Felice and her group – the Q4Q team – explore how software and algorithms designed for the latest quantum computing technologies can be adapted to suit the needs of researchers in diverse scientific disciplines. In a collaborative project, the Q4Q team sets out a roadmap for bringing accessible, user-friendly quantum computing into fields ranging from materials science, to pharmaceutical drug development.

Researchers from Elimu Informatics, the University of Florida and Brigham and Women's Hospital are also using the latest advances in computer science to bridge the gap between different fields. In their project, which we highlight next, the team has built software that can convert between the file format used in genomics, and that used in clinical informatics. Through future improvements, the team's software could soon transform the ways in which crucial clinical decisions are made.

Next, we introduce Dr Guoqing Zhang at the University of Windsor in Canada, who uses the latest computational techniques to streamline our modern supply chains. By integrating computing technologies and optimisation algorithms into the systems that bring products to consumers, Dr Zhang's methods could soon ensure that modern companies will not fall behind.

Meanwhile, at Rutgers University, Dr Hui Xiong has been leading efforts to develop computational tools based on artificial neural networks, which can accurately identify the right candidates for specific jobs. Over the past few years, Dr Xiong has led efforts to design a comprehensive intelligent HR management system that could bring significant intelligence to recruitment consultants.

From here, we move on to research focusing on virtual and augmented reality. Although these technologies have greatly improved in the last few years, they continue to face major challenges due to the wide variability of human vision. Now, Dr Gordon Wetzstein and his colleagues at Stanford University are exploring innovative new ways to overcome these challenges, through the latest advances in computing, optics and vision science.

Our final article showcases the pioneering work of John Sauter and his colleagues at SoarTech, who have developed SwarmMATE™ – a transformative software that enables drones to mimic the behaviours of swarming animals found in nature. The team's software now paves the way for numerous real-world applications – from tracking wildfires and storms to aiding search and rescue missions.

ADVANCING QUANTUM COMPUTING TO ACCELERATE SCIENTIFIC RESEARCH

Over the past few years, the capabilities of quantum computers have reached the stage where they can be used to pursue research with widespread technological impact. Through their research, the Q4Q team at the University of Southern California, University of North Texas, and Central Michigan University, explores how software and algorithms designed for the latest quantum computing technologies can be adapted to suit the needs of applied sciences. In a collaborative project, the Q4Q team sets out a roadmap for bringing accessible, user-friendly quantum computing into fields ranging from materials science, to pharmaceutical drug development.

Quantum Computing

Since it first emerged in the 1980s, the field of quantum computing has promised to transform the ways in which we process information. The technology is centred on the fact that quantum particles – such as electrons – exist in 'superpositions' of states. Quantum mechanics also dictates that particles will only collapse into one single measurable state when observed by a user. By harnessing these unique properties, physicists discovered that batches of quantum particles can act as more advanced counterparts to conventional binary bits – which only exist in one of two possible states (*on* or *off*) at a given time.

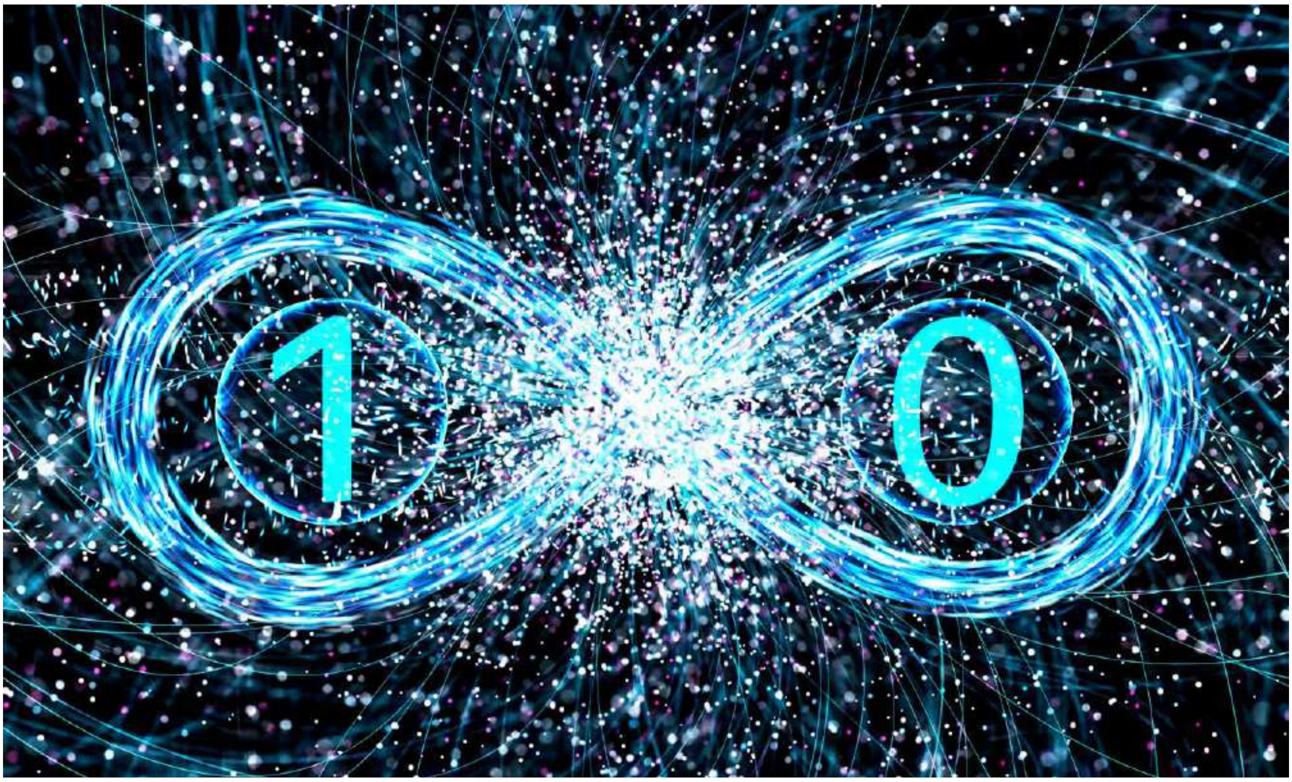
On classical computers, we write and process information in a binary form. Namely, the basic unit of information is a bit, which takes on the logical binary values 0 or 1. Similarly, quantum bits (also known as 'qubits') are the native information carriers on quantum computers. Much like bits, we read binary outcomes of qubits, that is 0 or 1 for each qubit.

However, in a stark contrast to bits, we can encode information on a qubit in the form of a superposition of logical values of 0 *and* 1. This means that we can encode much more information in a qubit than in a bit. In addition, when we have a collection of qubits, the principle of superposition leads to computational states that can encode *correlations* among the qubits, which are stronger than any type of correlations achieved within a collection of bits. Superposition and strong quantum correlations are, arguably, the foundations on which quantum computers rely on to provide faster processing speeds than their classical counterparts.

To realise computations, qubit states can be used in quantum logic gates, which perform operations on qubits, thus transforming the input state according to a programmed algorithm. This is a paradigm for quantum computation, analogous to conventional computers. In 1998, both qubits and quantum logic gates were realised experimentally for the first time – bringing the previously-theoretical concept of quantum computing into the real world.

Stalling Advances

From this basis, researchers then began to develop new software and algorithms, specially designed for operations using qubits. At the time, however, the widespread adoption of these techniques in everyday applications still seemed a long way off. The heart of the issue lay in the errors that are inevitably introduced to quantum systems by their surrounding environments. If uncorrected, these errors can cause qubits to lose their quantum information, rendering computations completely useless. Many studies at the time aimed to develop ways to correct these errors, but the



processes they came up with were invariably costly and time-consuming.

Unfortunately, the risk of introducing errors to quantum computations increases drastically as more qubits are added to a system. For over a decade after the initial experimental realisation of qubits and quantum logic gates, this meant that quantum computers showed little promise in rivalling the capabilities of their conventional counterparts.

In addition, quantum computing was largely limited to specialised research labs, meaning that many research groups that could have benefited from the technology were unable to access it.

Improving Accessibility

While error correction remains a hurdle, the technology has since moved beyond specialised research labs, becoming accessible to more users. This occurred for the first time in 2011, when the first quantum annealer was commercialised. With this event, feasible routes emerged towards reliable quantum processors containing thousands of qubits capable of useful computations.

Quantum annealing is an advanced technique for obtaining optimal solutions to complex mathematical problems. It is a quantum computation paradigm alternative to operating on qubits with quantum logic gates.

The availability of commercial quantum annealers spurned a new surge in interest for quantum computing, with consequent technological progress, especially fuelled by industrial capitals. In 2016, this culminated in the development of a new cloud system based on quantum logic gates, which enabled owners and users of quantum computers around the world to pool their resources together, expanding the use of the devices outside of specialised research labs. Before long, the widespread use of quantum software and algorithms for specific research scenarios began to look increasingly realistic.

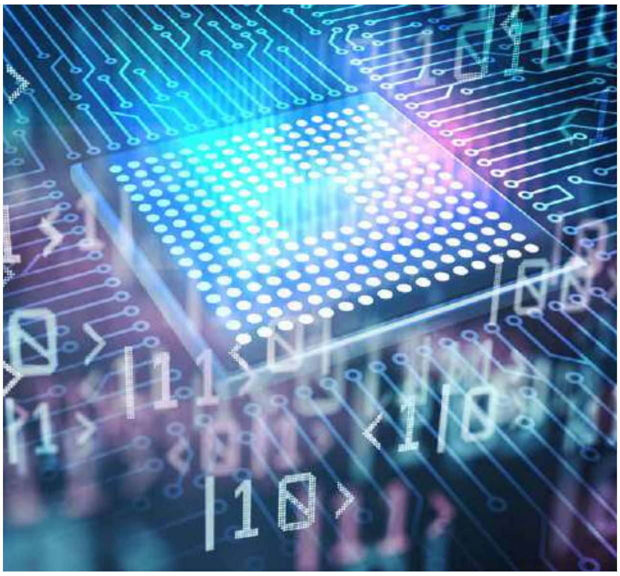
At the time, however, the technology still required high levels of expertise to operate. Without specific knowledge of the quantum processes involved, researchers in fields such as biology, chemistry, materials science, and drug development could not make full use of them. Further progress would be needed before the advantages of quantum computing could be widely applied outside the field of quantum mechanics itself.

Useful Quantum Simulations

Now, the Q4Q team aims to build on these previous advances – using user-friendly quantum algorithms and software packages to realise quantum simulations of physical systems. Where the deeply complex properties of these systems are incredibly difficult to recreate within conventional computers, there is now hope that this could be achieved using large systems of qubits.

To recreate the technologies that could realistically become widely available in the near future, the team's experiments will incorporate 'noisy intermediate-scale quantum' (NISQ) devices – which contain relatively large numbers of qubits, and by themselves are prone to environmental errors.

In their projects, the Q4Q team identifies three particular aspects of molecules and solid materials that could be better explored through the techniques they



aim to develop. The first of these concerns the 'band structures' of solids – which describe the range of energy levels that electrons can occupy within a solid, as well as the energies they are forbidden from possessing.

Secondly, they aim to describe the vibrations and electronic properties of individual molecules – each of which can heavily influence their physical properties. Finally, the researchers will explore how certain aspects of quantum annealing can be exploited to realise machine-learning algorithms – which automatically improve through their experience of processing data.

Molecules and Solids

As they apply these techniques, the Q4Q team predicts that their findings will lead to a better knowledge of the quantum properties of both molecules and solid materials. In particular, they hope to provide better descriptions of periodic solids, whose constituent atoms are arranged in reliably repeating patterns.

Previously, researchers struggled to reproduce the 'wavefunctions' of interacting quantum particles within these materials, which relate to the probability of finding the particles in particular positions when observed by a user. Through their techniques, the Q4Q team aims to reduce the number of qubits required to capture these wavefunctions, leading to more realistic quantum simulations of the solid materials.

Elsewhere, the Q4Q team will account for the often deeply complex quantum properties of individual molecules made up of large groups of atoms. During chemical reactions, any changes taking place within these molecules will be strongly driven by quantum processes, which are still poorly understood. By developing plugins to existing quantum software, the team hopes to accurately recreate this quantum chemistry in simulated reactions.

If they are successful in reaching these goals, the results of their work could open up many new avenues of research within a diverse array of fields – especially where the effects of quantum mechanics have not yet been widely considered. In particular, they will also contribute to identifying bottlenecks of current quantum processing units, which will aid the design of better quantum computers.

Expanding into New Fields

Perhaps most generally, the Q4Q team hopes that their techniques will enable researchers to better understand how matter responds to external perturbations, such as lasers and other light sources.

Elsewhere, widely accessible quantum software could become immensely useful in the design of new pharmaceutical drugs, as well as new fertilisers. By ascertaining how reactions between organic and biological molecules unfold within simulations, researchers could engineer molecular structures that are specifically tailored to treating certain medical conditions.

The ability to simulate these reactions could also lead to new advances in the field of biology as a whole, where processes involving large, deeply complex molecules including proteins and nucleic acids are critical to the function of every living organism.

Finally, a better knowledge of the vibrational and electronic properties of periodic solids could transform the field of materials physics. By precisely engineering structures to display certain physical properties on macroscopic scales, researchers could tailor new materials with a vast array of desirable characteristics: including durability, advanced interaction with light, and environmental sustainability.

Training a New Generation

If the impacts of the team's proposed research goals are as transformative as they hope, researchers in many different fields of the technological endeavour could soon be working with quantum technologies.

Such a clear shift away from traditional research practices could in turn create many new jobs – with required skillsets including the use of cutting-edge quantum software and algorithms. Therefore, a key element of the team's activity is to develop new strategies for training future generations of researchers. Members of the Q4Q team believe that this will present some of the clearest routes yet towards the widespread application of quantum computing in our everyday lives.

Meet the Q4Q Team

The Q4Q team was established in 2018, when the lead investigator Rosa Di Felice took the initiative to respond to a funding opportunity of the US Department of Energy (DOE). The team was consolidated with the DOE funding in September 2018. In addition to the lead investigator, the core team comprises Anna Krylov, Marco Fornari and Marco Buongiorno Nardelli. It has been recently expanded to include Itay Hen and Amir Kalev.

Rosa Di Felice is an Associate Professor of Physics and Astronomy and Quantitative and Computational Biology at the University of Southern California, and a Research Director of the Italian National Research Council, Institute of Nanoscience. She is an expert in computational predictions of structures and electronic properties of solids and molecules.

Anna Krylov is a Professor of Chemistry at the University of Southern California. She is an expert in quantum chemistry of open-shell and electronically excited species, and an inventor of models and methods for strong correlations and molecular properties.

Marco Fornari is a Professor of Physics at Central Michigan University. He is an expert in theoretical and computational condensed matter physics, particularly in high-throughput materials prediction for energy conversion and other technical applications.

Marco Buongiorno Nardelli is a professor of Physics and Chemistry at the University of North Texas in Denton. He is an expert in computational materials science and high-performance simulations.

Itay Hen is a Research Lead at the Information Sciences Institute of the University of Southern California and a Research Associate Professor with USC's Physics and Astronomy department. He is an expert in quantum algorithms, complexity, simulations and implementation.

Amir Kalev is a Research Scientist at the Information Sciences Institute of the University of Southern California. He is an expert in quantum physics and developer of quantum algorithms.

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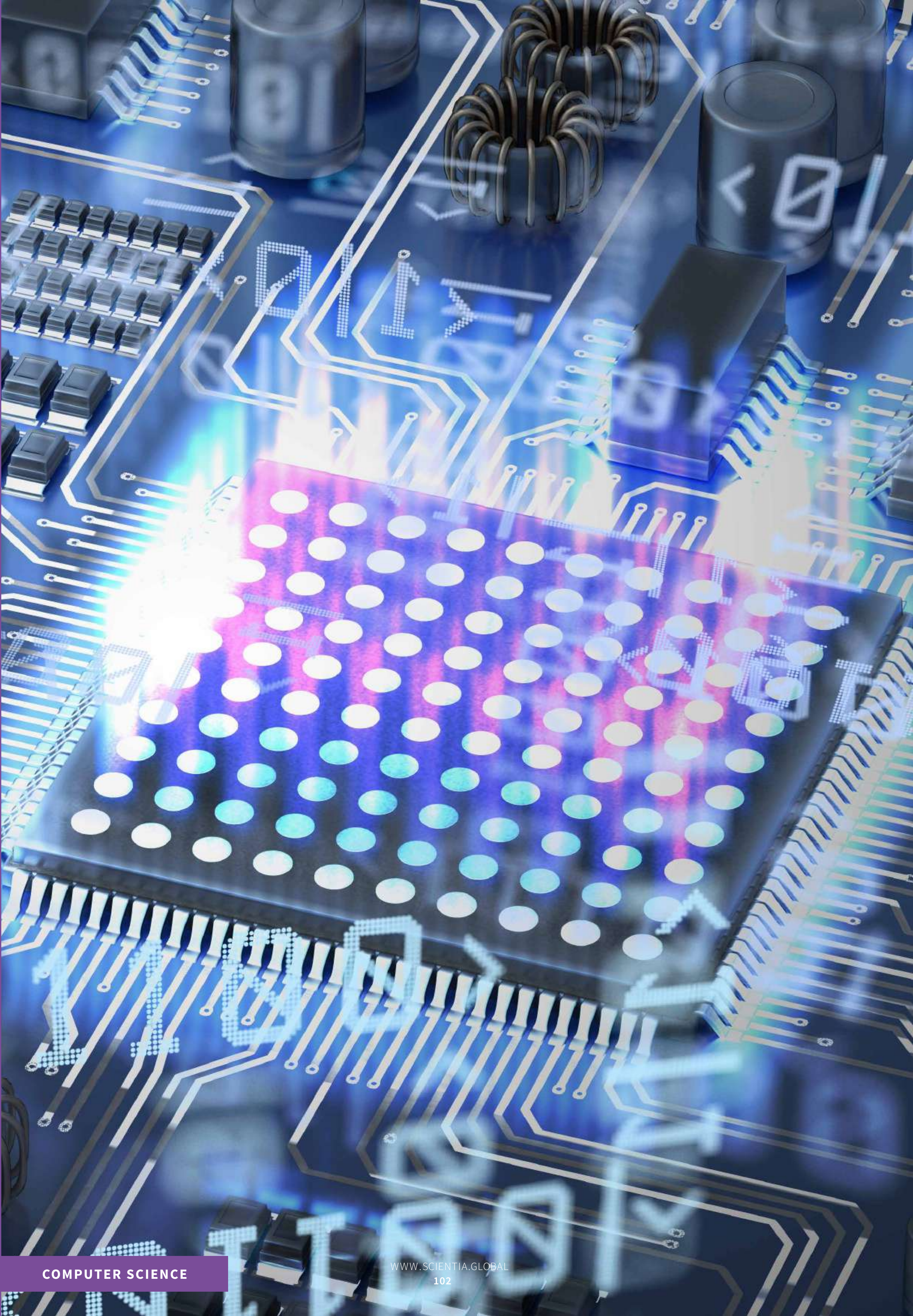
Quantum Computation
for Quantum Prediction
of Materials and Molecular Properties



vcf2fhir: BRIDGING THE GAP BETWEEN GENOMICS AND HEALTHCARE

On molecular scales, the responses of our bodies to particular medical treatments are deeply engrained in our unique genetic codes. Yet so far, the advanced computer science technologies used to study patient responses and molecular-scale mechanisms have remained entirely independent from each other. Now, **Dr Robert Dolin** of Elimu Informatics, **Dr Srikar Chamala** at the University of Florida, and **Dr Gil Alterovitz** at Brigham and Women's Hospital, address this issue through vcf2fhir: a resource capable of converting between the file formats used by both fields. Through future improvements, his team's approach could soon transform the ways in which crucial clinical decisions are made.

Informatics

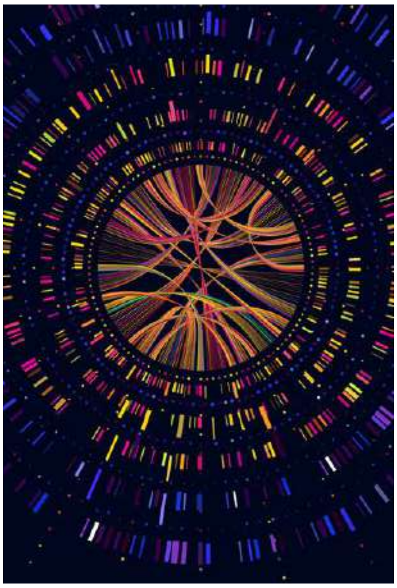
Today's technologies allow us to apply the data we gather from many different sources across numerous sectors of society. Such actions encompass an extensive range of fields, including artificial intelligence, robotics, and statistical analysis – yet as a whole, they can be described as part of a broader field, named 'informatics'. As one of the most important branches of modern computer science, this area of technological innovation ensures the continuing operation of many of the data-driven systems we have come to rely on.

Two specific branches of informatics are now key elements of genetic research, and digitised healthcare systems, respectively. On one hand, the field of 'bioinformatics' develops software that can interpret the deeply complex biological datasets describing living organisms. On the other, 'clinical informatics' deals with the application of data to assessing medical problems – allowing clinicians to make more informed decisions about diagnoses and treatments. Yet despite the fact that both fields appear to be highly relevant to one another, and could stand to benefit from each other's operations, there have been few efforts to unify them so far.

Genomics and Molecular Medicine

In modern healthcare systems, clinical informatics can be easily utilised using digital collections of medical information, named Electronic Health Records (EHRs). These records can contain systemised data relevant to both individual patients and wider populations, and can be freely shared across all relevant groups within healthcare systems – ensuring that medical procedures can be carried out as effectively as possible.

In a parallel field of research, the data gathered through bioinformatics can describe precisely how certain medical procedures will affect patients on a molecular level. As a result, this data would be immensely valuable to include in EHRs.



Two particular branches of science would be particularly useful. Firstly, the field of 'genomics' can map out a complete set of a patient's DNA, describing how all of their interrelated genes will collectively respond to certain treatments. Secondly, 'molecular medicine' explores how genomes will respond to the molecular structures and mechanisms contained in medicines – potentially allowing for highly targeted treatments.

‘Precision medicine aims to bring together all possible data sources to guide the care of an individual,’ describes Dr Robert Dolin of Elimu Informatics in California. ‘We are seeing tremendous growth in genomics and molecular medicine – these fields have such voluminous data that they pose challenges for today’s EHRs.’

Dr Dolin and his colleagues, Dr Srikar Chamala at the University of Florida, and Dr Gil Alterovitz at Brigham and Women’s Hospital in Massachusetts, aim to finally bridge the gap between bioinformatics and clinical informatics. To do this, they look to the latest advances in computer science.

Converting Between File Formats

Many of us will be familiar with the experience of converting files between different formats – whether saving a Word file as a PDF, or converting between JPG and PNG images. To allow us to do this, software developers have designed specialised programs that can essentially express the code underlying a file in a different language. Such translations enable programs that have been built to operate using one file format to handle those initially written in other formats – making them crucial to ensuring that many digital systems can run smoothly.

Through their work, Drs Dolin, Chamala and Alterovitz aimed to build software for carrying out similar conversions between file formats, albeit on colossal scales. In the language of bioinformatics, the data describing an organism’s unique genome is stored on a text file in a Variant Call Format (VCF) – which can be readily written, stored, and read out by geneticists.

In clinical informatics, a format named Fast Healthcare Interoperability Resources (FHIR) is used as a common standard for the files used in EHRs. This format stores data in ways that all healthcare providers can work with universally. Ultimately, the differences between these two formats are at the root of the difficulty in unifying bioinformatics and clinical informatics. However, as Dr Dolin and his colleagues have shown, the challenge is not insurmountable.

Bridging the Data Gap

In their latest research, Drs Dolin, Chamala and Alterovitz introduce an advanced piece of software named ‘vcf2fhir’ – which provides a robust way for researchers, healthcare providers, and any other relevant groups to reliably convert files in the VCF format into FHIR, and vice versa. ‘Our vcf2fhir converter is a bridge between molecular data and the EHR,’ Dr Dolin explains. ‘The converter can extract relevant slices of molecular data, package it up in a language the EHR understands, and deliver it to the EHR, where it can be used by precision medicine algorithms to improve patient care.’

Such advanced capabilities will be immensely useful to clinicians, who likely don’t have an in-depth knowledge of the precise molecular-scale mechanisms that take place when certain treatments are applied. Using vcf2fhir, they will be able to draw from the findings of cutting-edge research in genomics and molecular medicine – finally bridging the gap between the bioinformatics and clinical informatics communities.

In turn, two fields that have developed entirely independently of each other so far will be able to work more closely together – opening up advanced new capabilities in both healthcare and research. Having developed vcf2fhir, Drs Dolin, Chamala and Alterovitz next aimed to test their converter's ability to provide useful guidance in real-world healthcare scenarios.

Practical Decision Making

Perhaps one of the most immediately applicable areas of vcf2fhir is in 'pharmacogenomics' – a field that studies the role of a patient's genome in their response to certain drugs. This is particularly important to consider when predicting allergic reactions in patients. Depending on their unique genome, their reaction of a patient to a particular chemical can cause damaging side-effects, which may appear unexpectedly if the patient hasn't received that treatment before.

Some recent studies have discovered that as many as 7% of all FDA-approved treatments in the US, and some 18% of all written prescriptions, are affected by patient pharmacogenomics. This is now driving a crucial need for clinicians to easily identify how drugs will affect patients on a molecular level, before deciding to prescribe them. In their study, Drs Dolin, Chamala and Alterovitz tested a functional prototype of vcf2fhir for its ability to develop a reliable clinical decision support service – where genomic data could be used to make practical decisions through patient EHRs.

Assessing Drug-gene Interactions

In many medical procedures, it is common for clinicians to require certain information about a patient's genetic code, which may have never been recorded before. In these cases, a conversion from the patient's FHIR files into a VCF format could allow them to determine the exact genetic information they need to obtain to carry out the procedure effectively. By interfacing the vcf2fhir software with patient EHRs, such important clinical decisions could be made quickly and easily, allowing for treatments which are specifically tailored to the pharmacogenomic needs of patients.

'We showed that we could provide drug-gene interaction checking to clinicians right when they are ordering a medication, thereby avoiding potentially serious drug reactions,' says Dr Dolin. Leading on from their initial research, Drs Dolin, Chamala and Alterovitz have now applied vcf2fhir in two further case studies.

Firstly, the SMART Cancer Navigator is a web application that can link patient EHR data with information describing the genetics of various types of cancer. This enables far more coordination between the many medical groups involved in the treatment of cancer patients – leading to more beneficial clinical decisions in turn.

Secondly, the Precision Genomics Integration Platform enables clinicians to intersect a patient's clinical and genomic data with their own knowledge – allowing for the efficient delivery of new, relevant genomic findings to the patient's EHR. From the success of these initial case studies, Drs Dolin, Chamala and Alterovitz now hope that the use of vcf2fhir could be greatly expanded in the near future.

A Bright Future

As an open-source software facility, vcf2fhir could soon become widely accessible, and has already attracted early interest from a wide variety of healthcare institutions across the US. 'Project collaborators come from the University of Florida, Intermountain Healthcare, Cincinnati Children's Hospital, Boston Children's Hospital, Brigham and Women's Hospital, the Harvard/MIT Division of Health Sciences and Technology, and Harvard Medical School,' Dr Dolin concludes.

For now, additional testing will be crucial before vcf2fhir can be realistically applied in real-world healthcare and genomics settings. Yet through this further research, Drs Dolin, Chamala and Alterovitz are hopeful that future efforts to bridge the long-present gap between both fields could lead to profound improvements in the ways that they both operate.

Meet the researchers

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Dr Robert Dolin completed his MD at the University of California, Irvine in 1986. Ever since, his career has been driven by a goal to improve healthcare through the use of computer technology. In 1989, he became the Chief Resident in Internal Medicine at UCLA, where he designed and implemented the first adaptive Electronic Health Record for patient data. Afterwards, he was instrumental in the development of the Clinical Document Architecture standard; and also developed an interest in genetics along the way. Dr Dolin joined Elimu Informatics in 2009, where he now works as a Senior Informaticist. He now strives to continue his efforts to developing robust clinical standards, and using them to integrate genetic information into Electronic Health Records.

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Dr Gil Alterovitz completed his PhD in Electrical and Biomedical Engineering at MIT and Harvard University in 2006. He has since taken research positions at institutions including Harvard Medical School, and the Children's Hospital Boston – before becoming a Lead Investigator at the Brigham and Women's Hospital in 2020. Dr Alterovitz's main research interests focus on the development of novel, interdisciplinary approaches for machine learning in computational biomedicine for infectious diseases. This has led him to develop new ways for studying aspects including drug resistance in tuberculosis, and single-nucleotide polymorphism in DNA.

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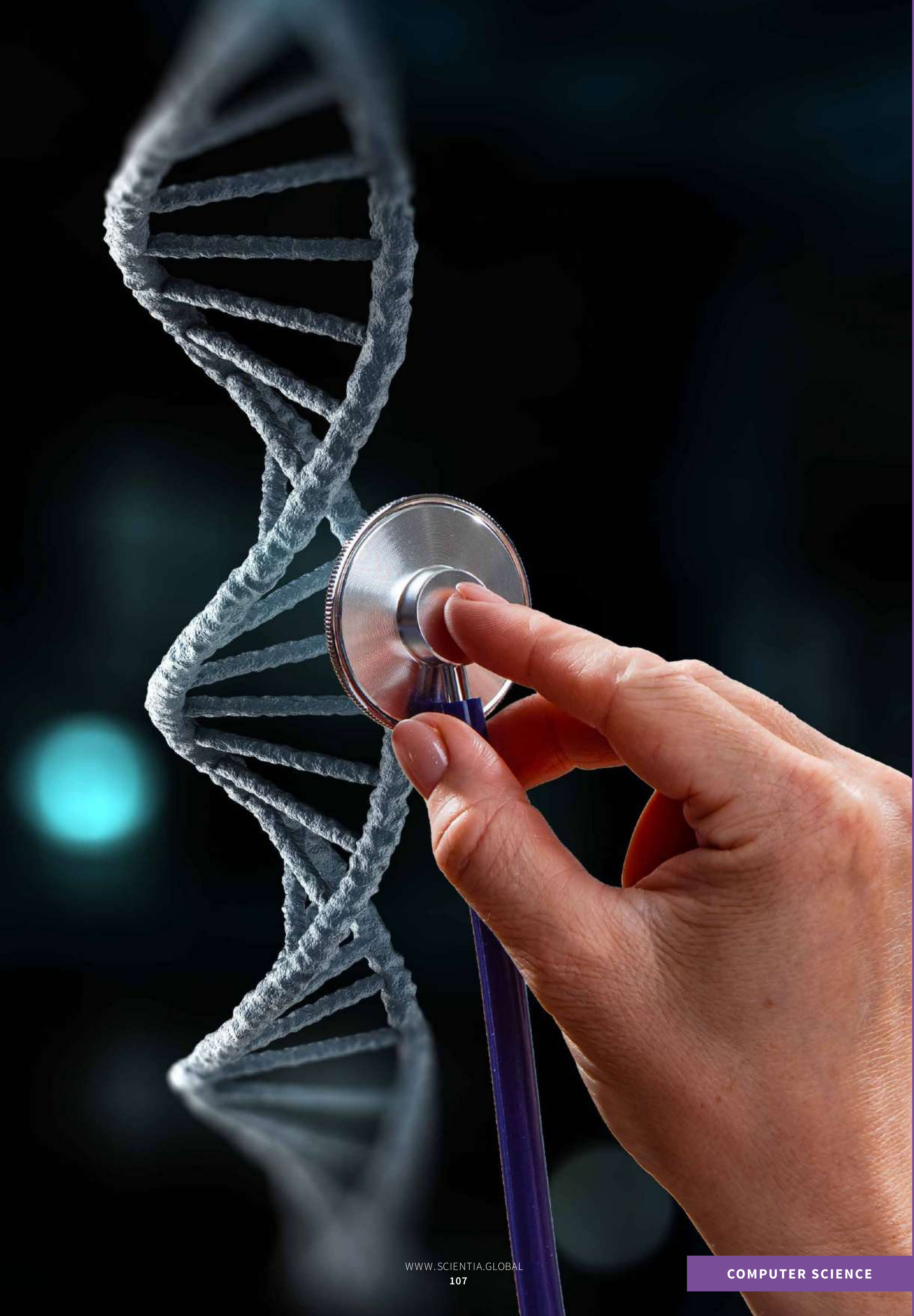

STREAMLINING THE MODERN SUPPLY CHAIN

The digital age has seen a profound shift in how we consume products. Not only have many of us shifted to doing most of our shopping online; new technologies are also transforming how products are produced. These shifts have brought about similarly monumental changes to the supply chains that bring products to the doorstep, presenting significant new challenges to the complex networks of groups involved. In his research, **Dr Guoqing Zhang** at the University of Windsor in Canada uses the latest computational techniques and optimisation algorithms to present smart solutions to these issues.

Profound Change

In little over two decades, the ways in which most people in the developed world buy and consume products has changed almost beyond recognition. Previously, our only option to shop was to visit a physical store, whereas now, most of us frequently go online to buy products ranging from food to the latest technologies. Throughout the COVID-19 pandemic, online shopping has allowed millions of people to obtain essential supplies while remaining in the safety of their homes, helping to curb the spread of the virus.

In the US, the convenience of online shopping meant that total sales reached almost $350 billion in 2015 – a figure which was then predicted to grow annually by 6% until 2020. This profound shift spurred many companies to migrate from physical retail alone, to an approach that combines both physical and online channels.

Although this has largely occurred behind the scenes, such a significant transformation in behaviour has had a large influence on product supply chains, which encompass broad networks of people, companies, activities, information, and resources. Throughout their operation, these systems take in raw materials; transform them into finished products over successive stages; and finally, deliver them to consumers. This intricate process can be severely disrupted if any changes are not implemented effectively. In turn, this has required a substantial rethink amongst industries about how the movement and storage of materials and final products should be managed.

The Modern-age Newsboy Problem

Although this is a distinctly modern problem, Dr Guoqing Zhang at the University of Windsor shows that links can be drawn with the far older 'newsboy problem', which considers how managers need to make decisions about their inventory over limited periods.

In the past, news vendors faced constant uncertainty in the demand for their products. To deal with this problem, they needed to make smart decisions about how many papers to buy from a supplier each morning: if they bought too many, their leftover products would be worthless the next day; but if they bought too few, they would miss out on crucial opportunities to make more profit.

For modern industries, this problem becomes highly relevant when considering how multiple products should be sold – a situation that has now been widely studied for decades. In a 2008 study, Dr Zhang developed an algorithm that offered new solutions to this problem, accounting for factors including budget constraints, which limit the number of products that can be sold, and promotional price discounts, which would diminish profits if not enough products are sold. Since then, Dr Zhang has expanded on these advanced algorithms and mathematical techniques to explore how solutions to the newsboy problem can inform the supply chains of the digital age.

Recently, he also used a newsvendor model to formulate some supply chain risk management problems, and analysed the impacts of a manufacturer

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or retailer's risk attitude (such as risk-neutral or risk-averse) on ordering and marketing strategies. His team then developed an optimal capacity strategy for new product development with risk consideration, and applied it to the automotive industry.

Closed-loop Supply Chains

In a 2013 study, Dr Zhang became the first to consider how the newsboy problem is simultaneously affected by both supplier discounts and budget constraints: a situation that required an entirely new approach to analysis compared to previous approaches to the newsboy problem. His proposed algorithm was extremely effective in solving the problem on both small and large scales, even when it was extended to consider multiple realistic constraints. In particular, he considered 'closed-loop' supply chains – which involve products and materials travelling both forwards and backwards among networks of actors.

In this research, Dr Zhang investigated the characteristics of such a system made up of multiple interconnected plants, collection centres, demand-generating markets, and products. His methods led to a model that minimises the total costs for these supply chains, and that could be extended to consider external factors leading to unexpected variations in their operation. In addition, it could account for the impact of uncertainties in demand along both directions in the chain. To achieve this, Dr Zhang needed to incorporate elements of randomness into his models – a factor that would be crucial in his subsequent research.

More recently, his team studied production quantity, pricing and collection network decisions for manufacturing enterprises under either the 'take-back' or 'carbon emission capacity' regulations, and applied it to electronic waste collection and a tyre closed-loop supply chain.

Handling Two Channels

The dual physical and online channels described by Dr Zhang have brought about significant new challenges to the operation of modern supply chains. Together, they need to handle customers who can be distributed across wide geographical regions; deal with large volumes of orders that are often very small; and achieve short, flexible delivery times, often at night. As in the original newsboy problem, variations in demand across both of these channels can create significant uncertainties regarding how they should be operated.

Following on from his previous findings, Dr Zhang next aimed to analyse the impact of this type of commerce and 'omni-channel' commerce (referring to retailers with both a physical and digital presence to provide seamless shopping experience) on the management and logistics of supply chains, and to provide concrete solutions to how they should be configured effectively. In doing this, he used his algorithms to design new approaches to dual- or omni-channel commerce with random demand, which consider factors including facility locations, inventories, warehouse storage, and transportation. Through this approach, he hoped that his findings would provide key guidance to retail and manufacturing industries as they shift their operations to incorporate dual-channel supply chains.

Managing Warehouses and Inventory

Through a subsequent study, published in 2018, Dr Zhang drew on these cutting-edge techniques to suggest how optimised supply chains could be specifically designed to account for modern behaviours. To do this, he examined the inventory policies for newly emerging dual-channel warehouses, which are uniquely divided into two areas: one for fulfilling online orders; and the other for both storing products and fulfilling offline orders.

Dr Zhang also studied warehouse layout problems where both horizontal and vertical travel costs need to be considered, and developed several algorithms to solve these complex issues. Motivated by a real-world case, he also proposed an integrated strategy to combine production planning and storage layout, and analyse the impact of the 'Internet of Things' (IoT) on warehouse operations, in the first research to combine these two problems. His strategy ensures the availability of warehouse space, and saves costs during production and warehouse operation.

Realising Smart Supply Chains

Since the time of Dr Zhang's earlier research, an almost bewildering array of new technologies have emerged, including the internet of things, cloud

computing, and artificial intelligence. Although these terms can encompass widely varying systems, they are united in their ability to bridge the gap between advanced computational architectures, and everyday situations in the real world. Therefore, each of these technologies can be integrated into 'smart' supply chains to make them more cost-effective, share information more effectively amongst networks of companies, and better account for random uncertainties in the external environment.

However, these supply chains inevitably bring new challenges due to the manufacturing and business models they entail, and the high risks of uncertainty involved with applying new technologies. Therefore, it is critical to study how smart supply chains can be made to connect networks of companies and individuals with relevant technologies, and how industries can reconfigure and optimise their existing networks. Ideally, these systems would even have the capacity to intelligently plan, control, and adjust the systems to match supplies with ever shifting demands in real time.

Developing Optimisation Algorithms

To realise these capabilities, Dr Zhang and his colleagues are now working towards the development of advanced optimisation algorithms – which can find the best possible solutions out of all possibilities. This has involved exploring a variety of techniques and case studies. In his earlier research, Dr Zhang developed a software package for solving large-scale linear optimisation problems, which can be applied to various fields of study. Leading on from this, his team used these techniques to determine how the operation of a world-leading airline's vast cargo network could be optimised. From analysis of real data, the researchers solved routing problems, which would have once taken over 450 hours of calculation, in just 7 minutes.

More recently, Dr Zhang developed novel optimisation algorithms for solving diverse problems, including healthcare supply network issues and supply chain problems, such as warehouse layout and operation. Through their optimisation algorithms, his team showed how the operation costs of complex warehouses could be reduced by 26%.

Incorporating New Technologies

In his upcoming research, Dr Zhang will rigorously study the challenges faced by the supply chains of the digital age, resulting in new frameworks and optimisation algorithms for smart supply chains. In particular, he will focus on four key areas. Firstly, he will study the impacts and opportunities for new digital technologies like the internet of things and cloud computing, and will design new business models that can incorporate them effectively. Secondly, he will develop new concepts and methods for smart supply chain manufacturing – focusing on problems as wide ranging as uncertainty, tactical planning decisions, procurement, distribution, sales, and smart warehouse operation.

Thirdly, Dr Zhang will develop data-driven optimisation models, methods, and algorithms, which will enable him to study how modern data analysis can be combined with classical optimisation techniques to solve complex management problems. Finally, he will work with partners in real industries, including car manufacturing, energy, retailing, food, and medicine, enabling him to effectively solve the problems which arise for real-world supply chains, and to verify the solutions which have already been proposed.

Recently, Dr Zhang has also proposed an IoT-assisted randomised storage layout policy, and developed an integrated strategy to combine this with production planning. Through rigorous analysis, the IoT-assisted randomised storage policy can reduce operation costs by up to 28% and increase space utilisation by up to 17%.

Ensuring Success in Future Supply Chains

Through over a decade of research into how modern supply chains have been transformed by the digital age, Dr Zhang has made important advances in our understanding of how industrial practices have adapted. In the coming years, the technical landscape now looks set to transform in more profound ways than ever before – meaning his results have never been more relevant. By fully integrating the latest technologies and optimisation algorithms into the systems we rely on to bring products to consumers, while fully accounting for rapid improvements, Dr Zhang's methods could soon ensure that modern companies will not fall behind.

Meet the researcher

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Dr Guoqing Zhang achieved his PhD in Management Sciences from City University of Hong Kong in 2000. He has since worked at a variety of institutions worldwide, including as a postdoctoral fellow at McMaster University in Canada, a visiting associate professor at the University of Pittsburgh in the US, and a JSPS fellow at Osaka University in Japan. He joined the University of Windsor in 2002 as an Assistant Professor, then became an Associate Professor in 2005, and has been a Full Professor since 2011. His current research interests include smart supply chain and logistics management, the design of intelligent decision support systems, and optimisation algorithm design and development. He has earned numerous awards for his important findings in these areas, including the first practice prize of Canadian Operational Research Society in 2015 and the Outstanding Paper Award at the IEEM International Conference in 2014. He has also developed an effective optimisation software for solving large-scale linear programming.

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MATCHING PEOPLE WITH THEIR IDEAL JOB USING ARTIFICIAL INTELLIGENCE

The main responsibility of recruitment consultants is to match individuals to jobs that best suit their professional experience, skills, capabilities, dispositions, and academic background. **Dr Hui Xiong** at Rutgers University has been leading efforts to develop tools based on artificial neural networks that can automatically identify the right individuals for specific roles. Over the past few years, he has led efforts to design a comprehensive intelligent HR management system that could bring significant intelligence in human resource management.

Tech-fuelled Evolution of Recruitment

Practices in the field of human resources (HR) management have been continuously evolving over the past decade or so, in large part due to the emergence and proliferation of online recruitment platforms. Platforms such as LinkedIn, Lagou, Glassdoor and Indeed have opened new possibilities for recruiters to seek out and source fresh talent, allowing HR agents to easily advertise new job opportunities to a wider range of potential applicants. For instance, in 2017 alone, LinkedIn had 467 million users and 3 million active job listings.

In addition to allowing employers and HR agencies to conveniently access talent worldwide, online recruitment platforms have enabled the collection of vast amounts of employment-related data. This data could aid the development of tools to automate or simplify the recruitment process, such as job recommendation systems or models that match individuals to suitable jobs.

The main responsibility and objective of recruitment agents is to identify the best person-job fit. Past studies suggest that a person's suitability for a given job depends on several factors, including obvious ones such as their practical skills, academic background, and past professional experience, as well as psychological features, such as their personality traits, attitude, abilities, and preferences.

Dr Hui Xiong, a Distinguished Professor at Rutgers, the State University of New Jersey, has been developing artificial intelligence (AI) approaches that could help recruiters to identify ideal candidates for a given job faster and more efficiently. These tools are trained on datasets containing a wide range of real employment-related data.

'Our suite of algorithms and tools have been developed for supporting intelligent decision-making in talent management, organisation management, and culture management,' Dr Xiong says. 'At the talent level, this powerful set of innovative AI techniques can support talent recruiting, performance evaluation, talent retention, talent development, and person-job matching. At the organisation level, they can help to support organisation stability analysis, leadership development and management, and intelligent team development. Finally, at the culture level, they can help to identify key factors for the development of creative culture and perform organisation culture analysis.'

Tackling the Person-Job Fit Problem

In recent years, many computer scientists worldwide have been trying to

‘Our suite of algorithms and tools have been developed for supporting intelligent decision-making in talent management, organisation management, and culture management.’

develop computational tools that could speed up or simplify online recruitment, such as recommender systems. These systems, which are often trained on data collected by online recruitment platforms, can learn to recommend suitable jobs for individual candidates by analysing their employment history and background information, as well as different features of job advertisements available online.

Unfortunately, automatic job recommendation systems typically need to be trained on large amounts of data reviewed and annotated by humans. This makes their development expensive and time-consuming, which in turn prevents their large-scale and widespread implementation. Over the past few years, Dr Xiong and his team created new systems based on artificial neural networks that could significantly simplify and innovate HR management practices.

‘The big data trend has made its way to talent management,’ explains Dr Xiong. ‘Indeed, the availability of large-scale HR data provide unparalleled opportunities for business leaders to understand talent behaviours and generate useful talent knowledge, which can be used to develop intelligence for real-time decision making and effective people management at work.’

The PJFNN Model

In 2018, Dr Xiong and other researchers at Baidu’s Talent Intelligence Centre developed a new computational model called the Person-Job Fit Neural Network, or ‘PJFNN’. This model is based on a convolutional neural network, which is a machine-learning algorithm commonly used by computer scientists to tackle tasks that involve the analysis of large amounts of images or other data.

The model created by Dr Xiong and his colleagues can learn the joint representation of person-job fitness by analysing past online job applications. In other words, it can match a candidate’s qualification to the requirements for a specific role. Its unique structure allows the model to estimate whether a given candidate matches a role, while also identifying specific requirements in the job posting that are satisfied by the candidate.

Dr Xiong and his colleagues evaluated the PJFNN model in a series of experiments, using a large-scale dataset containing employment-related information. The model performed remarkably well and could predict the person-job fit with high levels of reliability and accuracy.

The TAPJFNN Model

After they published their first paper on the PJFNN model, Dr Xiong and his colleagues continued working on the model, with the aim of broadening its capabilities and further improving its performance. In 2020, they proposed a new version of the model, dubbed the Topic-based Ability-aware Person-Job Fit Neural Network (TAPJFNN) framework.

The TAPJFNN framework, which was also trained on job application data gathered in the past, utilises a recurrent neural network with a hierarchical attention mechanism to create semantic representations of requirements listed in job postings and the experiences of candidates. Subsequently, the model employs two strategies to quantify the importance of different job requirements, as well as the extent to which individual professional experiences mean that a candidate meets a specific requirement.

As part of their study, Dr Xiong and his colleagues also devised a strategy to refine the model's ability to predict the best person-job fit based on a candidate and employer's past recruitment records. They also showed how the TAPJFNN model could be used for two different HR-related applications, namely to source new talent and recommend suitable jobs to candidates.

Finally, the researchers evaluated their model and compared it with other machine-learning tools for sourcing new talent or recommender systems. In their experiments, the TAPJFNN model performed remarkably well, outperforming several baseline techniques for HR management.

The SSCN Model

Earlier this year, Dr Xiong and his colleagues also introduced a technique to assess the value of individual professional skills within the global job market. This technique was designed to help companies and HR agencies worldwide to identify the most suitable type of candidates for a given role.

Initially, Dr Xiong and his collaborators represented the task of assessing the value of job skills as the composition of a set of requirements associated with contextual job-related information. In their representation, a job's salary is assumed to be dependent on the context-related value of individual professional skills.

Subsequently, the researchers developed an enhanced neural network-based model, dubbed the Salary-Skill Composition Network (SSCN). This model can discern between different job skills and evaluate their individual value based on how much they contribute to the job salary. In a series of experiments and evaluations, the SSCN model effectively assigned value to multiple job skills, while also outperforming benchmark job salary prediction models.

New Tools to Improve Recruitment

In the future, the research carried out by Dr Xiong could help to significantly improve HR practices and speed up recruitment processes. So far, the tools his team has developed have achieved highly promising results, and they could soon be tested and employed by real recruitment agents.

The computational tools developed by Dr Xiong and his colleagues have several advantages over traditional HR practices. 'Traditional HR management systems are usually based on rules extracted from experts' long-term experiences and have various disadvantages in practice,' explains Dr Xiong. 'For instance, traditional HR management decisions are based on fragmented information and are subjective. The predictive management of risks in HR is highly desired but difficult to implement with traditional HR systems.'

His team's approaches can analyse vast amounts of employment-related data and identify good person-job fits much faster than human agents would. 'My team has exploited advanced big data and AI technologies for smart HR management and designed the pioneering talent intelligent management system, which can support HR management in a transparent, objective, comprehensive, and predictive manner,' Dr Xiong says.

The three models presented in Dr Xiong's recent papers, namely the JFNN, TAPJFNN, and SSCN models, could be highly valuable tools for both employers and recruitment agencies, as they could help them to identify suitable candidates for specific roles faster and more reliably. In addition, the researchers developed the talent intelligent management system, a management system that could greatly enhance current HR practices.

'The talent intelligent management system is the first comprehensive intelligent HR management system that has changed the paradigm for traditional HR management,' concludes Dr Xiong.

Meet the researcher

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Dr Hui Xiong holds a PhD in Computer Science from the University of Minnesota, an MSc in Computer Science from the National University of Singapore and a BE in Automation from the University of Science and Technology of China. He is currently a Distinguished Professor at Rutgers University. His research primarily focuses on data and knowledge engineering, especially on the development of data analysis techniques for a variety of applications. Over the past decade or so, he has published over 80 journal articles, three books and more than 120 conference papers in numerous renowned scientific journals. In addition to his work as an educator and research scientist, he is an ACM Distinguished Scientist, AAAS Fellow, and IEEE Fellow. Dr Xiong has also received several awards, including the ICDM-2011 Best Research Paper Award, the 2017 IEEE ICDM Outstanding Service Award, a Grand Prix Ram Charan Management Practice Award from the Harvard Business Review in 2018, and the AAAI-2021 Best Paper Award.

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RUTGERS

A HUMAN-CENTRIC APPROACH TO NEAR-EYE DISPLAY ENGINEERING

Virtual and augmented reality technologies are now rapidly gaining traction in our society. Yet even as they improve, these devices continue to face major challenges relating to the wide variability of human vision. In their research, **Dr Gordon Wetzstein** and his colleagues at Stanford University explore innovative new ways to overcome these challenges, through the latest advances in both optics and vision science. In demonstrating ground-breaking innovations to near-eye displays and sensors, the team's work could soon bring enormous benefits to users spanning a diverse spectrum of visual ability.

Near-eye Displays

Virtual reality is among the most captivating technologies available today – enabling users to view and manipulate virtual 3D scenes through the movements of their eyes and bodies. As its capabilities rapidly improve, this technology is now offering an increasingly abundant range of applications: from allowing us to explore virtual worlds in video games, to helping architects and city planners to better visualise their designs.

One crucial component of virtual reality hardware is the near-eye display, which provides the interface between a user, and the programs they interact with. These devices are cutting-edge in themselves, but still have one major hurdle to overcome before their widespread use can become cemented in our society. The problem relates to the widely varying capabilities of our eyes.

The human eye is a key element of virtual reality technologies – receiving all of the optical waves produced by near-eye displays so that our brains can interpret them as 3D images. However, it is also the one element of the overall system that designers of the systems ultimately have no control over. Naturally, the focusing responses of human eyes vary significantly between different people. Therefore, as researchers develop more realistic user experiences in near-eye displays, it is critical to consider how these diverse focusing responses can be recreated within the displays themselves.

Artificial Focusing

As light emanates from a specific point on an object, it will travel in many different directions. In order for us to properly focus on objects, this light must re-converge at a specific point on the retina, allowing our brains to reconstruct an image of the original object. This is made possible by the eye's crystalline lens, which uses the property of refraction to bend the paths of optical waves entering the pupil in different directions: focusing them onto a single spot on the retina. As objects become closer, the angles of the waves entering the eye become sharper, and require higher degrees of refraction to remain focused on the retina. To account for this, circular muscles surrounding the lens will contract – changing the shape of the lens to increase the refraction of the light passing through it.

However, when viewing a near-eye display, our eyes will no longer do this automatically, because the user perceives the image as a 2D plane floating in front of their eyes rather than an object in a 3D environment.Instead, natural focusing responses must be artificially rendered in the display. If this isn't done correctly, a user's brain will not be able to interpret displayed images as intended – diminishing the comfort of their viewing experience.

Circumventing a Conflict

Through a study published in 2015, Dr Wetzstein and his colleagues developed a technique to alleviate the nausea and discomfort commonly experienced by users of current virtual reality systems. The problem stems from a conflict between the simultaneous, opposite movements of both eyes to obtain single 3D images, and changes in the shape of the eye's lens to stay clearly focused images of moving objects. It arises in all 3D displays, and must be overcome in order for users to comfortably perceive objects at varying virtual distances.

To solve the issue, Dr Wetzstein's team combined the established principles of artificial focus rendering with emerging principles of 'light field' technology, in which light from a single source travels in multiple different directions. In their study, light fields were produced by two different displays: each displaying the 3D image from a slightly different perspective. Since each display was only slightly larger than the size of a pupil, and projected the image at a range of viewing angles, a separate focusing response could be presented to each eye independently. Ultimately, the innovation enabled high-resolution images, while significantly improving the user's viewing comfort.

Tracking a User's Gaze

One alternative technique for achieving reliable focus rendering involves 'gaze tracking', in which sensors built into near-eye displays continually monitor the direction in which a user is looking. So far, the technology has been held back both by its high-power requirements, and the long delay times in the images produced. This has meant that image rendering was too slow to capture the rapid, subtle movements of our eyes.

In a recent study, Dr Wetzstein and his colleagues proposed a more sophisticated system, which is about 100 times faster both in capturing eye movements, and rendering images. They achieved this through a unique combination of emerging ultra-fast sensors and novel algorithms that can estimate in real time where a user's gaze will point next, allowing displays to be updated as rapidly as 10,000 times per second – far more quickly than even our most rapid eye motions can detect. After demonstrating their ultra-fast gaze tracking devices on real users, the researchers demonstrated highly accurate images over wide fields of view, paving the way for their widespread use in virtual reality.

Variability in Vision

In most young people, lenses can seamlessly adjust themselves as they look around at objects in the real world. As we age, however, the material structure of the lens becomes stiffer, meaning we gradually lose the ability to easily focus on nearby objects, resulting in a condition known as 'presbyopia'. This ultimately means that the focusing responses of humans as a whole are extremely varied.

When viewing near-eye displays, all users will perceive images at a single distance. However, problems arise for younger people, who can more readily notice differences between their natural focusing responses, and those they perceive in near-eye displays.

Until recently, this diversity in vision was extremely difficult to accommodate. Dr Wetzstein addresses the issue both for near-eye displays, and for eyeglasses that correct for vision impairment.

Improving Experiences for Younger Users

In parallel with gaze tracking technology, other studies have worked towards 'varifocal' displays, which physically alter the distance between the eye and a display. These displays incorporate 'focus-tuneable lenses' that can mimic the function of the lenses in our own eyes, by changing their shapes to alter their refractive properties.

In each of these cases, the perceived distance between the eye and a display can be readily altered, enabling devices to reproduce far more realistic focusing responses for younger users. Crucially, both approaches can be readily combined with gaze tracking technology to alter the distance between the eye and a display, depending on the part of the image a user is looking at.

One principal advantage of this approach is that it enables the opposite motions of both eyes required for viewing 3D images to be directly coupled with the reshaping of both lenses, instead of being in conflict with it. This removes the previous conflict between both actions, while maintaining the use of gaze tracking. In addition, varifocal displays based on focus-tuneable lenses enable the focusing responses recreated in the images to be precisely tailored to the needs of specific users. This ability offered a breakthrough in the accessibility of near-eye displays for younger users.

Introducing: Autofocals

Dr Wetzstein and his colleagues have developed novel electronic eyeglasses named 'autofocals', which combines gaze tracking software with a depth sensor to drive focus-tuneable lenses automatically. This approach enables the devices to automatically correct for presbyopia in older users by externally mimicking the response of a healthy, non-stiffened lens. Furthermore, the level of this automatic adjustment can be tailored to the degree of presbyopia in specific users, significantly improving its accessibility.

To analyse the performance of their design, Dr Wetzstein's team tested it on 19 volunteers – each with varying levels of presbyopia. After completing a visual task, the participants found that the autofocals greatly improved the visual sharpness of 3D images compared with their own vision, and also reported an ultra-fast, highly accurate refocusing response.

Furthermore, the low power requirements of the apparatus, combined with its ability to function in diverse situations without the need for calibration, could soon allow the researchers to integrate their autofocals with small, wearable devices. If achieved, this may lead to a whole new generation of eyeglasses, which would improve the lives of many millions of vision-impaired people globally.

Branching into Holography

Following on from these achievements, the next steps of Dr Wetzstein's research involve holographic near-eye displays. Holography is now a rapidly growing field of research that exploits the principles of light diffraction – where waves spread out after passing through narrow gaps, to enable 3D images to be viewed from multiple different angles. If projected from near-eye displays, they can allow users to perceive these images without any need for special eyeglasses or external equipment. Currently, however, the technology faces numerous challenges in achieving both high image quality, and real-time performance.

By drawing on the achievements they have made so far, and combining them with the latest advances in artificial intelligence, optics and human vision science, Dr Wetzstein's team is now addressing these challenges in a variety of innovative new ways. Their work could soon pave the way for the widespread use of holography in a new generation of virtual reality displays.

A New Era for Near-eye Displays

Ultimately, Dr Wetzstein and his colleagues hope that the computational near-eye display technologies they develop could bring the widespread application of virtual and augmented reality in our everyday lives one step closer. If achieved, this could open up numerous new avenues of research.

The primary interface between a user and the computer software run by near-eye displays will be crucial in ensuring comfortable viewing experiences for all users. Through the use of these emerging technologies, designers of virtual reality systems will not only achieve this level of comfort, but will also ensure that the technology becomes accessible for all users, regardless of their visual ability.
The team will now continue to draw upon advances in optics, human vision science, and other cutting-edge fields to improve the human-centred capabilities of near-eye displays even further.

Meet the researcher

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Dr Wetzstein completed his PhD in Computer Science at the University of British Columbia in 2011. He has now been an Assistant Professor at Stanford's Electrical Engineering Department since 2014, where he also leads the Stanford Computational Imaging Lab. Dr Wetzstein's research interests combine the latest advances in computer graphics, computational optics, and applied vision science, which he applies in applications as wide-ranging as next-generation imaging, wearable electronics, and microscopy systems. His groundbreaking research has now earned him awards including the 2019 Presidential Early Career Award for Scientists and Engineers (PECASE), the 2018 ACM SIGGRAPH Significant New Researcher Award, a Sloan Fellowship in 2018 and an NSF CAREER Award in 2016.

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SWARMMATE™: SWARMING DRONES FOR REAL-WORLD MISSIONS

The idea of unmanned drones flying together in expansive swarms may at first sound chaotic and unpredictable – yet with the right approach, these machines can enable their users to carry out coordinated and highly advanced missions. Through their research, **John Sauter** and colleagues at SoarTech have developed SwarmMATE™ – a transformative software that enables drones to mimic the behaviours of swarming animals found in nature. Their architecture now paves the way for real-world applications – from tracking forest fires and storms to aiding rescue missions.

Complex Swarms

From the seas to the skies, swarms of insects, birds and fish can be found across the natural world. The reasons why these animals collect into swarms can be highly varied – but in every case, properties emerge in these expansive groups that are vastly more complex than any individual animal could conceive on its own. As John Sauter explains, this has led to some highly sophisticated feats of engineering.

'Natural systems have devised means to coordinate the activities of many simple agents for accomplishing complex tasks,' he says. 'Termites build large complex mounds with floors, chambers, arches, and cooling all without the aid of a single architect. Ants can find and build shortest paths from distant food sources to their nests without using a navigation app.'

Although we may not realise it, similar phenomena are also present in our own society. For example, in the markets that drive our economy, the simple acts of buyers and sellers aiming to maximise their own profits each contribute to a deeply intricate financial ecosystem. In each of these scenarios, there is no central authority telling each individual exactly what to do; instead, complexity emerges from sets of simple and intuitive rules, which enable individuals to collectively achieve impressive feats.

Recently, these behaviours have seen increasing interest across a wide variety of fields of research. In their work, Sauter and his colleagues at SoarTech study one particularly fascinating area: swarms of unmanned aerial drones, which work together to carry out complex tasks.

Similarities in Design

In recent years, technological advances have led to cutting-edge designs of compact, lightweight, and inexpensive drones; capable of communicating with each other even as their positions continually change. In principle, these characteristics are ideal for using swarms of drones to carry out complex tasks. However, such an ambitious goal is faced with numerous challenges. 'Researchers have tried to control these large systems using traditional top-down planning approaches,' says Sauter. 'But those approaches simply don't scale when you are talking about tens, hundreds, or thousands for unmanned systems.'

Within such an intricate web of interacting machines, system designers must determine how individual drones should best contribute to the overall goals of a mission, while also assessing the performance of the overall system. When operating in environments with unpredictable terrains, obstacles, and weather conditions, it can be extremely challenging for designers to come up with plans for each drone that ensure the whole swarm achieves the objectives of the mission.

While studying this problem in the mid-80s, Dr Van Parunak, a colleague of Sauter, turned to natural systems for a possible answer. There, he found many examples of complex swarm behaviours even though individually, the members were not doing anything very sophisticated. Through their analysis of swarms found in nature and human society, Sauter's team developed advanced algorithms that mimic the

ability of groups of animals or insects to overcome these challenges, producing a result much more powerful than the sum of its individual members.

'By studying these systems, we've identified some common design principles that determine how they organise and coordinate their activities,' Sauter illustrates. 'We can now create artificial societies in our computers, with many agents operating under simple rules; and train them to solve some really hard problems.' With over 20 years of experience conducting these tests and studies, the researchers at SoarTech are now well equipped for making the widespread societal use of swarming drones a step closer to reality.

Introducing: SwarmMATE™

The team's efforts have now culminated in the launch of their tool – Swarming Mobile Autonomous Teaming Environment (SwarmMATE™) – first introduced in 2017. This advanced framework addresses four core challenges associated with drone swarm design and deployment: firstly, it breaks down the overall goals of a mission into sets of smaller tasks that can be performed by a single drone or team of drones. Secondly, the software determines the sizes of swarms to fit the needs of the mission. Thirdly, SwarmMATE™ has tools to measure and verify that the swarm behaviours are consistent with the goals of their mission, to a high degree of confidence. Finally, SwarmMATE™ includes an execution framework that enables a highly distributed swarm to communicate and coordinate using the swarming algorithms developed by SoarTech.

Together, these measures enable engineers to develop high-performance drone swarms that are robust against obstacles, and which can adapt to dynamic, unpredictable conditions in the field. By following the algorithms built into the software, drones can both cover larger areas within regions that would be hard to reach from the ground, while performing more coordinated manoeuvres to maximise the amount of information they gain.

'Through our research, we have developed a truly revolutionary software architecture that encapsulates the best of what I've learned about swarm intelligence and control,' Sauter describes. 'SwarmMATE™ is a platform that coordinates the behaviours of groups of robots performing a range of missions.' With these measures in place, Sauter's team could next focus their attention on applying drone swarms in specific scenarios.

Real-world Missions

By fitting drones with scientific instruments such as sensors and cameras, they can become highly sophisticated tools in the coordination of advanced, potentially dangerous missions. Such a system now displays clear potential for immense societal benefits. 'We aim to coordinate robotic swarms for performing missions that are useful for human society,' describes Sauter. 'We can scale from just a few robots to massive swarms comprising thousands of robots using the same algorithms, so we can solve both the small and really large problems we face.'

These capabilities have already been explored for military applications – but increasingly, the SoarTech team have come to examine the immense societal benefits they could soon unlock. 'A common theme among these missions is the need to cover large, irregularly shaped, dynamically changing areas,' Sauter continues. 'Swarms are an ideal way to organise a team of vehicles to distribute the tasking, and dynamically adapt to changing mission requirements.' Among the many applications this enables is the tracking of forest fires and severe weather; informing search and rescue operations; and monitoring agricultural crops.

Mapping Forest Fires

Forest fires have grabbed many headlines in recent years – unleashing widespread devastation both on natural environments, and the communities living within them. In the face of this threat, there is a pressing need for firefighting operations to monitor and map the spread of fires in real time, to determine where and how quickly the fire is moving and where best to deploy limited firefighting resources. As Sauter describes, SwarmMATE™ algorithms can coordinate drone swarms to perform these functions.

'We developed swarming algorithms to control a swarm of air vehicles with thermal sensors to search a large,

mountainous, forested area for forest fires,' he says. 'This involved finding the hot spots, patrolling around the perimeters of fires, mapping their extents, and then continuing to track and update maps of their perimeters as they spread.' By consulting these maps, authorities would be far better equipped to direct firefighting teams to combat blazes as efficiently as possible.

Tracking Severe Weather

Through further studies, Sauter's team has shown how swarms can also be used to monitor extreme weather events – which can take place over expansive areas and ranges in altitude. Their techniques enable far more sophisticated measurements than those made by traditional instruments such as weather balloons and dropsondes dropped from manned aircraft, which have extremely limited monitoring ranges and operation times.

When equipped with weather sensors, swarming drones can smartly organise themselves into positions that give them the best possible meteorological data. 'Data needs to be collected on wind speeds, direction, temperatures, pressure and humidity, to better predict the severity and direction a storm,' Sauter illustrates. 'The swarm has the intelligence to adapt to the changing weather patterns as it moves across a region, ensuring continuous coverage and tracking.' In turn, this will enable meteorologists to generate far better forecasts of how storms will progress over time, giving communities time to prepare.

Informing Search and Rescue

Fast, thorough search techniques are particularly crucial for saving lives in search and rescue operations. Whether searching for hikers lost in the wilderness, or victims caught in disaster zones, these operations will often involve scanning expansive, remote, and possibly dangerous regions with difficult terrain. These are extremely difficult to cover extensively using manned aircraft – but are far less of an issue for intelligent drone swarms.

'An intelligent swarm of vehicles can cover a much broader area in a shorter time than manned aircraft and for much less cost,' says Sauter. 'They can fly closer to the ground and peer deep into valleys where it is difficult for manned aircraft to reach.' Equipped with tools such as infrared sensors, radar and radios, these swarms can search remote areas for signs of human life, while also providing cellular connectivity where there isn't otherwise any service available – allowing victims to communicate their positions.

Monitoring Agricultural Crops

As farmers around the world aim to improve the sustainability of their agricultural practices, while maintaining high yields to meet growing demands for food, they are increasingly seeking to minimise their use of chemicals and resources. Using drone swarms fitted with cameras capturing a wide region of the electromagnetic spectrum, they can scan large areas of farmland in a short space of time; identifying any areas where crops are suffering from factors such as insect-related disease or water stress.

As a result, these farmers can pinpoint exactly where additional water or chemical applications are needed. 'A swarm of drones can then deliver just the right kinds of chemical only when and where it is needed, instead of the current practices of broadcasting these chemicals everywhere as a preventative measure,' Sauter explains. This would enable farmers to greatly reduce the environmental impact of their operations – both reducing water usage in their local regions, and making fields more friendly to plants and animals that pose no threat to crops.

Diverse Societal Benefits

While intelligent drone swarms hold the potential to transform operations in each of these areas, the full extent of their capabilities extend far further still – ranging from law enforcement and drug interception, to logistics and traffic monitoring. In the future, Sauter and his colleagues at SoarTech will continue their efforts to expand the reach of their SwarmMATE™ software in numerous aspects of society. Ultimately, the team hopes that the benefits enabled by swarming drones could soon become a key feature of our everyday lives.

Meet the researcher

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John Sauter has over three decades of experience in research and development. He has a particular interest in using artificial and swarm intelligence for the control of complex systems – including systems of multiple vehicles, and the scheduling and control of distributed logistics. Sauter has served as Principal Investigator on numerous projects at DARPA, where he pioneered the development of one of the first swarming algorithms enabling fully distributed control over multiple unmanned vehicles. He has worked at Soar Technology, Inc (SoarTech) since 2013, where he is Director of Autonomy. Sauter is also an Instructor for the Unmanned Vehicle University, where he designed and teaches the graduate-level course, Autonomous Unmanned Systems.

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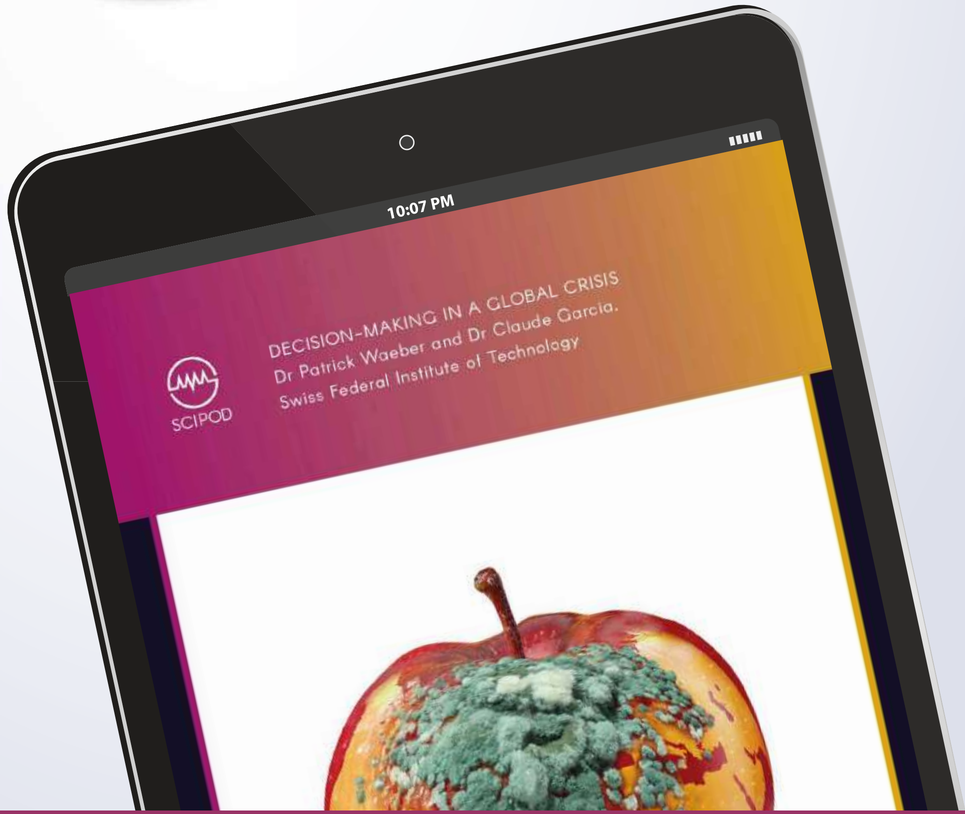
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