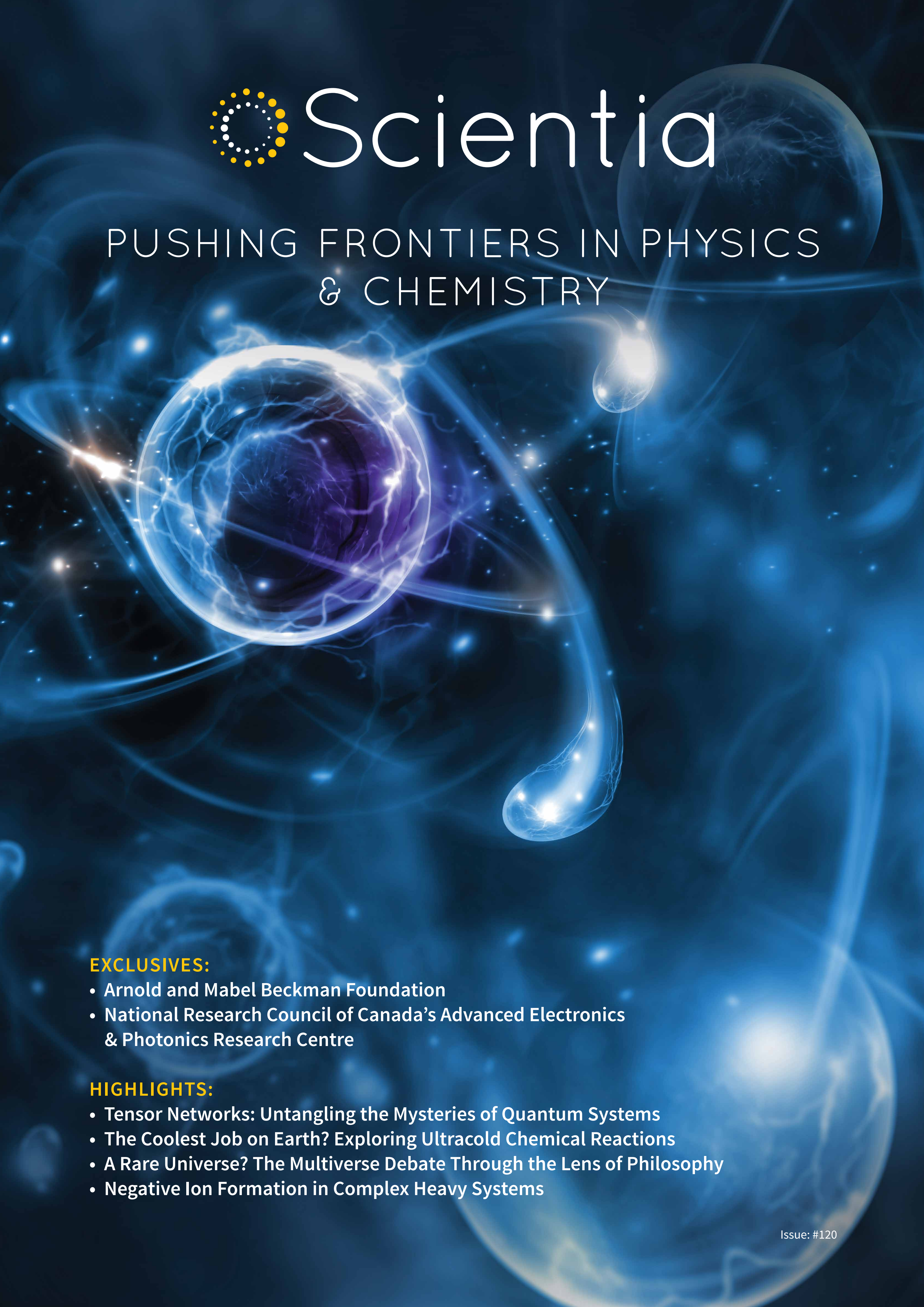

Scientia

PUSHING FRONTIERS IN PHYSICS & CHEMISTRY

EXCLUSIVES:

- Arnold and Mabel Beckman Foundation
- National Research Council of Canada's Advanced Electronics & Photonics Research Centre

HIGHLIGHTS:

- Tensor Networks: Untangling the Mysteries of Quantum Systems
- The Coolest Job on Earth? Exploring Ultracold Chemical Reactions
- A Rare Universe? The Multiverse Debate Through the Lens of Philosophy
- Negative Ion Formation in Complex Heavy Systems

Issue: #120

WELCOME...

In this thrilling edition of Scientia, we celebrate the pioneering scientists driving the latest discoveries and innovations in physics and chemical science.

To start, we deep dive into the quantum mechanical behaviour of subatomic particles, atoms and molecules. In this section, we meet researchers who are transforming our understanding of the weird and wonderful quantum world. We also introduce those who exploit quantum properties towards the development of futuristic computers and renewable energy technologies.

Our middle section of the edition is dedicated to the mind-bending fields of astrophysics and cosmology. Here, we meet many remarkable research teams – each dedicated to illuminating the mysteries of the cosmos. From hunting for dark matter to exploring whether we live in a multiverse, this collection of articles is sure to leave your mind reeling.

Finally, we showcase the latest innovations in the chemical sciences – an often-underappreciated field that has become an indispensable part of our daily lives. In this section, we meet an incredible ensemble of chemists and materials scientists, each aiming to improve our lives through painstaking chemical research. From creating lanthanide-based sensors that could be used in medical imaging, to developing catalysts for purifying water in developing countries, these inventive scientists are breaking boundaries and pushing frontiers to bring future innovations to fruition.

CONTACT

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E: info@sciencediffusion.com
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Meet The Team...

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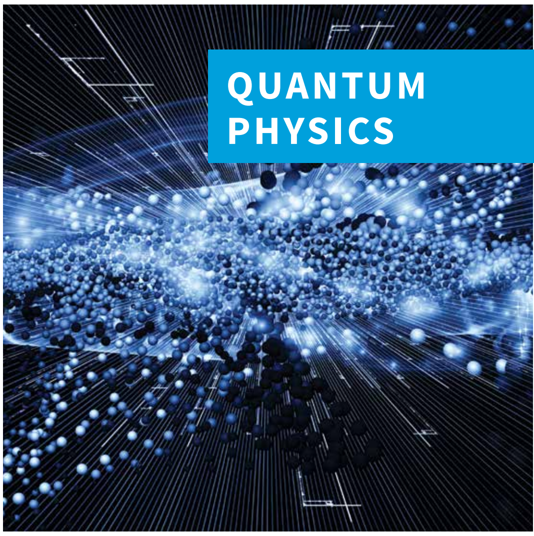

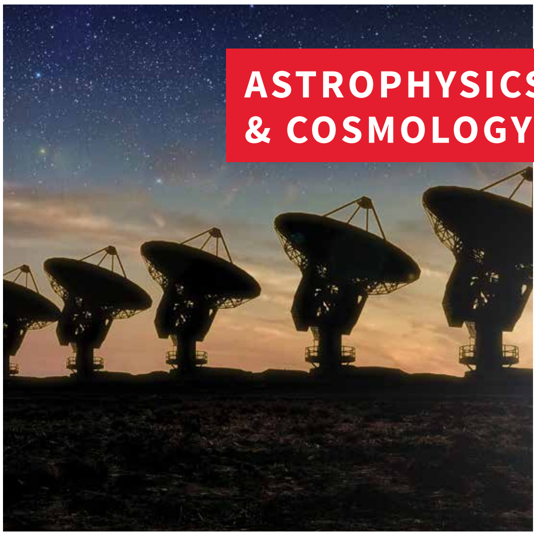

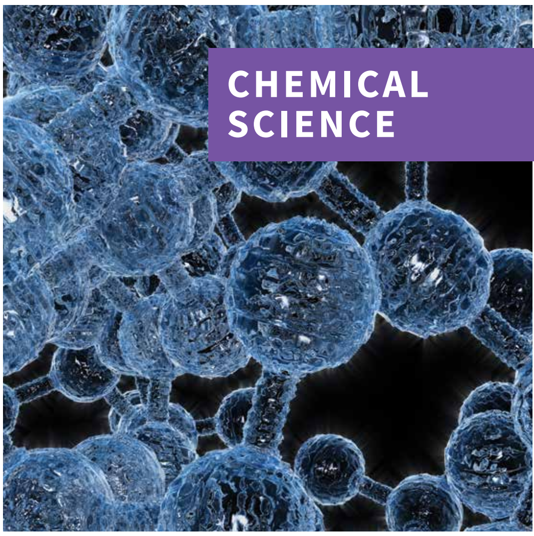

QUANTUM PHYSICS

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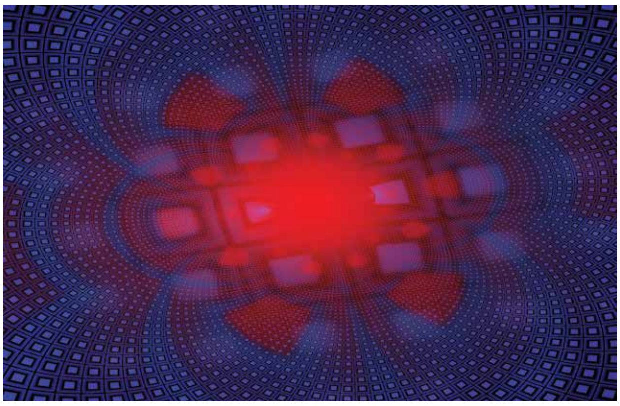
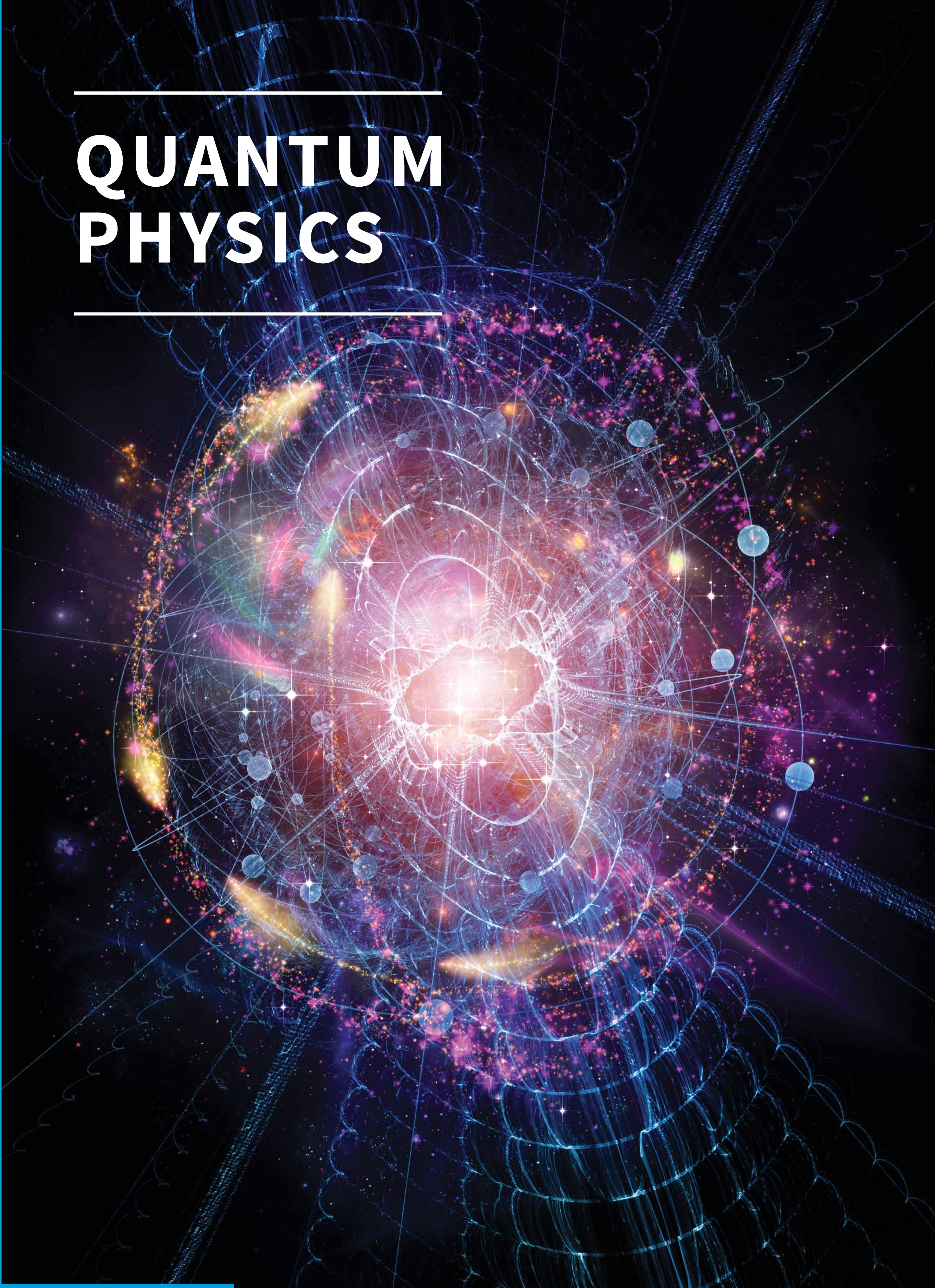


CHEMICAL SCIENCE

QUANTUM PHYSICS



SOLVING QUANTUM QUANDARIES

Founded by the German physicist Max Planck at the dawn of the 20th century, the unintuitive science of quantum mechanics radically transformed our understanding of the atomic and subatomic worlds.

Planck's ideas arose from his efforts to solve problems associated with black-body radiation. The classical theory of electromagnetism, in which light is treated as a wave, could not explain why the frequency of light emitted from a black body varied depending on the temperature of the black body.

A common example of an approximate black body is a fire iron. At room temperature, the fire iron emits low-energy infrared radiation, which cannot be seen. However, upon heating in a fire, it can release red, yellow or even blue light, depending on its temperature.

Planck explained this phenomenon by proposing that electromagnetic energy could only be emitted as discrete packets of energy, which he called 'quanta'. This means that energy can only exist as a multiple of an elementary unit, or quantum, rather than existing in any arbitrary quantity. He devised the equation $E = hf$, where f is the frequency of the light emitted and h is a proportionality constant, now known as Planck's constant.

Although Planck was unconvinced by his findings (and even considered his equation to be a trick employed to make the mathematics work), his ideas would go on to revolutionise physics forever. Five years later, Albert Einstein used Planck's quantum hypothesis to explain a phenomenon called the photoelectric effect.

This effect occurs when light shone onto a 'photoelectric' material causes electrons to be ejected from its surface. Using Planck's quantum concept, Einstein was able to explain this observation by proposing that a beam of light is composed of many individual quanta, whose energy is proportional to the frequency of the light. These discrete packets of light are now called photons. Photons with energies above a certain threshold value for a given photoelectric material can expel electrons from their atomic orbits. However, low-energy photons are unable to do so, regardless of the number of photons hitting the surface (the intensity of the light).

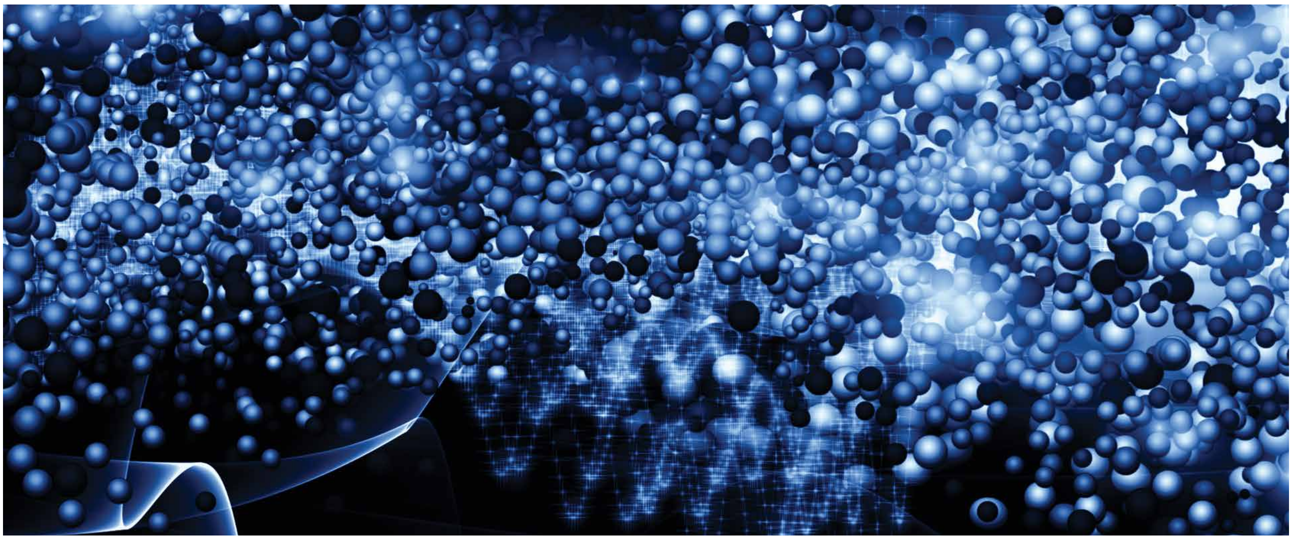
Although photons exhibit particle-like properties, such as location and momentum, they also have wave-like characteristics, including frequency, interference and refraction. Planck and Einstein's pioneering work gave rise to the concept that electromagnetic waves and subatomic particles are neither particles nor waves but have properties of both. Thus, the concept of wave–particle duality was born.

Through further work carried out by Planck and Einstein, in addition to Louis de Broglie, Niels Bohr and Arthur Compton (to name just a few), our current scientific theory maintains that all particles exhibit wave-like behaviour and vice versa. This not only applies to subatomic particles but has also been observed for larger particles such as atoms and molecules.

From these initial ground-breaking discoveries, quantum mechanics has since grown to become one of the fundamental pillars of physics. Indeed, quantum mechanics is the mathematical foundation of many fields within both physics and chemistry. Innumerable applications rely on our understanding of the quantum world, including superconducting magnets, lasers, LEDs and the transistors and semiconductors in computer hardware, along with many medical technologies such as MRI.

In this section of the edition, we introduce several scientists across the globe who are pushing the frontiers of our knowledge in quantum physics. We also meet several researchers who are expanding the applications of quantum phenomena, towards efficient quantum heat engines and viable quantum computers.

First up is Dr Román Orús and his team at the Johannes Guttenberg Universität in Germany, who are deepening our



understanding of quantum many-body systems – systems containing multiple quanta. Although we now have a well-established understanding of single quantum particles, the ways in which quantum many-body systems behave are unpredictable when using conventional mathematics, making theoretical simulations virtually impossible. Dr Orús is at the forefront of research into tensor network algorithms, which he believes are vital to simulating and thus explaining a wide range of quantum phenomena.

Next, we introduce the research of Dr Timur Tscherbul and his research team at the University of Nevada, who also develop algorithms to further our understanding of the quantum mechanical nature of matter. In particular, they use their algorithms to study chemical reactions at temperatures close to absolute zero, when molecules occupy the lowest possible quantum states. Their work is challenging 100-year-old conventional wisdom surrounding chemical reactions.

From here, we go on to showcase the latest research into quantum computing. In regular digital computers, data is encoded into two definite states: 1 and 0. In quantum computers, however, quantum properties can be exploited to superimpose multiple states onto individual particles. These particles, known as quantum bits, or 'qubits', can essentially carry multiple 0s and 1s at the same time. This ability of qubits means that quantum computers can theoretically perform calculations at much greater speeds than our current supercomputers.

However, we are still far from building complex, functional quantum computers. In the meantime, scientists need to test the capabilities of quantum computers using simulations on conventional computers. Understandably, this requires enormous amounts of computing power. In this section we meet Dr Hans De Raedt at the University of Groningen, who has been working on a remarkable piece of software called the Massively Parallel Quantum Dynamics Simulator. Unlike previously developed software to simulate quantum computations, the Massively Parallel Quantum Dynamics Simulator can be used to realistically simulate quantum systems containing 46 simulated qubits and perform experiments with them.

Next, we feature the research of Dr Philip Walther at the University of Vienna, who is also working hard to make quantum computing a reality. His team has shown that the orders in which quantum computers carry out operations can be superimposed, which means that two or more operations can be carried out at the same time. Their findings could pave the way for the development of quantum computers that operate with even greater efficiencies than researchers had predicted.

Our next article showcases the work of Dr Gernot Schaller and his colleagues at the Technical University of Berlin, who focus their efforts on a different application of quantum physics – energy conversion. They are working to obtain a device known as 'Maxwell's demon' – a highly desirable yet supposedly unattainable means of extracting energy from disordered particles. Dr Schaller and his team suggested how Maxwell's demon could take the form of a device called a 'quantum dot' coupled to two electronic leads. This semiconducting quantum dot could effectively act as a 'feedback-controlled single-electron transistor', deciding on which particles are allowed through to the other lead.

To close our quantum physics section, we feature an exclusive interview with Ruth Rayman, Director General of The National Research Council of Canada's Advanced Electronics & Photonics Research Centre. Here, we discuss how the Centre accelerates the development of next-generation semiconductor-based photonics and electronics. Following on from Dr Schaller's work on quantum dots, Rayman explains how the Centre has developed innovative quantum dot technology for applications in the telecommunications and information technology industries.

TENSOR NETWORKS: UNTANGLING THE MYSTERIES OF QUANTUM SYSTEMS

For decades, physicists have struggled endlessly with the problem of quantum many-body systems – systems containing multiple quantum particles. Because of quantum properties, the ways in which these systems behave are unpredictable when using conventional mathematics, making theoretical simulations virtually impossible. Now, **Dr Román Orús** at the Johannes Guttenberg Universität in Germany (soon moving to the Donostia International Physics Centre in Spain) believes that tensor networks will become a vital tool when exploring these unconventional properties. He hopes that the cutting-edge mathematical technique will have implications in fields from artificial intelligence to quantum gravity.

The Many-body Problem

When quantum particles are on their own, theoretical physicists have little trouble in predicting how they will behave. Using the Schrödinger equation, they can predict how the characteristics of the particle will change over time, accounting for quantum properties such as the particle's spin and momentum.

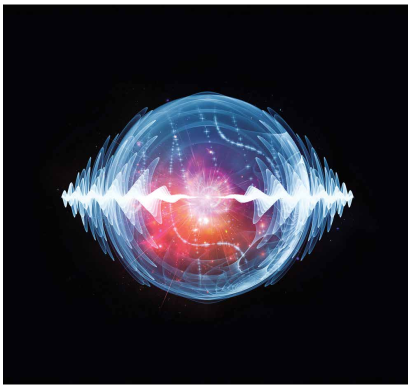
However, for systems where many of these particles are in play, calculations are notoriously difficult. In these so-called 'quantum many-body systems', the fates of two or more particles can become entwined through the little-understood property of entanglement. Due to this phenomenon, the locations, spins, and momenta of two particular particles can be directly connected with each other, regardless of the distance between them. Meanwhile, observers ultimately have no easy way to determine how entangled two particles are – a nightmare situation when many particles are involved.

To begin to understand the behaviour of quantum many-body systems, theoretical physicists have long realised that they need to construct simplified models in order to study the complex interactions that occur. To do this, they require reliable numerical simulations – the construction of which has created the need for an entirely new branch of mathematics. Since the 1990s, the idea of constructing so-called 'tensor networks' has propelled the mission to construct simulation methods, but the complex mathematics behind them has required years of research to perfect.

Dr Román Orús and his colleagues are at the forefront of this work, and believe that tensor networks are vital in explaining a wide range of quantum phenomena.

The Mathematical Power of Tensors

Ask just about any physicist, and they will tell you that among their earliest memories as students of the subject was the study of vectors. In physics, we can attach numbers to many quantities: speed, distance and mass, to name a few. These 'scalar' quantities are useful in simple problems, but most often in physics, we need information about

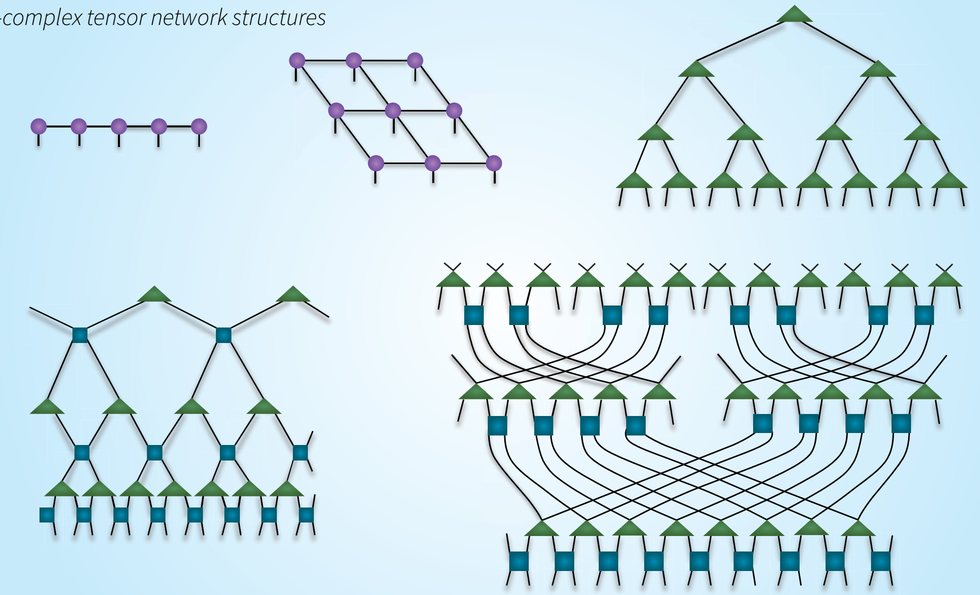


the direction in which these scalars act. By assigning direction coordinates to scalars, they can be turned into more useful vectors: velocity, displacement, acceleration.

However, as is so often the case in physics, problems rapidly become far more complex than before, as even Einstein found out the hard way. When constructing his theory of general relativity, Einstein struggled to make his calculations using vectors alone. He famously enlisted the help of his mathematician friend Marcel Grossmann, who would enlighten him on a mathematical construct a degree of complexity higher than vectors, known as tensors.

‘The topic of tensor networks has exploded a lot in recent years, and is now finding applications in many fields, including condensed matter physics, quantum gravity, lattice gauge theories, open systems, machine learning, and many other places.’

Increasingly-complex tensor network structures



Now part of the toolbox of skills for many physicists, tensors contain information about the relationships between scalars, vectors and even other tensors. The concept was a breakthrough for Einstein, who used tensors as a fundamental building block in his explanation of the union of space and time.

However, in more recent decades, problems have inevitably been thrown up that require yet another layer of complexity – perhaps the most notorious of these is the quantum many-body problem. This is the stage of complexity where Dr Orús joined, and at the heart of his solution for creating simulations of complex quantum phenomena, is the concept of tensor networks. ‘The topic of tensor networks has exploded a lot in recent years,’ he says. ‘It is now finding applications in many fields, including condensed matter physics, quantum gravity, lattice gauge theories, open systems, machine learning, and many other places.’

A New Layer of Complexity

To visualise the structure of tensor networks, Dr Orús and his colleagues use the analogy of DNA, and how its structure determines the overall makeup of the human body. Molecules of DNA act as the fundamental building blocks of our biological characteristics – aspects ranging from our height to our personality traits can ultimately be explained by how these blocks are positioned and interact within a highly complex network.

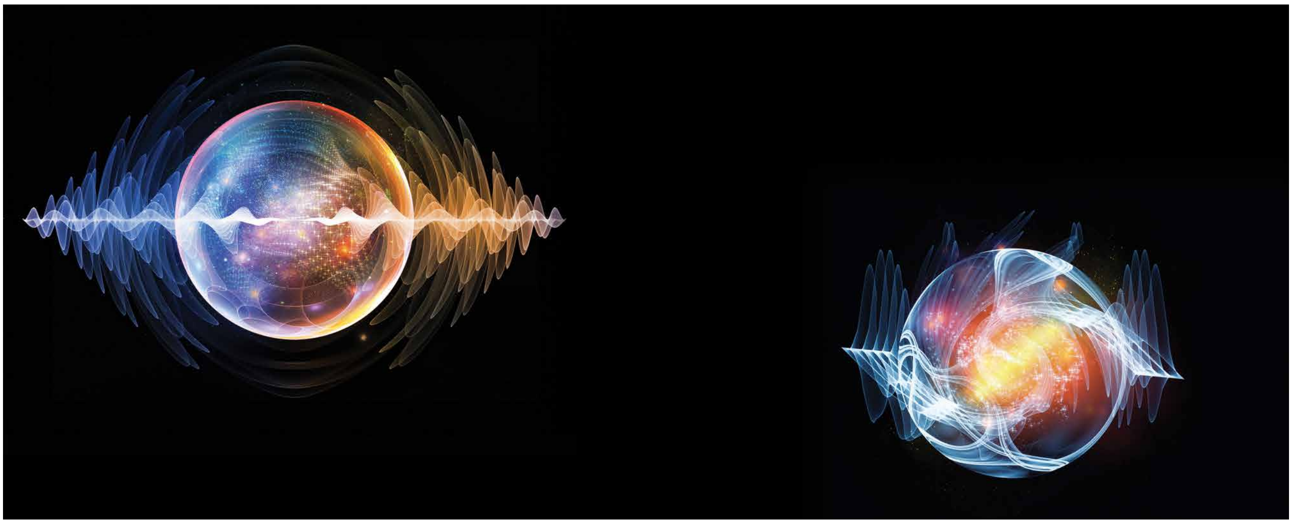
In the same way, individual tensors act as the DNA of an overall complex system, which can be described by its ‘wave function’. The characteristics and interactions of each individual tensor in the network play a part in determining what the overall wave function will look like, therefore providing insight into how the quantum system will behave. But to get to this stage, some highly sophisticated mathematics – the product of decades of research – is required.

Essentially, constructing the simplest tensor network first involves arranging tensors in an orderly line. Known as ‘Matrix Product States’ (MPS), these one-dimensional arrays allow tensors to interact with their neighbours, already allowing some advanced predictions to take place. To improve the construct further, a two-dimensional lattice can be created by replicating the one-dimensional structure repeatedly, using a technique named ‘Projected Entangled Pair States’ (PEPS).

With this infrastructure in place, reliable numerical simulations of quantum many-body systems can now take place with some further mathematical modifications. ‘My main focus now is the development of simulation techniques for quantum lattice systems using tensor networks, and the mathematical investigation of quantum many-body entanglement,’ Dr Orús explains. ‘My plan is to apply these methods to study a number of important phenomena.’

Long-awaited Numerical Simulations

By exploiting the mathematics behind MPS and PEPS, Dr Orús and his colleagues have worked towards fine-tuning tensor networks to display



quantum properties reliably. Using the models, they have analysed how tensor networks can be used to simulate fermions – a family of quantum particles that includes electrons and quarks, whose dynamics are incredibly hard to predict using conventional mathematics.

The team has also studied symmetries in tensor network states – a special case in which the quantum state of the system was not changed during an interaction with other systems. In addition, they have explored how tensor network simulations can be used to account for complex patterns of entanglement – perhaps the most important requirement for replicating truly realistic properties of many-body systems.

Using these ingredients, Dr Orús and his team have recently investigated a wide range of special cases of the behaviour of quantum many-body systems. In 2016, they studied how a theoretical system of magnetic particles in two dimensions would dissipate over time when immersed in an environment. Previous difficulties had arisen from the unpredictable behaviour of entangled particles, yet the algorithms used by Dr Orús and his colleagues managed to reliably predict how the system would evolve.

One year later, the team analysed how infinite tensor networks could be constructed to analyse Quantum Electrodynamics (i.e., the theory of electromagnetic interactions), allowing them to be used to simulate a system large enough to display macroscopic properties. This was particularly useful, as it allowed a first theoretical glimpse into how the so-called 'standard model', which is our deepest understanding of how particles interact in nature, could be eventually studied thanks to the new simulation methods based on entanglement – an unthinkable feat just a few decades ago.

Promising Potential for Tensor Networks

Dr Orús is confident that tensor networks could be put to an almost bewildering array of uses in the near future. 'Examples of problems are topological quantum order, frustrated quantum antiferromagnets, quantum dissipation, quantum transport, many-body localisation, lattice gauge theories, holographic entanglement, new numerical simulation methods, the connection to artificial intelligence, and possible connections of all these topics to experiments,' he lists.

Each of these uses is an in-depth area of physics in itself, but they are all unified in their need for the accurate simulations of the properties of quantum many-body systems. The study of antiferromagnets, for example, involves simulating the behaviour of many electrons at low temperatures. Artificial intelligence and machine learning solve problems using algorithms that act out scenarios repeatedly – gradually improving their methods for completing tasks, until becoming expertly skilled. Just as in our brains, computers will need to make complex connections between ideas and concepts in their own hardware, making simulations with tensor networks particularly useful.

Perhaps the most intriguing consequence of Dr Orús's research will be an insight into the most infamous problem in physics to date: quantum gravity. In their own right, the theories of quantum mechanics and Einstein's theory of general relativity seem to work remarkably well, and yet a single theory that marries them both together has eluded physicists for the best part of a century. In a macroscopic system of quantum particles, however, quantum effects play a significant role in determining the behaviour of the system. Dr Orús believes that by studying such a system using tensor networks, the path towards a unified theory would be clear: the equations of gravity would be nothing but those governing the quantum many-body entanglement. This deep connection between quantum physics and gravity has become increasingly evident in recent years.

It is fitting that the very mathematical concept that allowed Einstein to make his most important discovery, in a more advanced form, could soon provide us with a more advanced understanding of the consequences of his work.

Meet the researcher

Dr Román Orús

Johannes Guttenberg Universität

Mainz

Germany

Dr Román Orús is a Junior Professor of Condensed Matter Theory at the Johannes Guttenberg Universität in Mainz, Germany. After obtaining his degree and PhD in Physics at the University of Barcelona in 2006, he has worked as a Research Fellow at the University of Queensland, Australia, and the Max Planck Institute, Germany, as well as visiting Professor at the Universitè Paul Sabatier – CNRS, France, and the Donostia International Physics Center – DIPC, Spain. In September 2018 he will become a tenured Ikerbasque Research Professor at DIPC and a Visiting Professor at the Barcelona Supercomputing Center. With research interests in the diverse applications of quantum many-body systems and quantum technologies, Dr Orús has achieved several awards for his work, including a Marie Curie Incoming International Fellowship, and the Early Career Prize (2014) by the European Physical Society. He has written around 60 scientific articles about quantum research (cited around 3000 times), and is Founding Editor of the journal Quantum, member of the 'Quantum for Quants' commission of the Quantum World Association, and partner at Entanglement Partners SL.

CONTACT

E: roman.orus@gmail.com
W: http://www.romanorus.com

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THE COOLEST JOB ON EARTH? EXPLORING ULTRACOLD CHEMICAL REACTIONS

Algorithms are everywhere. From the targeted ads that flood your Facebook feed, to the split-second decision making of self-driving cars, they can be surprisingly simple or considerably complicated. At the University of Nevada, **Dr Tscherbul** and his research team are using algorithms to further our understanding of the exciting field of ultracold molecular dynamics. Their work is challenging the 100-year-old conventional wisdom surrounding chemical reactions.

An Absolute Temperature Scale

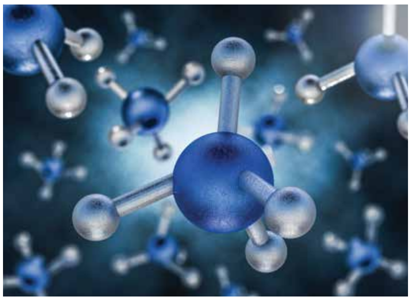
Sir William Thomson – later, Lord Kelvin of Largs – was an Irish mathematician and physicist who held the position of Professor of Natural Philosophy at the University of Glasgow for over 50 years. His contributions to science and engineering are vast, but his most notable achievement (still honoured in Physics today with the use of the unit Kelvin) was the insight he provided into temperature. Have you ever wondered why water just happens to boil at 100°C and freeze at 0°C? Setting our default temperature scale to one of the most widely available, naturally occurring chemical (water) makes a lot of sense, but is there a better option?

In physics, an 'ideal' gas follows a specific relationship that shows that its volume, pressure and temperature are related. In essence, both pressure and volume increase as the temperature increases and, if you know two of the above variables, it is simple to calculate the third. The so-called 'Ideal Gas Law' is one of the cornerstones of thermodynamics and without it, the internal combustion engine could not exist. If you flip the process around and decrease the temperature of any gas at a steady rate, the volume and pressure of the gas also decrease.

Lord Kelvin demonstrated that if you plot the volume and pressure of a gas against its temperature, they both reduce towards zero at a very specific point: −273.15°C, or 0K (zero Kelvin). We call this temperature 'absolute zero', as it is commonly thought of as the lowest temperature possible. It's also the temperature at which all chemical activity stops – or so we thought.

Ultracold Molecular Dynamics

'While conventional chemical wisdom tells us that as the molecules are cooled down, all chemistry must grind to a halt, recent experiments with chilled molecules show that chemical reactions can be as fast near absolute zero as they are at room temperature,' says Dr Timur Tscherbul, of the University of Nevada, Reno. 'This happens due to the quantum mechanical nature of matter, which becomes more and more pronounced as the temperature approaches absolute zero.' Dr Tscherbul and his research team specialise in this emerging area of physics. It's science in its most cardinal form: not limited solely to the search for new knowledge, but also thoroughly testing those theories that we have long held as truth. Inspired by the pioneering experiments by Professor Jun Ye and collaborators at JILA and the University of Colorado, Boulder, and by Professor Jonathan Weinstein at the University of Nevada, Reno, measurements on chemical reactions of ultracold molecules are now carried out in several laboratories around the world.



It turns out that the unexpected enthusiasm of atoms and molecules close to absolute zero can be explained by the effects of quantum mechanics, which become more pronounced as the temperature decreases. In 'traditional' chemistry, molecular dynamics are usually studied at around – or above – 300K (approximately room temperature), where the outcome of a chemical reaction is determined by billions of molecular quantum states.

Ultracold molecular dynamics changes things. At temperatures close to absolute zero, all of the reacting molecules

‘While conventional chemical wisdom tells us that as the molecules are cooled down, all chemistry must grind to a halt, recent experiments with chilled molecules show that chemical reactions can be as fast near absolute zero as they are at room temperature’

occupy the lowest quantum states – at this level, chemical reactions can be controlled by applying external electromagnetic fields.

To observe how molecules behave at such low temperatures, scientists use a technique called ‘sympathetic cooling’. The process involves bringing a gas of cold molecules into contact with an ultracold gas of atoms and watching it cool down. The idea might sound slightly complicated, but it’s surprisingly similar to what happens when you put something in the refrigerator at home. Dr Tscherbul explains why the technique is so useful: ‘Despite its apparent simplicity, this technique is quite powerful and has been used to create ultracold samples of neutral atoms and atomic ions, which could not be cooled by any other method.’

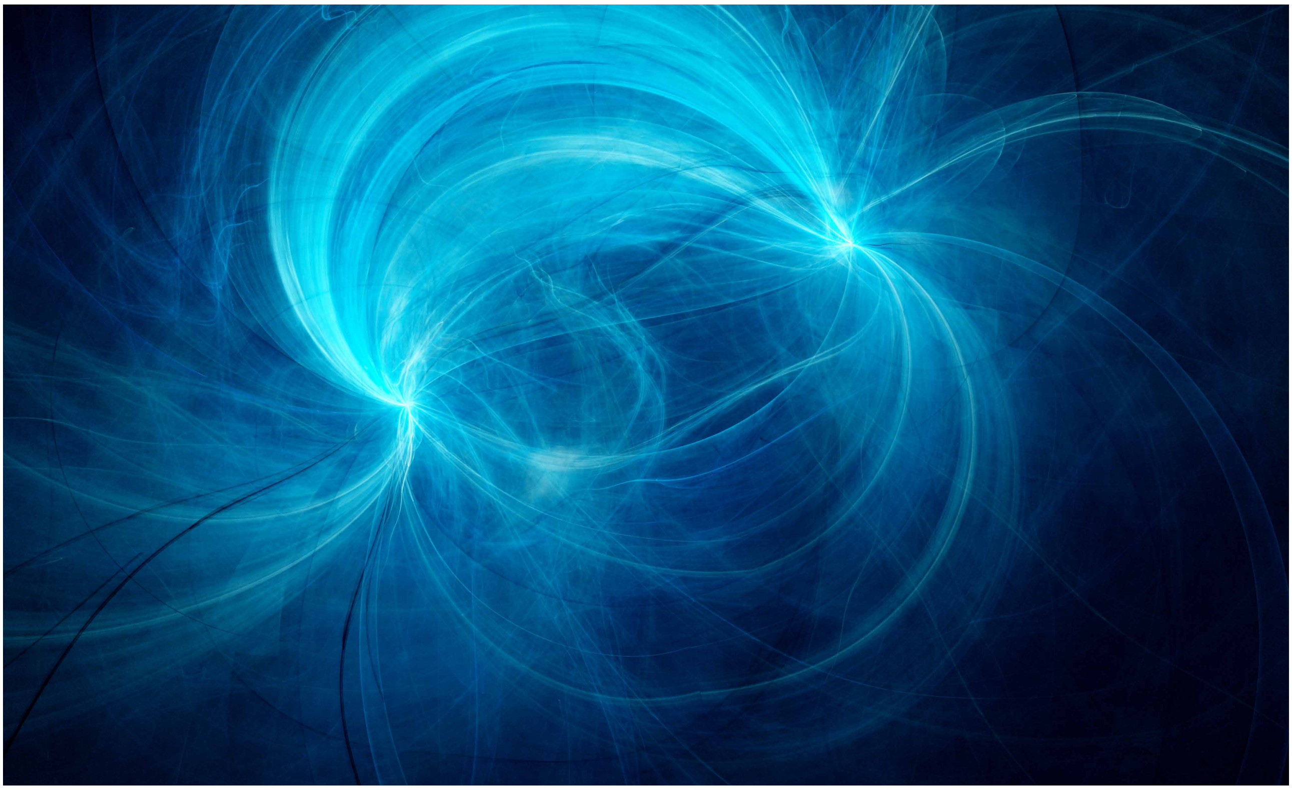
The trouble is that monitoring how molecules behave when they interact is extremely complicated and, until now, a clear understanding of this field has remained tantalisingly out of reach. Dr Tscherbul and his research team have resolved this problem by developing an algorithm to efficiently solve the ‘quantum mechanical equations of motion’, which describe how the molecules of interacting gases collide and react with each other as they mix. This is no easy feat – these equations are extremely difficult to solve using standard computational techniques.

The Algorithm

In the world of computing, scientists and programmers use algorithms to accomplish tasks, process data and solve problems. An algorithm is a process – or set of rules – that is automatically followed to process information. On the most basic level, an algorithm makes decisions using the mantra of *if this, then that* – where *this* is a set of predefined conditions and that is a set of actions. But as the information fed into the algorithm becomes more complicated (or the problem more difficult), what starts out as a simple set of rules and actions can quickly increase in complexity. Once an algorithm is defined, however, data can automatically be processed, analysed or ignored without any conscious input from the user. The algorithms created by Dr Tscherbul and his team go far beyond the simple *‘if this, then that’* process outlined above.

By taking advantage of an underlying symmetry in the apparent chaos of the interacting gases, the research team were able to simplify the problem and uncover completely new physics. ‘We developed efficient theoretical algorithms for solving the quantum mechanical equations of motion, which describe how ultracold molecules collide and react with each other,’ explains Dr Tscherbul. ‘Using these algorithms, we can uncover novel ways of manipulating ultracold chemical phenomena with external electromagnetic fields.’

The main focus of Dr Tscherbul’s research is optimising the sympathetic cooling technique by reducing the intrinsic losses as much as possible by preserving specific arrangements of molecular spins. This could help create ultracold molecular ensembles, which are required for new applications in quantum information processing, quantum simulation, and precision tests of physics beyond the Standard Model,’ Dr Tscherbul says.



New Insights

In a series of articles in 2010–2012, Dr Tscherbul and his team introduced their algorithm to the world and showed that it was capable of solving problems previously thought to be out of reach. 'The algorithm is interesting because it allows us to efficiently solve the intricate multichannel quantum scattering equations, which describe the scattering of complex molecules in the presence of external electromagnetic fields,' explains Dr Tscherbul. 'Prior to the development of the algorithm, these problems were intractable.'

In two subsequent papers in 2011 and 2017, Dr Tscherbul and his collaborators Drs Masato Morita, Jacek Klos, and Alexei Buchachenko demonstrated their application of the algorithm to the sympathetic cooling process. This allowed them to uncover the properties of molecular and atomic collisions on a microscopic level. 'As a result, we identified a new class of molecules suitable for sympathetic cooling in a magnetic field,' states Dr Tscherbul.

In 2015, with his paper *Tuning Bimolecular Chemical Reactions by Electric Fields*, Dr Tscherbul in collaboration with Professor Roman Krems demonstrated that it is actually possible to control chemical reactions at ultracold temperatures by applying electric fields within a lab environment. This paper was the first accurate calculation on a chemical reaction within an external electric field using the quantum mechanical equations of motion, and opens the door to a new area of physics and chemistry.

Future Plans

On the future of his work, Dr Tscherbul is optimistic about what his team can achieve using their new approach. One of the main areas he plans to focus on is extending the algorithm from the electric into the magnetic domain. 'This will allow us to explore the use of magnetic fields as a tool to control atom-molecule chemical reactivity at ultralow temperatures,' he says.

In particular, his team plans to focus on a phenomenon known as the 'magnetic Feshbach resonance' – which is currently used in the field of ultracold atom physics to control atomic interactions – to investigate whether the same effect can be used for controlling chemical reactions at the molecular level. The team will further refine their algorithm to enhance the efficiency of quantum scattering calculations.

Once these adaptations have been made, the team's ultimate goal is to use their algorithm to study how specific molecules react and interact with various ultracold atoms (such as lithium) held within a magnetic field. The potential payoff on reaching this stage is huge, as described by Dr Tscherbul: 'The calculations of elastic and inelastic collision rates will enable the experimentalists to optimise the conditions for atom–molecule sympathetic cooling experiments, potentially leading to the production of a wide variety of ultracold molecular gases, the sought-after goal in the field of cold molecules.'

The work being undertaken by Dr Tscherbul and his research team might, at first, appear to be extremely technical, but it contains within it the potential to transform our understanding of how chemical reactions occur at the most fundamental level.

Meet the researcher

Dr Timur Tscherbul
Department of Physics
University of Nevada, Reno
Reno, NV
USA

Dr Timur Tscherbul completed his education at Moscow State University with an undergraduate degree in Chemistry in 2002 and a PhD in Physical Chemistry in 2005. He has since worked in a variety of research positions at the University of British Columbia, the Harvard-MIT Center for Ultracold Atoms, and the University of Toronto. He is currently an Assistant Professor at the University of Nevada, Reno, where his research focuses on ultracold molecular dynamics and the theory of open quantum systems. He was awarded the Killam Postdoctoral Research Fellowship in 2006 and has helped organise a number of workshops within his field. Over the past ten years Dr Tscherbul has been an invited speaker at over thirty talks around the world.

CONTACT

T: (+1) 775 784 1079
E: ttscherbul@unr.edu
W: https://www.unr.edu/physics/people/timur-tscherbul

KEY COLLABORATORS

Dr Masato Morita, University of Nevada
Professor Roman Krems, University of British Columbia
Professor Jun Ye, University of Colorado
Professor Jacek Klos, University of Maryland

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FURTHER READING

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University of Nevada, Reno

SOFTWARE FOR REALISTIC SIMULATIONS OF QUANTUM SYSTEMS

The potential capabilities of universal quantum computers have many of us excited, but there's one problem – we aren't close to building complex, functional quantum computers just yet. In the meantime, scientists need to test the capabilities of quantum computing using simulations on conventional computers, which requires enormous amounts of computing power. However, over the last decade, **Professor Hans De Raedt** at the University of Groningen and his collaborators have been working on a piece of software that has already greatly improved these simulations.

Challenges for Quantum Computer Simulations

Since the 1990s, computer scientists have known of algorithms that would be performed much faster using quantum computers than even the most powerful supercomputers of today.

In conventional computing, data is encoded into binary digits in two definite states – 0 and 1. These 'bits' of data are processed by logic gates, which output further bits whose states depend on those of the input bits. In quantum computers, however, quantum properties are exploited to superimpose multiple states onto individual objects. These objects, known as quantum bits, or 'qubits', can essentially carry combinations of 0s and 1s at the same time. Using qubits to carry data would allow scientists to solve mathematical problems that are so complex that they would take far too long to calculate using our current resources.

However, during their earlier research in 2000, Dr De Raedt and his colleagues realised that physical models of quantum computers of fewer than sixteen qubits could be simulated on a conventional computer. Using such a simulation would allow scientists to carry out realistic experiments to probe the capabilities of quantum computers, without going to the trouble of actually building them.

The problem was that adding extra qubits to the simulations, making them more useful to scientists, quickly ate up memory. 'Simulation models of quantum computers share the feature that with every qubit added to the system, the memory required to represent the state of the system doubles in size,' Dr De Raedt explains. 'For instance, to simulate a system with 30 qubits, one needs a little bit more than 16 gigabytes of memory. While it is not rare these days to have PCs with more memory than this, to simulate say 40 qubits, one would have to increase the memory by a factor of 1024 – around 16 terabytes.'

Chances are, you won't be able to generate this amount of computing power using your laptop. 'Machines that have this amount of memory are not that common,' Dr De Raedt continues. 'Simulating 46 qubits can only be done on a handful of supercomputers. From this simple counting argument, it follows immediately that for these simulations, the amount of available memory is the limiting factor.'

But even when qubits are successfully stored in a computer's memory, the problems don't end for scientists wishing to manipulate them to perform calculations. 'We also need to do

‘The “Massively Parallel Quantum Dynamics Simulator” is software that is designed to handle the memory, computer and communication problems using the available hardware as efficiently as possible. The software is portable and runs, without modification, on hardware ranging from PCs to the largest supercomputers that are available today.’

something useful with the numbers stored in this memory,’ adds Dr De Raedt. If just 40 qubits are involved, he describes in an example, trillions of calculations need to be made for every individual step that the quantum computer takes. ‘It is not difficult to imagine that performing this calculation requires a lot of computing power.’

Software up for the Task

Dr De Raedt and his colleagues realised that in order to prevent the computational requirements of more complex quantum computer simulations from getting out of hand, a more calculated approach was needed. ‘Performing such calculations in a reasonable amount of real time is only feasible by using massively parallel computers,’ Dr De Raedt explains. ‘Such computers have their memory distributed over many computer nodes.’ A computer node is a physically self-contained computer unit in a distributed computing architecture. Such a node has its own processors, memory and input-output channels.

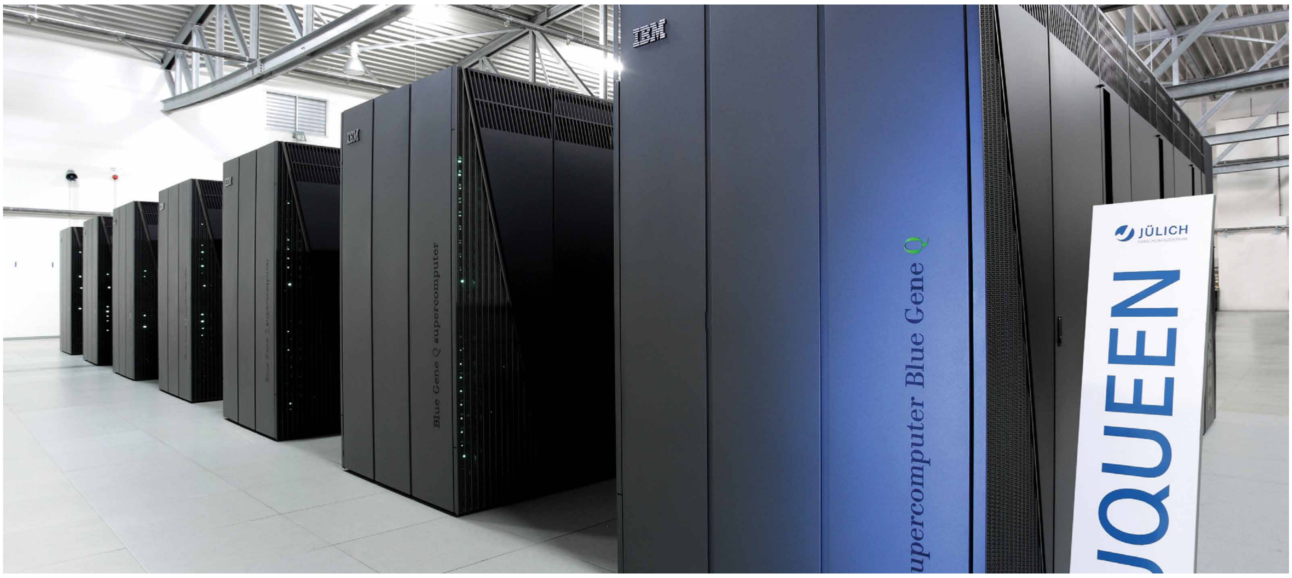
With Dr De Raedt’s research, however, the task required of these computer node networks was more involved than can be achieved with everyday hardware. ‘The problem that arises is to efficiently exchange data between compute nodes,’ he explains. ‘A characteristic feature of the problems that we are interested in is that the communication patterns are not fixed and can be rather complicated.’ With networks of millions of nodes that were constantly exchanging data, a more sophisticated method was needed to ensure that operations were being carried out as efficiently as possible by the computer.

A breakthrough came in 2007 when Dr De Raedt and his team developed a piece of software capable of exploiting massively parallel computers. In 2011, they were awarded the Wim Nieuwpoort Award in recognition of their outstanding achievement – the most efficient deployment of modern massively parallel supercomputers.

‘The “Massively Parallel Quantum Dynamics Simulator” is software that is designed to handle the memory, computer and communication problems using the available hardware as efficiently as possible,’ Dr De Raedt says. ‘The software is portable and runs, without modification, on hardware ranging from PCs to the largest supercomputers that are available today.’ With the software up and running, his team could begin conducting real experiments using quantum computer simulations.

Proving Capability

In 2017, the Massively Parallel Quantum Dynamics Simulator software was used to simulate the behaviour of quantum particles. The scenario involved two quantum particles interacting with a ‘bath’ of 34 similar particles. Before, the quantum behaviour of the particles would be far too complex for a computer to simulate how the system evolves over time. However, by using simulated qubits to represent each quantum particle in the system, Dr De Raedt and his colleagues were able to observe how the two particles relaxed to lower energy states, and eventually reached thermal equilibrium with the rest of the particles in the bath.



To confirm that their simulation was a realistic representation of the scenario, the research team compared their results to those calculated using the theoretical principles of 'Markovian dynamics'. This theory describes the motions of particles in different systems as they interact – in this case, the interaction of the two test particles with the bath. Overall, the researchers showed for the first time that their predictions, made using a simulated quantum computer, were consistent with theoretical principles.

In a further experiment, the team simulated the evolution of a one-dimensional system of electrons (which are also quantum particles) over time. Initially, the simulated electrons were clumped together at a single, dense point. As a static system where time isn't involved, the properties of such a clump of charged particles could already be described fairly well using previous simulations. However, the quantum behaviour of the electrons as they interacted with each other over time is far more difficult to simulate.

Again testing the reliability of their simulation using theoretical principles, the researchers compared the behaviour of the electrons represented by simulated qubits with predictions arising from mathematical calculations of 'linear response theory'. Within the limits of high temperatures, and the regime of strong particle-particle interactions, the way in which the electrons evolved as they spread out from the initial clump over time was again fairly consistent with theoretical calculations. This time, however, the team's simulations involved up to 40 electrons – so far the most complex simulations of the dynamics of quantum particles ever performed on conventional computers.

At the same time as the team were conducting these experiments, a system containing a record-breaking 46 simulated qubits was developed in a project led by Dr De Raedt's colleague, Dr Kristel Michielsen. By reducing the memory required to represent a quantum state from 16 bytes down to just two bytes, they were able to increase the efficiency of quantum computer simulations far beyond previous capabilities.

Using the JUQUEEN supercomputer at the Jülich Supercomputing Centre in Germany, as well as the world's fastest supercomputer – Sunway TaihuLight in China – the teams involved created the largest simulated quantum computers to date. Already, it seems that Dr De Raedt will be able to adapt his software to perform even more complex simulations in the near future.

Keeping up with the Times

Having successfully demonstrated how his software can be used to realistically simulate quantum systems and perform experiments with them, Dr De Raedt is now well prepared for future advances. 'The next steps for our work will be to adapt the software to make effective use of the new hardware features like accelerators that are available in the latest generation of supercomputers,' he says. Such advances can only increase the capabilities of the Massively Parallel Quantum Dynamics Simulator software, in terms of the number of qubits it can simulate, and the efficiency with which operations can be carried out across computer nodes.

Dr De Raedt also has his eyes on solving more conventional problems in quantum mechanics. 'We would like to use the simulation software to address issues such as decoherence and error detection and correction in realistic models of quantum computers which interact with an external environment,' he continues. With an ever-increasing number of simulated qubits available to act as quantum particles, Dr De Raedt will be able to test increasingly complex theoretical predictions of quantum mechanics. His discoveries, both present and future, offer a satisfying alternative to experiments involving real quantum computers, for which we may have a few more years to wait.

Meet the researcher

Professor Hans De Raedt
Zernike Institute for Advanced Materials
University of Groningen
Groningen
The Netherlands

Dr Hans De Raedt received his PhD in 1976 from the University of Antwerp for work on magnetism in one dimension. Since 1990, he has been Professor of Computational Physics at the Zernike Institute for Advanced Materials at the University of Groningen. After contributing to the early development of quantum Monte Carlo methods, his interest shifted towards the simulation of physical phenomena in the time domain, including computational electrodynamics, and simulations of physical models for quantum computers. Currently, his work focusses on foundational issues of quantum physics, which includes the development of event-based simulation methods of quantum phenomena.

CONTACT

E: h.a.de.raedt@rug.nl
W: http://www.compphys.org/compphys0/

KEY COLLABORATORS

Prof. Dr Kristel Michielsen, Jülich Supercomputer Centre
Dr Fengping Jin, Jülich Supercomputer Centre
Koen De Raedt, Bright Computing

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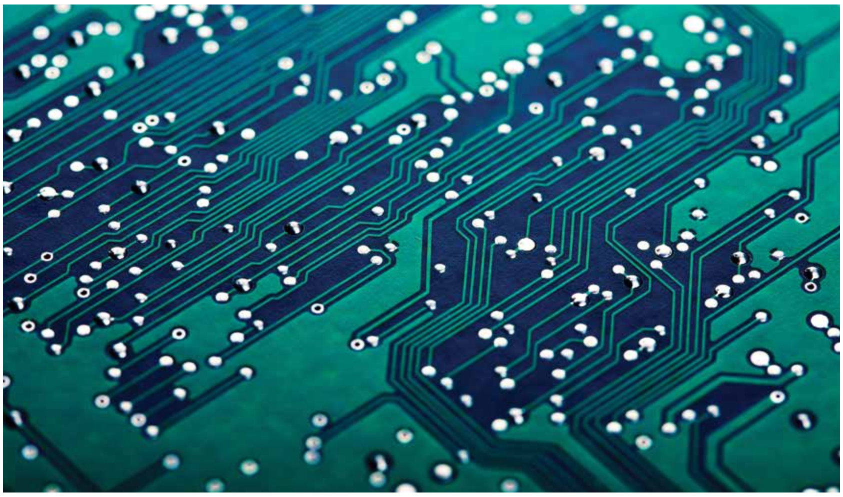
Link to the software: http://www.compphys.org/QCE/

university of groningen / faculty of science and engineering / zernike institute for advanced materials

INDEFINITE CAUSAL ORDER: FASTER COMPUTERS AND FUNDAMENTAL QUESTIONS

Quantum mechanics has greatly improved the speeds at which computers make calculations, but new research shows that quantum computers can be made to run even faster. **Professor Philip Walther** and his team at the University of Vienna have shown that the very orders in which quantum computers carry out operations can be superimposed, essentially meaning that two or more operations can be carried out at the same time. This work could give rise to even more efficient quantum computers in the near future, but also leaves some baffling questions about our physical understanding of the Universe.



A Computational Revolution

Over recent decades, research into quantum computing has laid the foundation for devices that will greatly improve the efficiency of classical computers. In regular digital computers, data is encoded into binary digits in two definite states – 0 and 1. These 'bits' of data are processed by logic gates, which output further bits whose states depend on those of the input bits. When sequences of these logic gates are arranged into circuits, they output information that acts as instructions to the computer, telling it what to do next.

In quantum computers, however, quantum properties can be exploited to superimpose multiple states onto individual particles. These particles, known as quantum bits, or 'qubits', can essentially carry multiple 0s and 1s at the same time. As they pass through a quantum logic gate, all 0s and 1s are processed simultaneously.

Quantum algorithms are designed so that the co-existence of 0s and 1s is affected by destructive and constructive interference, until only the 0s and 1s that are the sole output of the calculation are left. This approach offers huge advantages over regular computers, as instead of every bit of data corresponding to a single input state, many input states can be encoded onto just a few qubits, enabling the co-existence or 'superposition' of many different input states.

This massive parallelism of input data and the possibility of having quantum circuits allows for quantum algorithms that require significantly fewer steps than classical algorithms in conventional computers. Overall, this means that quantum computers allow operations to be carried out far more efficiently, which reduces not only computational speeds, but energy consumption, and therefore costs.

However, Professor Philip Walther and his team at the University of Vienna believe that more complex quantum mechanical processes can be exploited to improve the efficiency of quantum computers even further.

Even Faster Speeds for Quantum Computers

In a 2015 study, Professor Walther and his colleagues showed that quantum

‘It is truly remarkable that quantum physics keeps surprising us about possible concepts and applications for which quantum mechanical features can be exploited – and I am sure that we are still at the beginning of this journey’

mechanics allows for the superposition of not just quantum states on a single particle, but of entire circuits of quantum gates. This means that the order in which operations are carried out on sequences of quantum gates is indefinite. In other words, multiple operations could essentially be carried out at the same time.

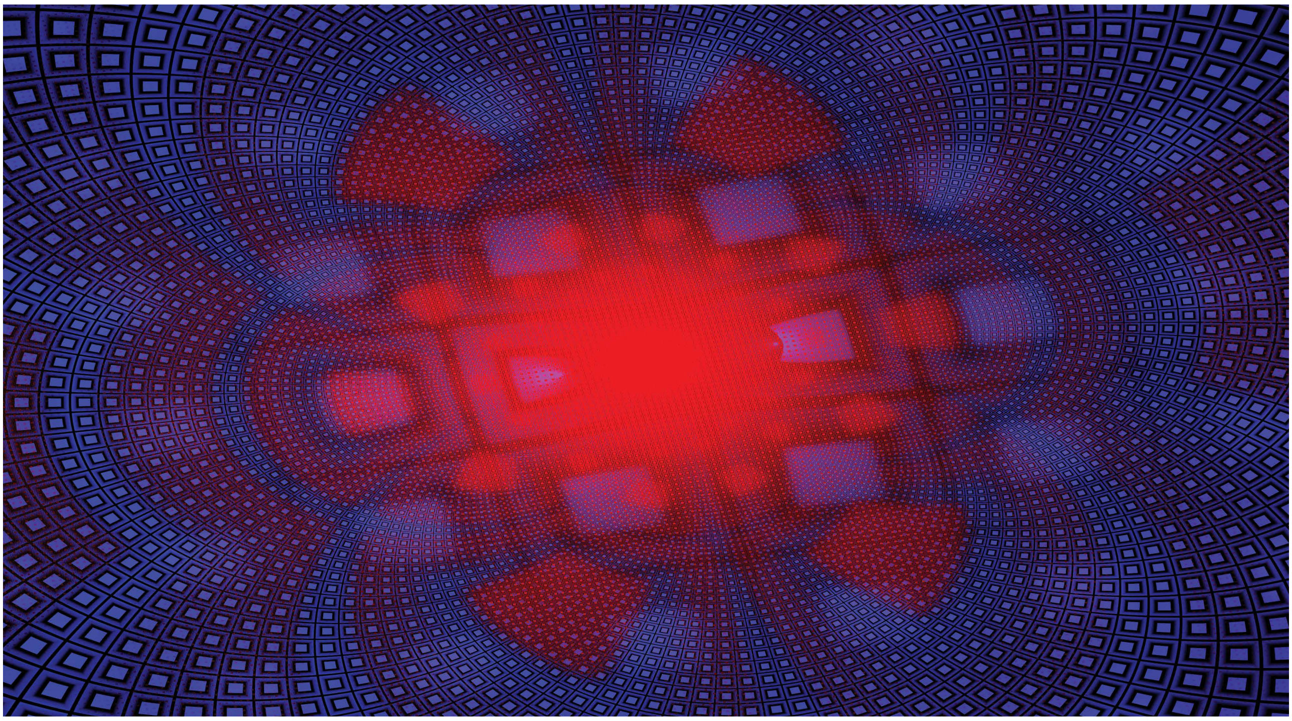
The team demonstrated that if a gate can be used multiple times, fewer gates need to be used overall, increasing the efficiency of the computer. By superimposing multiple circuits, the researchers could control which circuit was applied to an input qubit. Therefore, they could test whether the superposition of multiple circuits really improved computation speed by calculating the reduction in ‘query complexity’ (calculated from the smallest number of queries required to calculate a function) compared with conventional quantum computers.

To implement their ideas experimentally, Professor Walther’s team created a simple quantum circuit, consisting of two logic gates they named Alice and Bob. Typically, an input qubit would either be sent from Alice to Bob or from Bob to Alice, resulting in two possible paths. However, the researchers added a layer of complexity to the scenario by encoding two qubits into the same photon (light particle) by using its path and polarisation as the variable parameters. The two qubits were named the ‘control qubit’, which would be acted upon by the scientists, and the ‘target qubit’, which would itself pass through the logic gates.

The control qubit acts on the target qubit by defining the order of gate operations through which the target (input) qubit will propagate. When the control qubit is in one state, then the target qubit will first pass through Alice, and then through Bob, while when the control qubit is in the other state, the target qubit will pass through Bob first, and then Alice. Now, when the control bit is prepared in the superposition of both states, then the target qubit will have superimposed or indefinite orders: both Alice to Bob, and Bob to Alice. Therefore, the path taken by the target qubit depends entirely on the preparation of the control qubit.

How Much Faster?

When Alice and Bob are quantum gates, then this superposition of quantum gate orders is indefinite and does not allow us to know, even in principle, if one operation occurred before another operation, or the other way around. This means that two quantum logic gates A (for Alice) and B (for Bob) can be applied in both orders at the same time. In other words, gate A acts before B and B acts before A. Professor Walther’s team designed an experiment in which the two quantum logic gates were applied to single photons in both orders.



The results of their experiment confirm that it is impossible to determine which gate acted first – but the experiment was not simply a curiosity. In fact, they were able to run a quantum algorithm to characterise the gates more efficiently than any previously known algorithm. From a single measurement on the photon, they probed a specific property of the two quantum gates thereby confirming that the gates were applied in both orders at once.

For future developments as more gates are added to the task, this new method for quantum computers becomes even more efficient compared to previous techniques.

Fundamental Questions

The idea of 'causality' is fundamental to our understanding of how the Universe works. It defines the link between physical events that follow each other chronologically. If one event happens before a second event it's linked to, it seems logical to us that the first event was the cause of the second – in other words, a 'definite causal order'.

However, in their exploration of the properties of quantum mechanics that allowed them to achieve faster computational speeds, Professor Walther's team realised that their experiment appeared to utilise 'indefinite causal order'. In their initial experiment, Professor Walther's team could not observe indefinite causal order directly. The researchers had confirmed and quantified its apparent consequences with the faster computational speeds achieved, but they hadn't yet measured the quantum mechanical properties that would confirm whether the causal order of the use of Alice and Bob was truly indefinite.

To do this, they had to go significantly beyond the previous experiment by experimentally superimposing more complex processes for A and B. These processes included quantum measurements acting on the target bit when passing through Alice. Importantly, for enabling this in a circuit, the order of multiple quantum operations can be superimposed, and both possible outcomes of Alice were processed into Bob, or vice versa.

From then on, there would be no chance to ever read the outcome of the initial gate – a measurement could only be made at the very end of the process, meaning it could never be determined which path was actually taken. This allowed the team to characterise the indefinite causal order by acquiring information from inside (where the superposition of causal orders take place) and outside, where the result after the processing through the circuit can be measured.

As Professor Walther's team mention in their paper, 'this can lead to disconcerting consequences, forcing one to question concepts that are commonly viewed as the main ingredients of our physical description of the world. But these effects can be exploited to achieve improvements in computational complexity and quantum communications.' It's a somewhat startling idea. On a quantum scale, the comfortable notion that an outcome can be directly attributed to distinct previous events does not always hold, and yet this mysterious property can be exploited for our benefit.

The work of Professor Walther and his colleagues has opened up a wide avenue of possibilities in quantum computing. There is now much progress both in increasing speeds and reducing costs of quantum computers in the near future – a significant step towards making them widely commercially available.

Meet the researcher

Professor Philip Walther
Faculty of Physics
University of Vienna
Vienna
Austria

Professor Philip Walther completed his PhD in Physics at the University of Vienna in 2005, after which he took a post as a postdoctoral researcher at Harvard University. He returned to Vienna in 2009, and is now a tenured Professor at the Faculty of Physics. His areas of research include various fields in the development of quantum computing, and investigating the interface between quantum physics and gravity. Professor Walther co-founded the TURIS research platform in 2017. He has received a variety of prestigious awards for his work and has been elected as a member of the Young Academy at the Austrian Academy of Sciences and as fellow of the American Physical Society.

CONTACT

E: philip.walther@univie.ac.at
W: http://walther.univie.at
W: http://turis.univie.ac.at
W: http://vcq.quantum.at

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UNIVERSITY OF VIENNA

MAXWELL'S DEMON: EXTRACTING ENERGY FROM CHAOS

Since it was theorised over 150 years ago, physicists have viewed the concept of 'Maxwell's demon' as a highly desirable yet ultimately unattainable source of energy. For over a century, the device seemed to work theoretically, but a fundamental barrier prevented it from being realised: the second law of thermodynamics. Unperturbed, a team of physicists including **Dr Gernot Schaller** at the Technical University of Berlin have shown that Maxwell's demon can be practically implemented when the second law is extended. Their findings may help to improve the performance of quantum heat engines.

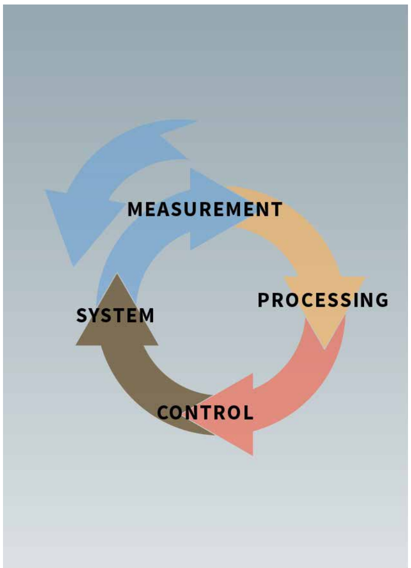
In 1867, Scottish physicist James Clerk Maxwell, regarded by many as the founding father of electromagnetism, proposed a puzzling thought experiment. In a letter, he described an intelligent device in a box that could sort particles of gas into two separate cavities: one for cold, slow-moving particles, and the other for hot, fast-moving particles.

'Maxwell's demon', as the device came to be known, operated by intuitively opening up a hole between the cavities, which allowed fast-moving particles in the cold cavity to move into the hot cavity, and vice versa – increasing the temperature difference between the cavities over time. Perplexingly, Maxwell showed that the demon wouldn't require any work to open and close the hole under ideal conditions. However, beyond this reasoning, the demon faced an immediate problem.

The second law of thermodynamics states that when a system of particles undergoes a process, the overall order of the system cannot increase. In other words, the level of disorder, or 'entropy', can only become greater. Interacting with a gas should, therefore, make the behaviour of its particles more chaotic, yet Maxwell's demon appeared to do the exact opposite. A gas separated into its hot and cold constituent particles would clearly be more ordered than before it interacted with the demon. Importantly, a heat engine could extract useful work from this thermal gradient.

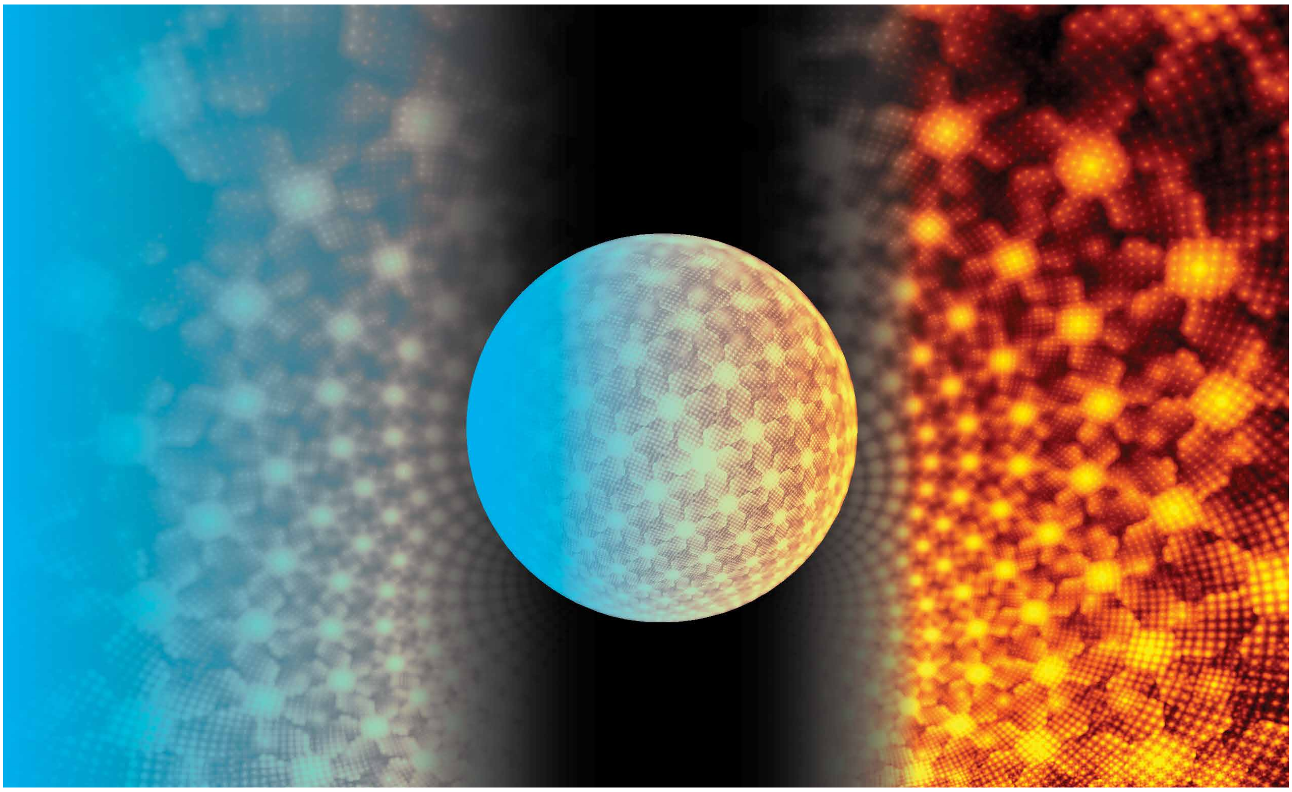
The apparent violation of the second law was a subject of debate for decades until 1961, when German-American physicist Rolf Landauer proposed how Maxwell's demon could operate without decreasing the entropy. He suggested that a periodically operating demon must – after processing each particle – delete information from its memory. This would ultimately increase the net entropy of the overall system and resolve the contradiction with the second law.

From this theoretical basis, a team of researchers including Dr Gernot Schaller and his colleagues at the Technical University of Berlin have proposed to implement Maxwell's demon in real life, and aim to use the device to improve practical energy generators.



Ways to Build a Demon

In 2011, the Berlin researchers – at that time led by Professor Tobias Brandes – suggested how Maxwell's demon could take the form of a device called a 'quantum dot' coupled to two electronic leads. Consisting of a semiconductor made from just a few hundred atoms, the dot could effectively act as a 'feedback-controlled single-electron transistor', deciding on which particles are allowed through to the other lead.



In this setup, the leads are at the same finite temperature, which leads to slow fluctuations of the charge of the dot. However, the potential of the leads is different, such that the demon directly generates electric power by driving electrons against a bias.

At the start of the process, the demon makes a measurement of the dot with a charge detector, deciding whether it is empty or filled. Depending on the outcome of the measurement, the demon opens a hole either in the left or the right wall to perform the sorting operation. When the information gained by the measurements is taken into account properly, the second law is not violated. However, to perform this operation automatically, the research team noted that they needed a further degree of complexity in their theoretical setup.

To operate autonomously, the demon could be implemented by a second quantum dot that continuously monitors the state of the first. The state of this second dot would depend entirely on that of the first – if it changed to a state that caused the demon to open the wall, the second dot would also change accordingly.

To make use of the state of the second quantum dot, the team, backed up by Dr Philipp Strasberg and Dr Massimiliano Esposito, proposed a devious trick. The second quantum dot would be connected to a third thermal lead – itself entirely separate from the leads connected to the first quantum dot. In line with Landauer's principle, the memory of the demon, which allowed it to perform the feedback loop, is thereby the single bit of information stored in the second dot, and its deletion is directly connected to the dissipation of heat into the third thermal lead.

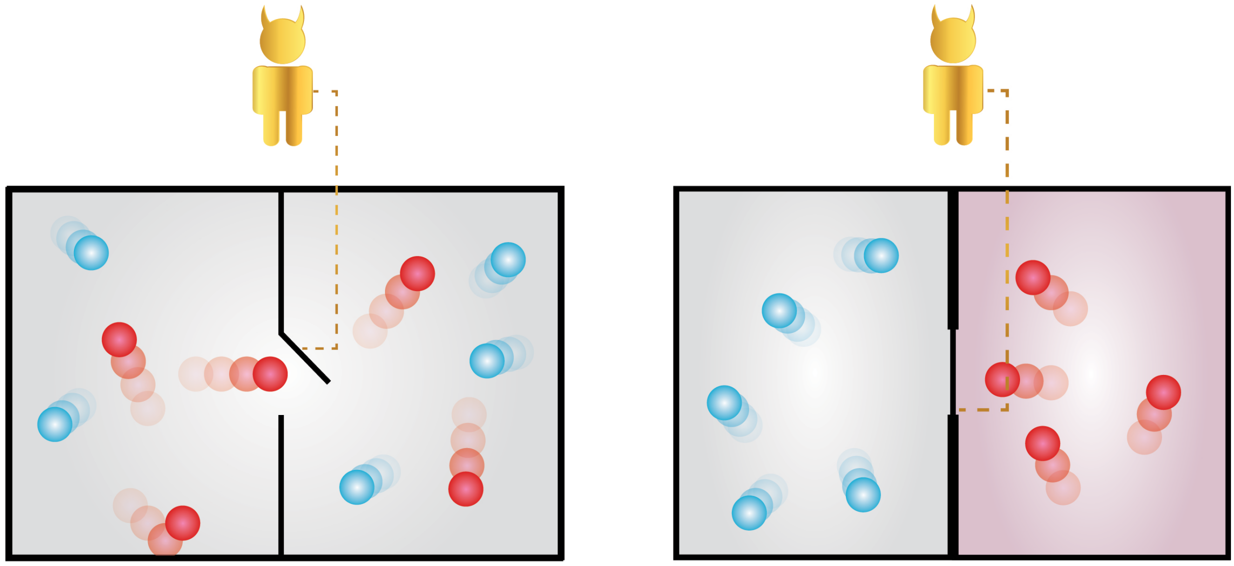
Although entropy increased in the system as a whole, nonequilibrium quantum effects could be smartly exploited to 'delete' the demon's memory after every decision. Using an autonomously operating microscopic model, the researchers demonstrated that the second law was globally valid without the need to invoke Landauer's principle.

Methods for Implementation

In reality, the situation where the demon 'opens up a hole between the two cavities' is more complex than this initial description. For the system to work, the central dot and the lead would be entirely separate from each other in a classical sense. In fact, the 'hole' represents how the electron continuously 'tunnels' between the dot and lead – travelling through a barrier instead of jumping over it.

In presence of a thermal gradient between the third lead and the two original leads, this quantum tunnelling induces a spontaneous electric current across the single-electron transistor. Since the two quantum dots are interacting with each other, the occupation of the demon dot will equilibrate depending on the occupation of the first dot. For appropriate parameters, this in turn will back-act on the current induced in the device, creating a closed feedback loop between the two contacts.

The Berlin team derived the equations needed to describe this feedback



loop, giving them an idea of how tunnelling rates could be modified to optimise the power generated by the demon. In 2015, a corresponding autonomous demon was experimentally implemented by researchers from Aalto university in Finland.

Such autonomous devices have the disadvantage that they always follow the same feedback protocol and thereby achieve the same function. In contrast, Maxwell's original demon could in principle also change its mind and sort the particles the other way. Therefore, it was still an open question whether the 2011 proposal could be implemented with an external feedback loop.

Creating an Optimised Power Generator

Inspired by these advances, a team led by Dr Akira Fujiwara at the NTT Basic Research Laboratories in Japan aimed to create Maxwell's demon, and use it to convert the free energy it generates into work that acts on its surroundings.

In their 2017 experiment, Dr Fujiwara's team followed an approach similar to the 2011 theoretical study proposed by the Berlin researchers. They demonstrated that information can be used to control the electric current through an artificial quantum dot. Moreover, the device was capable of generating electric current and power from information. Through numerical calculations, the Japanese researchers showed that power generation could be increased by miniaturising the cavity space within which electrons are confined.

These concepts work well when the opening or closing of a shutter does not cost relative amounts of energy and if the feedback loop is slower than the electronic equilibration time in the leads. To go beyond these limitations, Dr Schaller and Dr Georg Engelhardt at the Technical University of Berlin investigated what would happen when charge measurements were performed at an infinite rate.

The duo used a 'dynamical coarse-graining' method, which allowed them to reach the non-Markovian regime – where the evolution of the system at a given point in time not only depends on a snapshot at that time, but requires knowledge of all previous times. They discovered an optimal feedback protocol, where as much energy was extracted from the feedback loop as possible. In addition, they found that the Quantum Zeno effect (a feature whereby a quantum particle's movement is arrested by frequently taking measurements of it) would ultimately limit the output power by freezing the system.

Potential for Heat Engines

Through years of research, the team and their collaborators have gained an in-depth understanding of how Maxwell's demon can be used to extract energy from a variety of quantum systems. Yet until now, many issues have remained – for example, whether these insights can be used to improve the design of quantum heat engines. In thermodynamics, heat engines on macroscopic scales are incredibly important. On a quantum scale, however, their performance so is far too poor to be of practical relevance.

Unlike other quantum devices, such as quantum computers, which require complete isolation from their surrounding environments, Maxwell's demon actually needs to interact with its surroundings.

In the future, the team hopes that further fine-tuning of the quantum characteristics of the demon will allow for hugely efficient devices that extract useful energy from the heat of individual particles. For a concept that seemed to defy a fundamental physical law just a few decades ago, the practical uses of Maxwell's demon seem to have an incredibly promising future.

Meet the researcher

Gernot Schaller
Institute for Theoretical Physics
Technical University Berlin
Berlin
Germany

Gernot completed his PhD in Physics at Frankfurt University in 2006, after which he worked as a postdoctoral researcher in the field of Theoretical Physics at Technical University Dresden and Technical University Berlin. He is now a visiting professor in Computer-aided Material Physics at this university. His major research focus includes the dynamics of quantum systems far from equilibrium, in particular quantum transport. He is specifically interested in advancing concepts and methods.

CONTACT

E: gernot.schaller-AT-tu-berlin.de
W: www1.itp.tu-berlin.de/schaller/

KEY COLLABORATORS

Philipp Strasberg, Technical University Berlin and University of Luxembourg
Massimiliano Esposito, University of Luxembourg
Georg Engelhardt, Technical University Berlin and Beijing Computational Science Research Center

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Technische Universität Berlin

THE NATIONAL RESEARCH COUNCIL OF CANADA'S ADVANCED ELECTRONICS & PHOTONICS RESEARCH CENTRE

Headquartered in Ottawa, the National Research Council (NRC) is the primary national research and technology organisation of the Government of Canada. As one of its many research centres, the Advanced Electronics and Photonics Research Centre serves the information and communication technology industries by providing firms with access to expertise and state-of-the-art facilities. In this exclusive interview, we speak to **Ruth Rayman**, Director General of NRC's Advanced Electronics and Photonics Research Centre, who tells us all about the Centre and its varied activities.

To begin, please give us a brief introduction to NRC's Advanced Electronics and Photonics Research Centre.

The National Research Council of Canada and its Advanced Electronics and Photonics Research Centre (AEP) develop advanced sensing and communications technologies that collect and move data. The Centre enables Canada's infrastructure and services to become smarter, creating sustainable prosperity in the digital era.

Through world class researchers and facilities, we work with academia, other research organisations and industry to discover, de-risk, develop and commercialise technologies that address economic and social challenges critical to Canada and the world. We focus on next-generation semiconductor based photonics and electronics.

What types of research is conducted at this Centre, and for what applications?

We conduct innovative research and development in the areas of integrated photonics for telecommunications, Semiconductor lasers for medical applications, sensors and telecommunications, and printable electronics for autonomous energy collection, smart packaging, wearable electronics, advanced manufacturing, and internet of things applications.

Tell us about the importance of these technologies to the global and Canadian economies, and to improving people's quality of life.

The Government of Canada's priorities as expressed in the Innovation Agenda revolve around an improved quality of life for Canadians and a more sustainable society and economy. From Advanced Manufacturing to Smart Cities to Mobile Health, it's all about making the systems and processes we use smarter, more energy efficient and more secure so that we are more globally competitive.

Systems and processes become smarter when decisions are informed by data, which is created by distributed sensor arrays and transported by fast and secure networks. Our focus is to create the novel sensors and network components that enable Canada's infrastructure to be smart and support these goals.

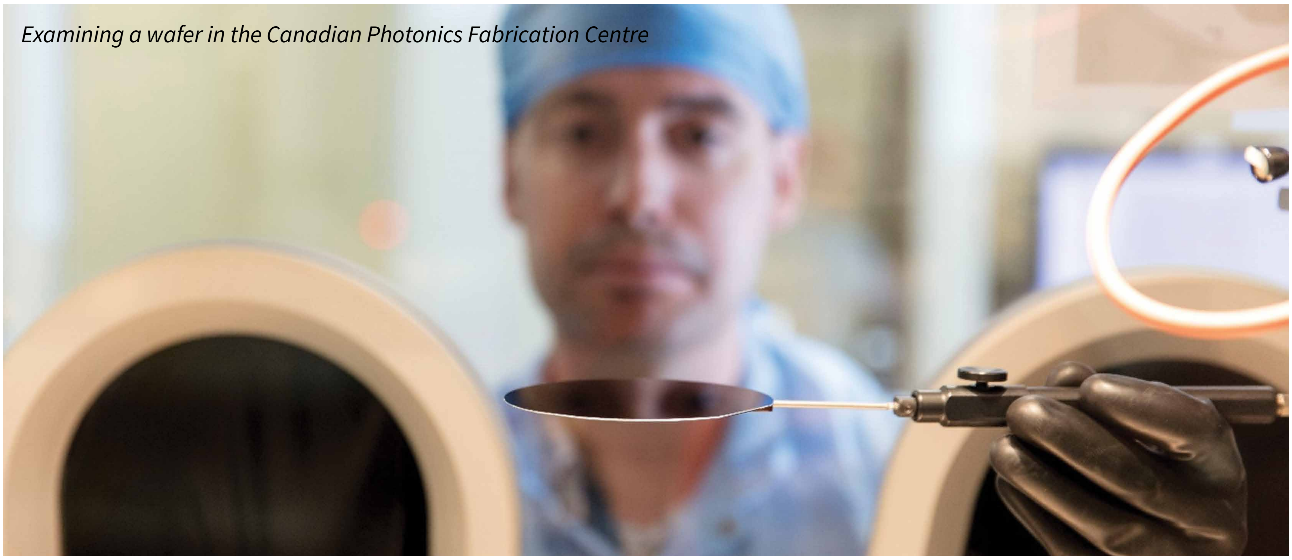
In what ways does NRC's Advanced Electronics and Photonics Research Centre help its collaborators to bridge the gap between innovation and commercialisation? How do you facilitate the introduction of new technologies into both national and global markets?

We are focused on developing innovative technology for commercialisation to create a sustainable competitive advantage for Canadian industry. We shorten the time to market and provide leading edge components with a primary focus on assisting industry in crossing the gap from R&D to manufacturability of innovation. Our unique value is our continuum of innovation, taking basic materials research, all the way through to production – very few places in the world boast this capability.

Please tell us more about some of the technical services offered by the Centre. Who is eligible to avail of these services?

We provide a number of different engagement mechanisms and collaboration models such as research service agreements, collaborative research agreements, technical services and technology licensing opportunities.

‘We focus on specific R&D areas where we can provide the greatest impact to Canadian organisations and ensure that despite the international pressures, Canada remains on the leading edge’



Examining a wafer in the Canadian Photonics Fabrication Centre

All of these services and mechanisms are available to small and medium-size enterprises, multinational enterprises and academic organisations.

Describe one or two recent success stories where you've helped to bring an innovative technology to the market.

We collaborated with GGI Solutions of Laval, Quebec to co-develop a new family of molecular inks for the printed electronics market. It has a number of exciting applications: In Mould Electronics (IME), sensors, antennae and displays. This collaboration has resulted in a large licensing agreement with one of the largest chemical multi-national organisations in the world, Sun Chemicals. The impact of this collaboration will further secure the growth and prosperity of GGI as well as the importance of Canada as a leader in printable electronics.

On another note, Ranovus develops and manufactures multi-terabit interconnect solutions for data centre and communications networks in the telecommunications and information technology industries, based on the NRC's Quantum Dot technology. Ranovus has raised over $35M in private equity to develop commercial products from this technology platform, and since 2012, has engaged in multiple rounds of collaborative research agreements, new product introductions, and most recently production agreements with us to drive the technology from inception through to general commercial availability.

This approach to leveraging multi-wavelength emission from a single laser chip (NRC quantum dot technology) puts Ranovus in a lower cost, lower power, smaller foot print, more environmentally sensitive position than competing technologies for the datacentre industry (DCI) and metro access applications. These advantages are highly valued in the multi-billion-dollar market space.

Finally, what do you see as the biggest challenges that lie ahead for the fields of advanced electronics and photonics in Canada and worldwide? How does the Centre aim to tackle these challenges?

With international demand for smart electronics and increased bandwidth in networks and data centres, the challenges to Canada are related to international competition and the

Pouring conductive molecular ink in the laboratories of the Canadian Photonics Fabrication Centre

ability to transition leading edge innovations to technologies. We enhance R&D and innovation capabilities for Canadian industry through our expertise and facilities to decrease time-to-market for innovators. We focus on specific R&D areas where we can provide the greatest impact to Canadian organisations and ensure that despite the international pressures, Canada remains on the leading edge.

The NRC also facilitates access to sources of innovation and commercialisation support through Industrial Research Assistance Program (IRAP) funding and business advisory services.

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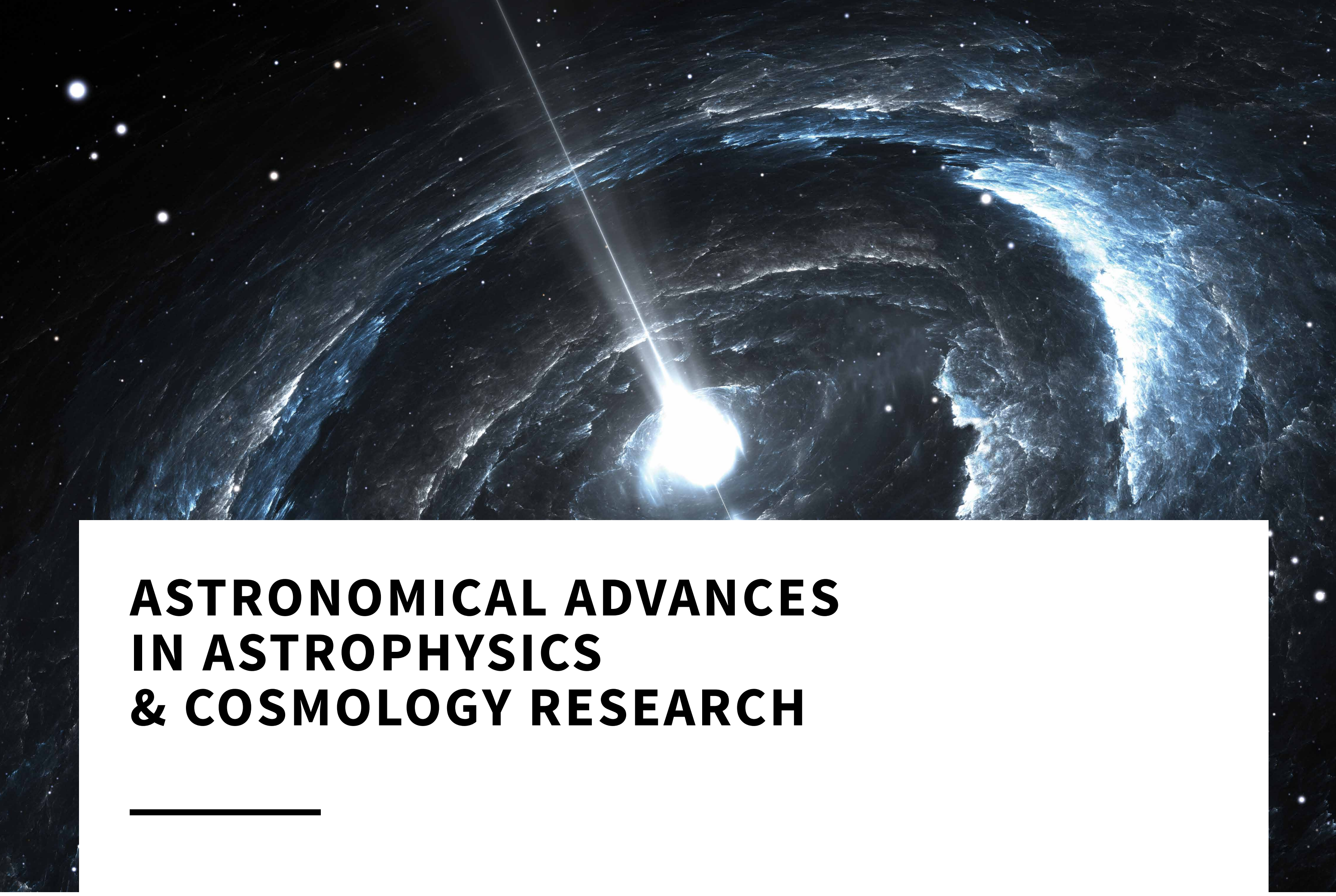
ASTROPHYSICS & COSMOLOGY



ASTRONOMICAL ADVANCES IN ASTROPHYSICS & COSMOLOGY RESEARCH

There has never been a more exciting time for astrophysics and cosmology research. For example, in 2016, scientists at the Laser Interferometer Gravitational-Wave Observatory (LIGO) announced their game-changing discovery of gravitational waves. These ripples in the fabric of spacetime, whose existence was first proposed by Albert Einstein a century ago, were caused by a pair of black holes merging together over one billion lightyears away.

Then, just earlier this year, scientists at Columbia University discovered that there could be as many as 10,000 black holes swarming around the supermassive black hole at the centre of our galaxy. This finding will greatly aid scientists who are deepening our knowledge of gravitational waves.

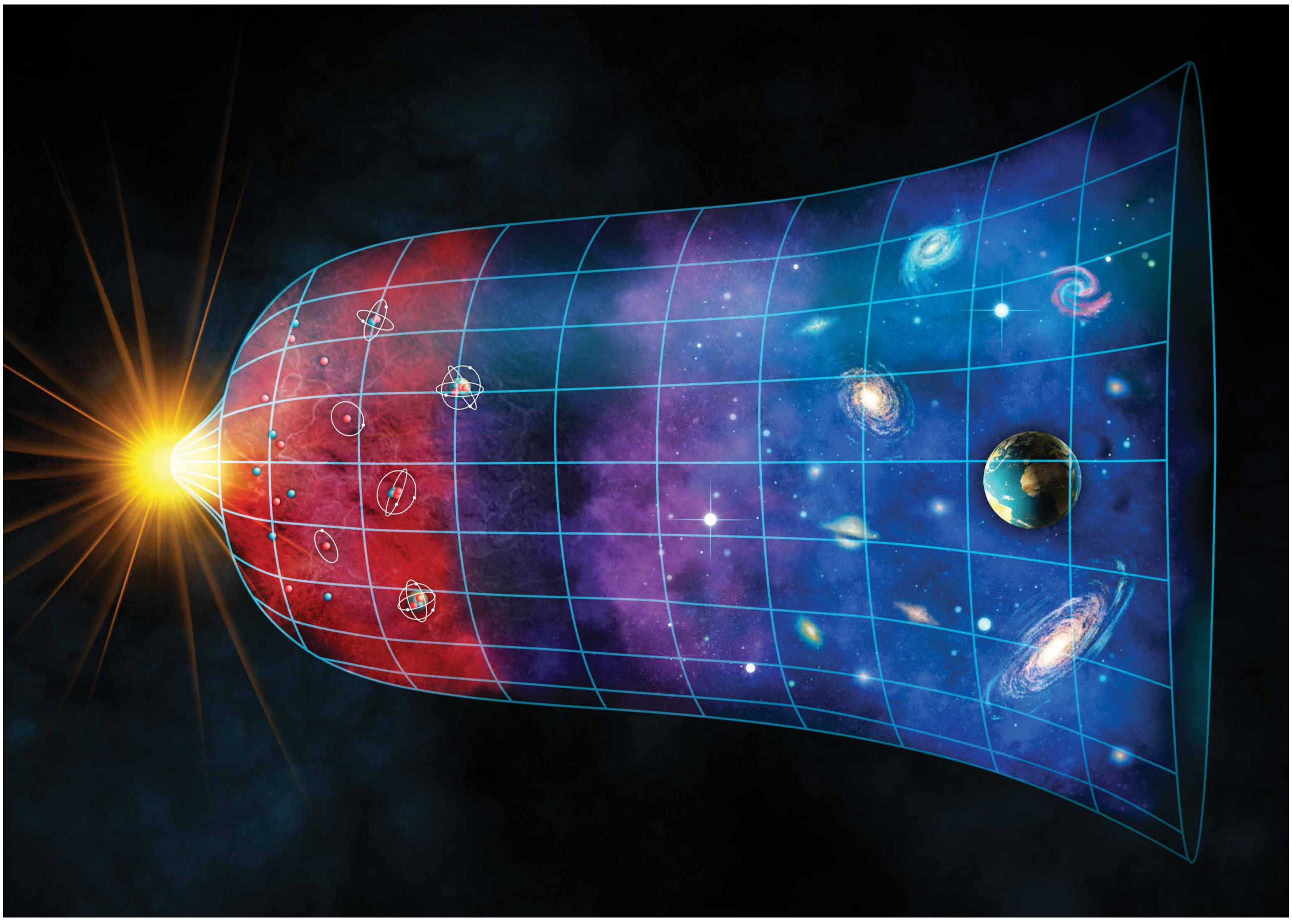
Now, one of the next big challenges for the fields of cosmology and astrophysics is to identify dark matter. Remarkably, this unidentified substance is estimated to make up a whopping 84% of all the matter in the universe, and it is not expected to be made up of normal matter. Even though we cannot directly observe dark matter, scientists know it is there, as it interacts gravitationally with both light and normal matter.

Some of the first strong evidence for this elusive substance came with the findings of an American astronomer called Dr Vera Rubin, who accurately measured the speed of stars in rotating galaxies. Although Kepler's law predicts that in spinning galaxies, a star further from the galactic centre should be rotating around it much slower than a closer one, Dr Rubin observed that all stars were rotating at roughly the same speed, regardless of their distance from the centre. This suggests that the stars are not really rotating around the supermassive black hole at the galaxy's centre, but around numerous other unknown clumps of 'dark matter' that provide a gravitational pull.

And galactic rotation speeds are not the only evidence indicating the existence of dark matter. Because of its mass, dark matter can bend spacetime – as described by Einstein's hundred-year-old theory of General Relativity (mentioned above). Warped spacetime leads to a phenomenon known as 'gravitational lensing', whereby light passing through a region of dense matter bends. Such bending can be observed using telescopes.

Finally, further evidence for dark matter is offered by the cosmic microwave background – light emitted in the early universe just 380,000 years after the Big Bang. Because of the universe's expansion over the past 15 years, this light has been stretched out to such an extent that we now detect it as low-energy microwave radiation. Unexplained fluctuations in this background radiation are believed to be caused by the presence of dark matter in the early universe.

Although there is much evidence for its existence, scientists have yet to detect dark matter directly. Furthermore, this elusive substance is highly unlikely to be composed of normal 'baryonic' matter (i.e. the protons and neutrons that comprise atoms). Therefore, many scientists predict that dark matter is made up of an as-yet unknown elementary particle – one that barely



interacts with normal matter or light, except through gravity. Because dark matter barely interacts with normal matter or light, this makes it extremely difficult to detect. However, many research groups across the globe are working to develop ingenious detectors to pin down the true nature of this mysterious substance. In our first two articles of this section, we meet two such teams of scientists – one headed by Dr Elena Aprile at Columbia University, USA, and the other led by Dr Gilles Gerbier of Queen's University, Canada. Both teams use large underground chambers of noble gases, which lie in wait for a miniscule flicker of energy that indicates the presence of dark matter.

Next, we meet Dr Liping Gan and her team at the Thomas Jefferson National Accelerator Facility, who perform experiments towards extending our current model of particle physics (the Standard Model). Using their new insights into the nature of force-carrier particles, the team hopes to adapt the Standard Model so that it accounts for the existence of dark matter, in addition to other elusive aspects of the universe.

In our fourth article of this section, we detail the impressive research career of the astronomer Dr Uli Klein. In just one aspect of his extensive work, Dr Klein has worked to map the distribution and quantity of dark matter in galaxies by investigating galactic radio emissions. His observations provide further evidence that dark matter is not composed of ordinary matter.

Rather than studying radio emissions, Dr Jeremy Drake at the Smithsonian Astrophysical Observatory and his collaborators analyse X-ray, optical and infrared radiation from star forming regions – dense complexes of young and newly forming stellar clusters. Their work, which we describe in detail in this section, is shedding light on the physics of how stars and planets form.

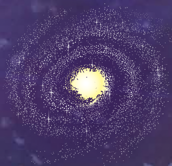
Also working to reveal the origin and evolution of planets is Dr David Jewitt and his team at the University of California, Los Angeles. In particular, Dr Jewitt and his colleagues investigate the nature of comets, as these cosmic snowballs provide unparalleled opportunities to learn about the earliest periods of our solar system's evolution.

In our final article of this section, we address the question of why the physical laws and constants in the universe appear to be 'fine-tuned' so that complex beings such as ourselves can arise. For example, if the masses of the lightest fundamental particles (the electron and the lightest quarks) had been remotely different, then stable atoms could not have formed. If the force of gravity were even slightly weaker, then galaxies and stars may never have coalesced.

Here, we meet physicist and philosopher Dr Simon Friederich of the University of Groningen, who explains this fine-tuning conundrum by the hypothetical existence of many universes beyond our own. His argument in favour of the 'multiverse' is compelling to say the least.

DARK MATTER

Evidence for dark matter
Though dark matter doesn't emit or interact with light, it has mass, and so interacts through gravity.
Three examples of such interactions are:

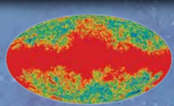


1.

GALAXY ROTATION CURVES
The rotation speeds of stars should decrease with distance from a galaxy's centre. However, this speed remains roughly constant, meaning that there must be clumps of invisible matter throughout the galaxy.

2.

GRAVITATIONAL LENSING
Regions of high dark matter density bend space, distorting light that travels past.
This distortion can be observed using telescopes.



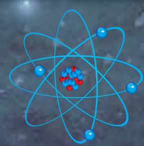
3.

COSMIC MICROWAVE BACKGROUND
This background radiation is light that was emitted soon after the Big Bang. Unexplained fluctuations in this radiation are believed to be caused by the presence of dark matter in the early universe.

What is dark matter?
Scientists do not know what dark matter is actually composed of. However, there are several candidates:

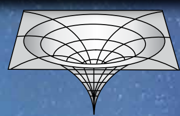
1.

AN UNDISCOVERED TYPE OF ELEMENTARY PARTICLE
This is the primary candidate for dark matter. Top possibilities are 'weakly-interacting massive particles' (WIMPs), and 'gravitationally-interacting massive particles' (GIMPs).



2.

NORMAL (BARYONIC) MATTER
In addition to normal protons and neutrons, baryonic matter also makes up black holes, neutron stars, faint white dwarfs and brown dwarfs (collectively known as MACHOs), which are hard to detect. However, much evidence suggests that dark matter is not composed of MACHOs.



3.

DARK MATTER DOESN'T ACTUALLY EXIST
Some scientists believe that our current theory of gravity (general relativity) needs to be revised to account for our observations. However, most astrophysicists agree that there is enough data from many different observations to conclude that dark matter exists.

Dark matter makes up
84%
of all the matter in the universe

DARK MATTER HUNTERS

Professor Elena Aprile and her collaborators, **Drs Kaixuan Ni** and **Luca Grandi**, join together with a worldwide consortium of scientists to design massive detectors for identifying the invisible matter that makes up the majority of our Universe.

For over 100 years, scientists have suspected that the 'empty' space between stars and other visible objects in our Universe is probably not empty. As far back as 1884, the Scots-Irish scientist and mathematician Lord Kelvin noted that the motion of stars in the Milky Way galaxy was inconsistent with the amount of matter observed – the stars and interstellar dust clouds we could see – and that much of the mass in the galaxy might be what he called 'dark bodies'. In 1906, the French scientist Jules Henri Poincaré termed Kelvin's dark bodies as 'matière obscure' – dark matter.

In the ensuing decades, a number of scientists had corroborated the fact that much or even most of the matter in our galaxy and others is dark matter. By the 1980s, this had become quite a problem in astrophysical circles. The majority of the Universe's was invisible to our instruments – so what is it, and how do we measure it?

This is a problem that Professor Elena Aprile of Columbia University has been working on for over 15 years. Theoretically, dark matter exists, but it does not interact with light or normal matter, so we cannot directly measure it. As Professor Aprile says: 'We know it's there, but it continues to escape instruments invented so far.' That leaves it up to her and her colleagues to directly measure it. To do that, they have built detectors containing increasing amounts of the inert element xenon, in the hope that some of the massive 'dark' particles that rain down on earth will collide with xenon atoms.

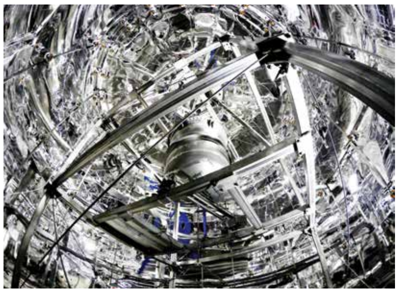
The XENON Project

Early in her physics career, Professor Aprile studied under Professor Carlo Rubbia, who shared the Nobel Prize in Physics in 1984 for discovering several subatomic particles using a particle accelerator at CERN. Inspired by Professor Rubbia, Professor Aprile became interested in detecting subatomic particles using the noble gases – specifically argon and xenon – which have the advantage of being inert, meaning that they rarely react with the electrons of other atoms and molecules.

If a high-energy particle travels through a tank of liquid argon or xenon and collides with its atoms and molecules, it transfers energy. This energy causes electrons of argon or xenon atoms to become dislodged and travel through the liquid to reach the detector. Not only does this process produce detectable electrons, but energised argon and xenon atoms can also release light – alerting scientists of a collision with a high-energy particle.

While Professor Aprile did her graduate work with argon, she then moved on to the heavier noble element xenon, and has since become a pioneer in the use of liquid xenon for particle detection. The design of these exquisitely sensitive xenon detectors is something that came in handy in the hunt for dark matter – especially if it is made up of dark particles called WIMPs.

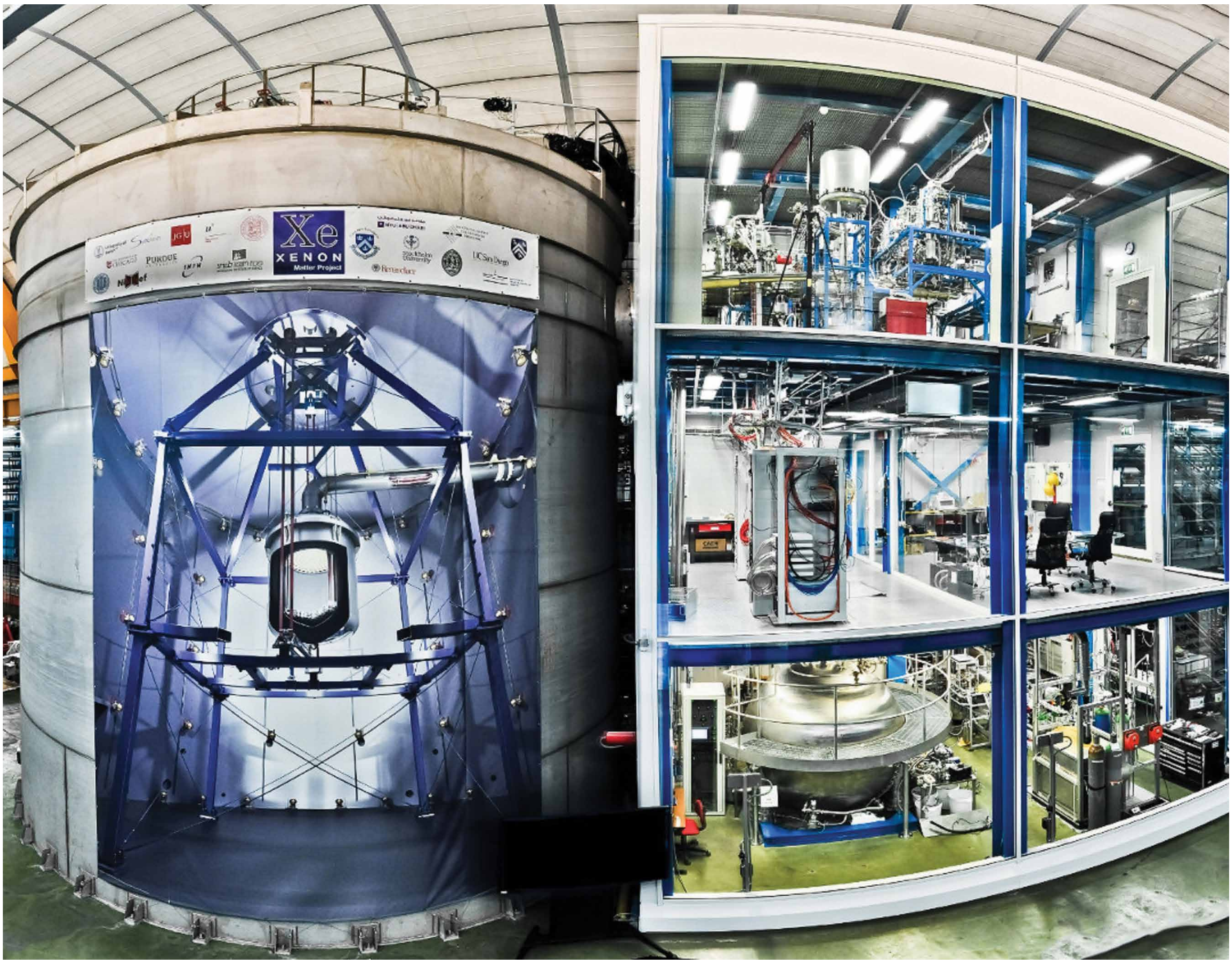
The WIMP – the 'weakly interacting massive particle' – is a theoretical



CREDIT: Roberto Corrieri, Luigi Di Carlo and Patrick DePerio

CREDIT: Roberto Corrieri, Luigi Di Carlo and Patrick DePerio

elementary particle of dark matter that does not interact with strong forces, such as electromagnetic forces, but only weakly, through gravity and the weak nuclear force. As well, to fulfil some of the observed effects of dark matter, the particle must have a very large mass compared with other subatomic particles. This is what makes the WIMP a WIMP – big mass, weak interaction. Because it only very weakly interacts, a very sensitive detector must be designed if WIMP interactions are to be picked up as they pass through.

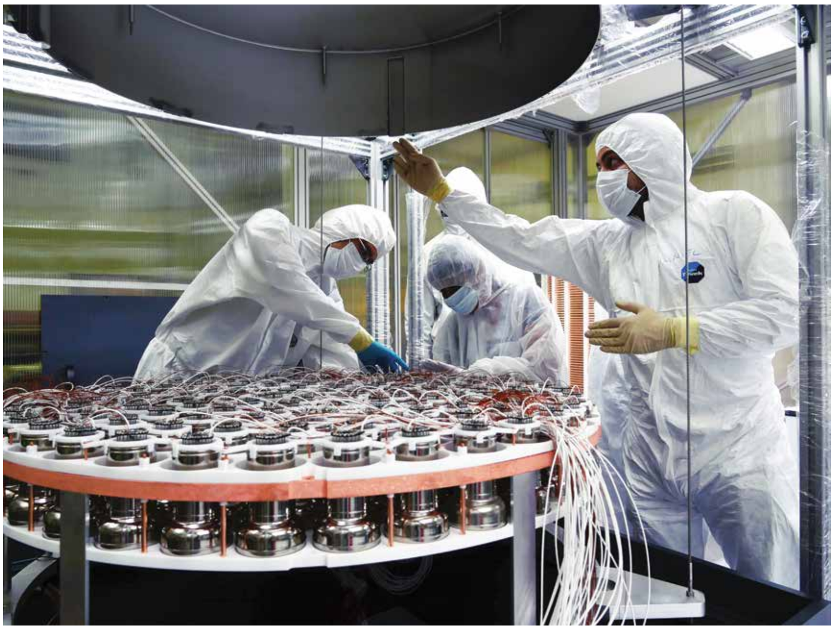


CREDIT: Roberto Corrieri, Luigi Di Carlo and Patrick DePerio

In 2001, Professor Aprile set her mind on using liquid xenon to design an experiment that would be very sensitive in the search for dark matter. With her experience gained from working with liquid xenon gamma ray detectors for NASA, Professor Aprile started a crusade that has almost circled the globe – the XENON project – a consortium of about 165 scientists in multiple centres around the world focused on finding the elusive WIMP. The idea is to detect these WIMPs as they collide with liquid xenon atoms in detectors that are operated deep underground to minimise noise from cosmic radiation. The combination of xenon's exquisite response to radiation and a deeply-buried location reduces background noise from other particles and will hopefully allow the weakly-interacting WIMP to be detected. While embarking on this great project, Professor Aprile, like Professor Rubbia before her, inspired others to follow her lead. Her very first graduate student on the XENON project was Kaixuan Ni. Ni came from Beijing to study at Columbia University and joined Professor Aprile's group at the beginning of the XENON project. The first stage of the project, XENON10, was a liquid xenon detector operated in record time underground at the Gran Sasso National Laboratory in Italy – the *Laboratori Nazionali del Gran Sasso*, or LNGS. About 120 km from Rome, the LNGS is billed as the largest underground research facility in the world, and is an ideal place for carrying out projects such as XENON. XENON10 consisted of a 25-kilogram liquid xenon detector and searched for WIMPs by simultaneously measuring the light emitted and ionisation produced by radiation in pure liquid xenon.

Dr Ni was apparently enthused with the concept of XENON and dark matter detection, and after he graduated from Columbia, he continued to work on data analysis for XENON10 as a postdoctoral fellow at Yale University. The first results of the project, published in 2008 in the journal *Physical Review Letters*, didn't actually detect any WIMPs, but it allowed the scientists to put a limit on how big they could be and how sensitive the detector could be designed. In Dr Ni's words, the results from XENON10, reported in one of the most cited papers in the field of dark matter, 'surpassed the results from the previously leading technology using cryogenic detectors and placed the liquid xenon detector technology on everyone's radar'.

After spending two years at Yale, Dr Ni returned to Professor Aprile's group at Columbia as a research scientist, to work on the next iteration of the XENON project, called XENON100. This time, the detector contained 62 kilograms of liquid xenon as the WIMP target,



CREDIT: Roberto Corrieri, Luigi Di Carlo and Patrick DePerio

surrounded by 99 kilograms of more xenon as active shielding, all inside a low-radioactivity stainless-steel vacuum insulated vessel, itself embedded in a passive radiation shield. The experiment was set up underground at the LNGS in Italy, where XENON10 had been housed. The results of XENON100, published in 2012 in *Physical Review Letters*, improved the limits of detection by more than a factor of 20 compared to XENON10, making the experiment the most sensitive in the world for several years.

But Dr Ni didn't stop there. Six years at Shanghai Jiao Tong University in Shanghai, China, was all it took for him, together with colleagues there, to put together a Chinese version of XENON, called PandaX, which was built at the JinPing underground laboratory located in the mountains in southwest China. Published in 2016 in Physical Review Letters, the first three months of operation of the PandaX-II with a 500-kilogram liquid xenon detection chamber witnessed no dark matter interactions. However, the target was getting larger and detector was getting better. From China, Dr Ni then took a faculty position at the University of California, San Diego, where he started yet another branch of the XENON project – XENON1T.

Darkside and XENON1T

Life sometimes takes interesting turns. For Dr Luca Grandi, his first conference on Dark Matter was a turning point. When he was still an undergraduate, he met Professor Aprile at a conference. 'We ended up sitting one next to the other,' he says. 'From some candy I had she figured out I was Italian like she was, and we discovered that we had both been students of Carlo Rubbia.' He kept in touch with Professor Aprile and the connection came in handy.

Dr Grandi went on to graduate and earn his PhD under Dr Rubbia, for his research with argon detectors. After working as a postdoctoral researcher in Italy on liquid argon detectors, Dr Grandi moved to the US and did postdoctoral work at Princeton, where he was one of the founders of the Darkside project. Darkside aimed to detect WIMPs using argon-based detectors, based on Dr Rubbia's work back in Italy. In fact, the successive Darkside projects, Darkside10 and Darkside50, were built at LNGS in Italy.

Dr Grandi then landed a faculty position at the University of Chicago and the famed Enrico Fermi Institute. Within a few months he started reconsidering his plans and soon realised that the xenon technology did indeed have a higher chance of detecting dark matter, due to its mature status, so he touched base with Professor Aprile at Columbia. Together with their worldwide collaborators, including Dr Ni in San Diego, they developed the latest iteration of the XENON project – XENON1T. Funded by the US National Science Foundation, like its predecessors, XENON1T is currently the largest and most sensitive liquid xenon detector, taking dark matter search data at the LNGS in Italy, and using 3.3 tonnes of liquid xenon. As the first tonne-scale xenon detector in the world, XENON1T is pushing detection limits to their lowest levels yet.

Bigger is Hopefully Better

XENON1T is, so far, the epitome of noble liquid WIMP detector technology. Already online since November of 2016, XENON1T has been putting out data that shows it to have the best sensitivity of any dark matter detector. The chamber contains a whopping 3,300 kilograms of xenon cooled to −95°C housed in a 1 m tall and 1 m wide cylindrical container. But even with that much xenon, detections may be few and far between. It is estimated that only one WIMP interaction should occur per year for every tonne of xenon. So, the plan is to wait and watch.

The detection sensitivity has been worked down to the minimum that is possibly attainable so far. When and if a WIMP shows its hand, Professor Aprile and her XENON team will be there to record it. If not, then it will be back to the drawing board for the astrophysicists. Professor Aprile admits that 'XENON1T won't see anything if the WIMP hypothesis is incorrect'. But there is all that dark matter out there that needs to be explained. And besides, at one potential interaction per tonne per year, we have only begun to wait for results. In the meantime, we have time to enjoy the stars and admire the constellations, and let XENON1T look at the dark spaces in between.

Meet the researchers

Professor Elena Aprile
Department of Physics
Columbia University
New York, NY
USA

Professor Elena Aprile received her Laurea in Physics from the University of Naples, Italy, in 1978. She then continued her studies at the University of Geneva, Switzerland, where she received a PhD in Physics in 1982. From 1982 to 1985 Dr Aprile was a postdoctoral fellow at Harvard University. Thereafter, she joined the faculty of Columbia University, where she is now Professor of Physics. Professor Aprile's research is currently focused on understanding Dark Matter through a direct detection experiment using noble liquids, currently liquid xenon. She is internationally recognised for her work with noble liquid detectors and her contributions to particle astrophysics in the search for Dark Matter.

CONTACT

E: age@astro.columbia.edu
W: http://physics.columbia.edu/people/profile/397

Professor Kaixuan Ni
Department of Physics
University of California
San Diego
La Jolla, CA
USA

Professor Kaixuan Ni received his Bachelors in Physics from Peking University, Beijing, China, in 2000. Thereafter, he pursued doctoral studies with Professor Elena Aprile at Columbia University in New York, where he received his PhD in 2006 with the first doctoral thesis in the XENON dark matter search program, 'Development of a Liquid Xenon Time Projection Chamber for the XENON Dark Matter Search'. After postdoctoral research at Yale University, Dr Ni worked at Columbia University as an associate research scientist and Shanghai Jiao Tong University as a distinguished fellow and associate professor. In 2015, he joined the faculty at the University of California - San Diego where he is currently Associate Professor in the Department of Physics. Dr Ni's research interests include the physics of Dark Matter and neutrinos. He is heavily involved in development of particle detectors based on liquid xenon for the investigation of Dark Matter.

CONTACT

E: nikx@ucsd.edu
W: https://nigroup.ucsd.edu/

Professor Luca Grandi
Department of Physics
University of Chicago
and Enrico Fermi
Institute
Chicago, IL
USA

Professor Luca Grandi received his Laurea in Physics in 2001 and his PhD in 2005 from University of Pavia in Italy. He then did postdoctoral work at National Institute of Nuclear Physics in Pavia, the National Laboratory of Gran Sasso in Assergi, and at the University of L'Aquila. Dr Grandi then worked for three years as an Associate Research Scholar at the Princeton University before he joined the Department of Physics at the University of Chicago, where he is now Assistant Professor in the department. He is also a member of the Enrico Fermi Institute and of the Kavli Institute for Cosmological Physics at the University. Dr Grandi's research is currently focused on the development of two-phase noble liquids Time Projection Chamber technology for the direct detection of Dark Matter.

CONTACT

E: lgrandi@uchicago.edu
W: https://grandilab.uchicago.edu

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A FLICKERING IN THE DARKNESS

Deep, deep underground, surrounded by kilometres of solid rock, a team of scientists led by **Professor Gilles Gerbier** of Queen's University, Canada, watches for a miniscule flicker of energy. A flicker that will, they hope, betray the existence of the most elusive particle known to humankind – dark matter.

It is a humbling feeling to look up into the sky at night, when thousands of stars seem to coat the sky with a curtain of light. Bring out a telescope and it becomes even more impressive, with millions of stars springing into view wherever you look. Yet for all the splendour of the sky at night, it is but a tiny fraction of what is really out there. Less than 20% of the Universe's mass is found within the safe, comforting world of stars and planets. The rest is… something else. Something we have not detected yet, but that leaves traces in our familiar world. It is known as dark matter, and it is one of the last great enigmas of modern physics.

The obvious question here is – if you have not detected it, how do you know it is there? In a nutshell, we cannot see dark matter but we can see the gravitational shadow it casts on everything else. Early astrophysicists noted that galaxies were spinning faster than was theoretically possible, and the gravity of visible stars would not be enough to hold each galaxy together. Therefore, entire galaxies should be disintegrating at a tremendous speed. As exploding galaxies are fairly rare, there was clearly some other source of gravity that was holding everything together. This mysterious substance was dubbed dark matter.

There have been many hypotheses regarding the identity of dark matter and they have spawned an alphabet-spaghetti worth of acronyms. The current favourite is known as a WIMP, or Weakly Interacting Massive Particle – a new form of subatomic particle that can interact through gravity and hopefully a miniscule amount of something else. This property means that a WIMP could theoretically pass right through the planet without leaving a trace – something that, naturally enough, makes it difficult to detect.

Efforts have been made, of course, to detect it in underground labs around the world, and to tentatively 'make' it in the Large Hadron Collider. Many of these attempts have focused on 'heavy' dark matter – particles with masses close to what popular theories would predict. However, none of these have been successful, and dark matter has remained as elusive as ever. Fortunately, physicists are nothing if not optimistic, and so they soon turned their attention to alternatives, one of these being 'light' dark matter. Unfortunately, the detectors that have already been built are designed to search for WIMPs, and few have the sensitivity to detect the smaller, less-massive WIMPs that are proposed.

The Noble Charge

So how do you actually detect light dark matter, given that it is essentially invisible to our instruments? This is the challenge ahead of an international collaboration headed by Professor Gilles Gerbier, holder of the Canada Excellence Research Chair in Particle Astrophysics at Queen's University. The research team is running two projects, the first of which is known as NEWS-G (New Experiments With Spheres – Gas), one of the most promising experiments to detect low-mass WIMPs. Developed by collaboration member Dr Giomataris, the equipment in use in NEWS-G is known as a Spherical Proportional Counter, or SPC. At its most basic, the SPC is a large metallic vessel filled with a noble gas (think Helium, Neon, etc) with a sensor at the centre.

Every so often, a weakly-interacting particle (such as the proposed dark matter particle) will come screaming through the vessel and smack directly into one of the atomic nuclei of the noble gas. This impact will knock electrons out of orbit around the nucleus and allow them to move freely through the detector. As electrons are charged, they will be attracted to the high-voltage central sensor and will therefore drift in towards the middle of the vessel. As they get closer and closer, the electric field acting on them will get stronger and stronger – which in turn lets them move faster and faster. The high-speed electrons will bounce off a number of other atoms at this point, in turn booting out more electrons and creating an avalanche of charged particles. These particles find their way to the central sensor, creating a measurable electrical current.

The team's other project is known as CUTE (Cryogenic Underground Test facility), which looks for intermediate-mass WIMPs. A Canadian led project within a large North American collaboration, CUTE uses a dilution refrigerator as its main tool. The way to track dark matter here is to operate solid crystals of Germanium brought to temperature close to absolute zero (−273.15°C), thanks to the cryostat, or dilution fridge. At this freezing temperature, miniscule energy deposits expected from dark matter particles induce tiny but measurable elevations of temperature of the crystal.

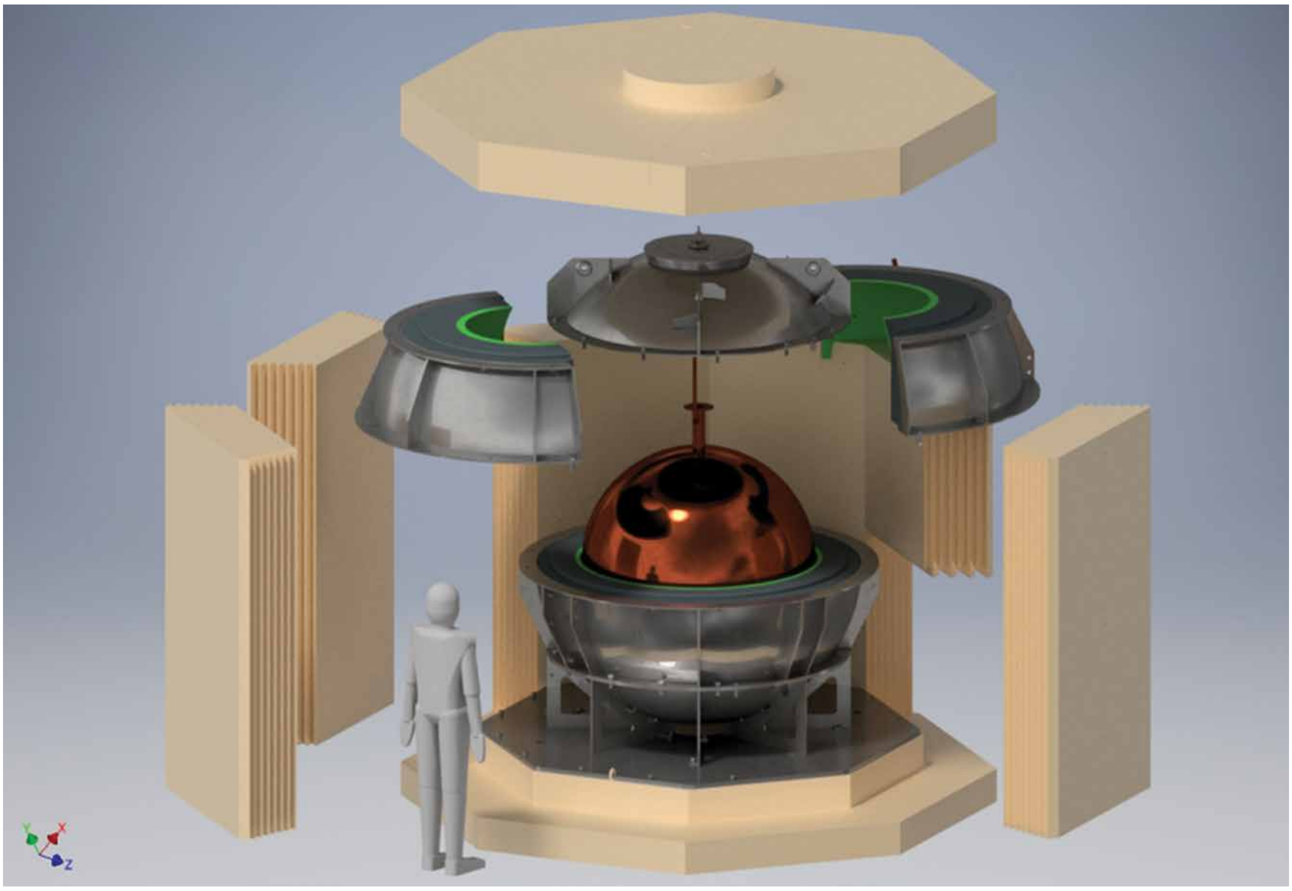
The combination of NEWS-G and CUTE detectors enlarges the range of explored masses, maximising the chances of finding the mysterious particles.

Hiding from the Background

One of the greatest challenges with this approach is that the research team's detectors are simply too sensitive. The world around us is awash with radiation coming from many different sources – a background level that is enough to flood out the rare dark-matter-related events. Thus, any successful detector needs to block out as much of the background radiation as possible in order to provide a clean signal. How is this possible? Well, it's not an easy process.

First, the researchers needed to find a location that is as free from background radiation as humanly possible. A major source of noise are so-called cosmic rays – high-energy radiation from outer space that hits our atmosphere, causing a burst of secondary radiation. As cosmic rays are, by definition, coming from above, the best way to avoid them is to go down, deep into the earth.

The SNOLAB is a perfect example of this. A specially-built laboratory for sensitive experiments such as these, the SNOLAB was built in a part of the Vale Creighton nickel mine – a sprawling network of mining tunnels located in Ontario, Canada. Burrowing deep into the earth, the tunnel system allows the SNOLAB to be positioned under two kilometres of solid rock. This impressive depth makes the SNOLAB the second-deepest laboratory of its kind in the world. The exceptional protection against cosmic radiation allows it to host a number of experiments searching for neutrinos and dark matter, both of which require extremely sensitive equipment and extremely low background radiation.



Second, the research team needed to shield their apparatus from further radiation. Rock is often slightly radioactive, and the radon gas that accumulates in closed environments such as mines is even more so. Even each one of you reading these lines is slightly radioactive: remember Carbon-14! The team's equipment thus uses multiple layers of protection. The most noticeable is the first layer, made of 'archaeological lead', which is taken from ancient sources. Freshly-smelted lead is slightly radioactive, due to the presence of a natural lead isotope, but this isotope decays with a half-life of decades. By taking old lead, say from a Roman shipwreck, you have a source of radioactivity-free metal to use as shielding.

Despite all of this effort, some background radiation does manage to make its way to the equipment. Therefore, the researchers needed to develop a technique to discriminate between a background signal and a true dark-matter signal. Thankfully, the two will tend to occur in different regions – a background signal will begin closer to the surface of the NEWG-G gas-filled vessel, while a dark-matter interaction will occur anywhere. This leads to a difference in the time it takes for an electron to reach the central sensor, which in turn allows the team to discard false signals.

Sensing the Dark

The radiation shielding and signal cascade effect means that the detector is able to detect the presence of a single electron – an incredibly miniscule amount. For comparison, a single second of current flow at 1 ampere (the typical charging current for most cell phones) involves the transfer of about 6,250,000,000,000,000,000 electrons – a, well, slightly higher number.

The choice of noble gas for the NEWS-G vessel also allows the detector to be tuned for certain particles. The lower mass of atoms such as Helium means that the tiny bit of energy imparted by dark matter has a much larger effect. Trying the same experiment with multiple gases will let the team identify which signals are background noise and which are truly coming from dark matter.

Initial studies with a prototype detector have already borne fruit for the collaboration, with the early work setting new constraints on the properties of very light WIMPs. The next generation detector, with a larger volume and better background radiation control, is set to be installed by the summer of 2019.

These projects are complex and involve the many different competencies available to the NEWS-G and CUTE collaborations. This combination of skill sets provides the team with instrumental set-ups of exceptional quality.

What will they detect? We cannot say. But we can say that the low background and unprecedented sensitivity of the NEWS-G and CUTE detectors will give Professor Gerbier and his international team an excellent basis for hunting the ever-elusive dark matter.

Meet the researchers at Queen's

Professor Gilles Gerbier

Professor Gilles Gerbier obtained his PhD at Université Paris XI (France) for his study of neutrino interactions in bubble chambers in 1983. He then completed a postdoctoral fellowship at the University of California, Berkeley, and later became team leader of the Beijing-Paris-Rome-Saclay Collaboration. He is now a world leader in the field of dark matter research and has been a professor in the Physics Department at Queen's University at Kingston since 2014. He also holds the Canada Excellence Research Chair in Astro-Particle Physics for his contributions to dark matter research.

E: gilles.gerbier@queensu.ca

Dr Philippe Gros

Dr Philippe Gros obtained his PhD at the Lund University (Sweden) in 2011 and then worked on gaseous detectors for detection of hadrons, electrons and photons in Switzerland, Denmark, Sweden, Japan and France. He joined the NEWS-G experiment in October 2017 as a research scientist where his main focus is performing characterisation measurements in the Queen's laboratory to prepare the SNOLAB scientific runs and coordinating operations at Queen's lab and SNOLAB.

Dr Quentin Arnaud

Dr Quentin Arnaud completed his PhD in France within the EDELWEISS collaboration (Direct dark matter searches using HP-Ge crystals). He joined the NEWS-G experiment at Queen's in early 2016 as a postdoctoral fellow. He has been leading the analysis of the first WIMP search data taken with a SPC prototype operated at Laboratoire Souterrain de Modane, allowing NEWS-G to obtain a world leading sensitivity at low mass. He is now focusing on lab activities and simulations to optimise the understanding and performance of SPCs.

Dr Serge Nagorny

Dr Serge Nagorny received his PhD from the Kiev Institute for Nuclear Research in 2011, and then worked on the CUPID-0 project at Gran Sasso Underground Laboratory (Italy), taking care of development, production, operations of the low-background enriched Zn82Se scintillating crystals. He joined the CUTE team at Queen's University in early 2018 as a postdoctoral fellow. His main activities include coordinating scientific operations of the CUTE facility and developing new detectors.

Marie Vidal

Marie Vidal is a PhD candidate whose project is related to the detection of the Coherent Elastic Neutrino-Nucleus Scattering (CEνNS) using a gaseous detector close to a nuclear power plant. She completed her Master's degree at the Universite Pierre et Marie Curie in France and then joined the NEWS-G team in September 2017. Her work is to estimate the feasibility of such an experiment. She is also involved in taking quenching factor measurements at TUNL.

Francisco Vazquez De Sola Fernandez

Francisco Vazquez De Sola Fernandez is a PhD student who joined the NEWS-G team in early 2015 after a Master's degree at the University of Cambridge, England. His focus has been mostly on data analysis, especially on understanding the pulse shape of events for better characterisation. He is now working on extracting a limit on solar KK axions, another form of Dark Matter, using the data from the 60 cm NEWS-G detector in the Laboratoire Souterrain de Modane.

Alexis Brossard

Alexis Brossard is a PhD candidate working on the NEWS-G experiment. He completed his Master's degree in France at the University of Strasbourg in 2014. His work has involved creating radioactive background simulations in order to understand data acquired with detectors in underground laboratories. He is also involved in building detector hardware, especially the design of the sensor to optimise detector response.

Daniel Durnford

Daniel Durnford is a Master's student who did his undergraduate degree at the University of Alberta, Canada, including work on the PICO and SNO+ experiments. His work at NEWS-G since September 2016 has centered primarily on exploring new calibration strategies for the detectors. He is also studying a new simulation method for very low numbers of electron signals and is setting up a likelihood analysis framework for the upcoming project at SNOLAB.

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Queen's UNIVERSITY

PROBING MATTER AND MORE: BEYOND THE STANDARD MODEL

Professor Liping Gan and her team at the Thomas Jefferson National Accelerator Facility are working to deepen our understanding of the matter that makes up our Universe. While key theories such as the Standard Model and Quantum Chromodynamics can provide accurate predictions about the smallest building blocks of matter, there are also notable limitations in the observed phenomena they can explain. Professor Gan continues to push these theoretical boundaries, giving way to a new era of contemporary physics, unrestricted by the Standard Model.

The Standard Model and Quantum Chromodynamics

Understanding what makes up the matter around us has been a unified goal of scientists around the world for decades. Since the 1970s, particle physics has used the Standard Model to describe fundamental particles and their interactions – a theory that encompasses the existence of the smallest building blocks of matter such as quarks and gluons. In fact, quarks are the most elementary matter particles to exist, and when they are bound together with force-transmitter particles called gluons, they form heavier particles such as neutrons, protons and the lesser-known 'pions'. In turn, these heavy particles make up all the matter we can see.

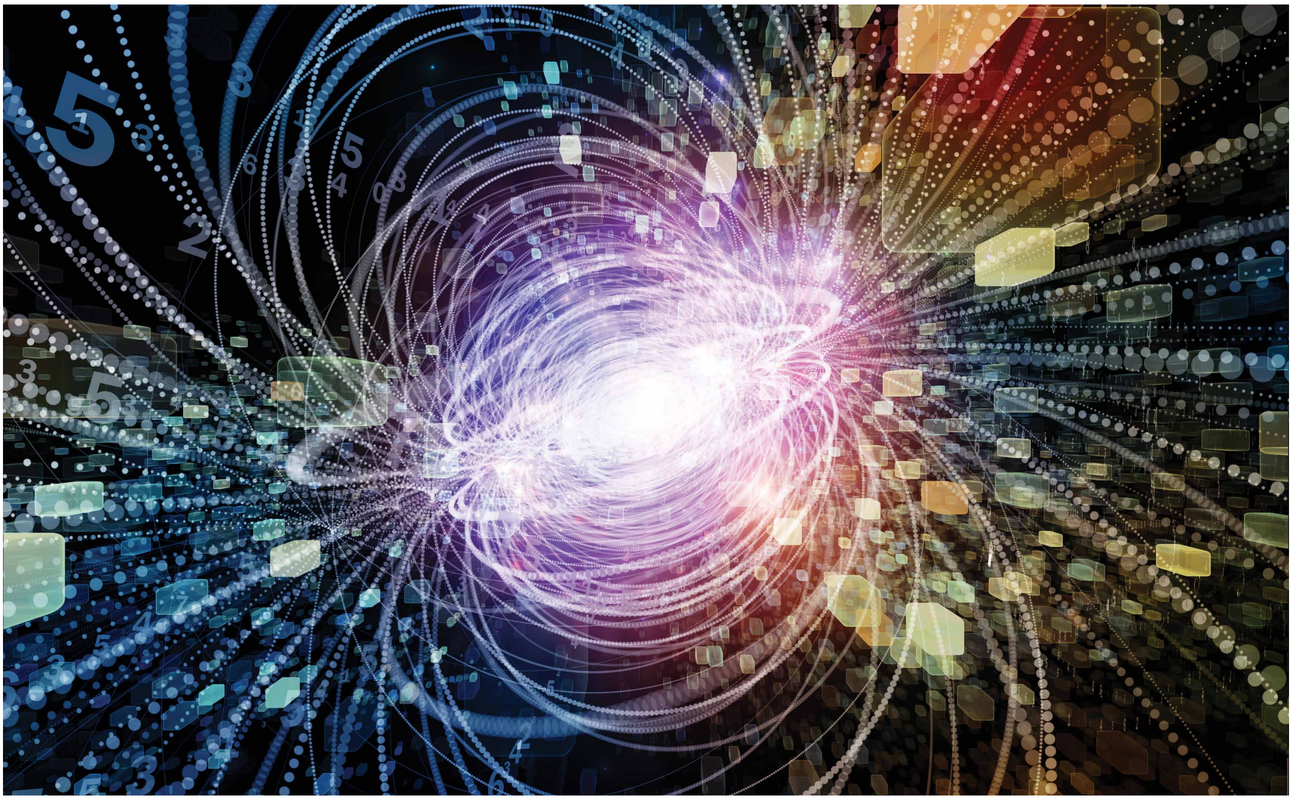
The Standard Model names 25 fundamental particles in total, from 12 force carrier bosons (including eight gluons) and all six types of quarks and leptons, to the Higgs boson which was discovered in 2012.

The theory of Quantum Chromodynamics (QCD) is an important aspect of the Standard Model, as it describes the strong force, which is transmitted by gluons to tightly bind quarks together. Much evidence has been gathered to support the Standard Model, including the discoveries of particles predicted by the Standard Model, such as the Higgs boson. Nonetheless, physicists have not turned a blind eye to some of the differences between the theoretical predictions of QCD and real observations.

One significant mystery of this theory is the confinement of quarks and gluons within subatomic particles. Although QCD theory suggests that more than 99% of visible matter is composed of these two important fundamental particles, quarks and gluons cannot exist on their own, outside the confines of subatomic particles such as protons and neutrons. Scientists agree that for QCD to be fully accepted, it must somehow also explain this observation of quark and gluon confinement. This problem is one of the most complicated challenges facing physicists today.

The search for new theories beyond the Standard Model motivates continued research in the fields of nuclear and particle physics. By uncovering more

about the smallest building blocks of matter, scientists hope to explain the more abstract and complex phenomena that dominate contemporary physics – such as dark matter and dark energy – in addition to increasing our understanding of QCD confinement. At the Thomas Jefferson National Accelerator Facility in Virginia, scientists are taking part in this endeavour.



The Jefferson Lab Experiments

Scientists at the Jefferson Lab use the Continuous Electron Beam Accelerator Facility (CEBAF) to probe atomic nuclei with continuous beams of high-energy electrons. Professor Liping Gan's group of the University of North Carolina, Wilmington, has continually been making significant strides at this facility, including measuring the lifetime of the neutral pion – an unstable particle made up of a quark and an antiquark.

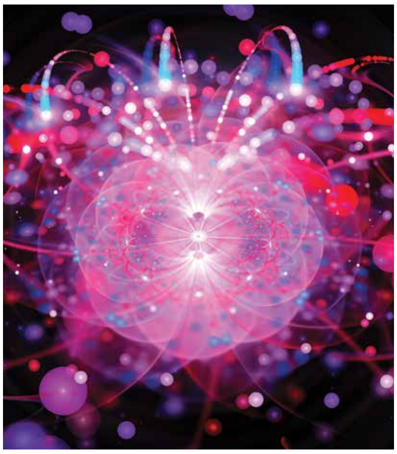
Pions are the lightest particles of all the 'mesons' – unstable particles that all contain a quark and an antiquark. To elaborate briefly on what exactly a neutral pion is, it must first be noted that an antiquark is the anti-matter version of a quark, meaning that it possesses the same mass as a quark, but has opposite charge. In fact, because the neutral pion is composed of a quark and its anti-particle, it has the potential to annihilate, which is why the lifetime of this pion is so brief before it decays into light energy (or photons). Because they are so unstable, pions are not abundant in nature, and mostly exist as short-lived by-products of high energy collisions in particle accelerators. Scientists at the Jefferson Lab have exploited a particular physical phenomenon that creates pions in this way, allowing them to experimentally probe these peculiar particles. Remarkably, the lifetime of the neutral pion is one of only a few quantities can be calculated accurately by QCD at the confinement scale, and as such, its precise measurement provides a robust way to test the theory.

Professor Gan is currently working on another experiment to measure the lifetime of another meson, called eta, which is also made up of pairs of quarks. She also aims to extend these measurements to a similar particle called eta-prime, using the same experimental techniques as those used to investigate the pion. Her team's precision measurements of the properties of the neutral pion, eta and eta-prime will offer a stringent test of some other aspects of QCD theory – more explicitly, to test the symmetry structure of QCD at low energy. These symmetries are key properties of QCD equations. As Professor Gan explains, her team's 'proposed measurements will have broad impact on QCD confinement that is widely considered as the last frontier within the Standard Model.'

This research could potentially shed some much-needed light on not only the nuts and bolts of matter, but also on far more elusive aspects of the Universe that cannot be explained by our current theories.

Other experiments at the Jefferson Lab that are drawing considerable interest is the search for a dark gauge boson. Observational evidence has shown that dark matter, an unknown invisible form of matter, makes up about 85% of all matter in the Universe. As direct detection methods to find out more about dark matter have been unsuccessful to date, physicists have started to broaden their searches to try and detect force-carrier particles that transmit forces between dark matter particles, and between dark matter and visible matter particles.

Scientists hypothesise that dark matter possesses a rich symmetry structure between its constituent forces and particles. To elaborate, specific types



of symmetries (referred to as 'gauge' and 'Lorentz' symmetries) of the Standard Model impose certain restrictions on the ways that a force-carrier particle of dark matter can behave. This is where the search for a dark gauge boson, a force-carrier particle, could provide a key extension of the Standard Model – potentially providing a way to expand this basic theory to include an explanation of the ever-elusive dark matter.

The Lifetime of the Neutral Pion

Professor Liping Gan and her colleagues obtained ultra-precise measurements that tested vital aspects of QCD theory, by conducting the so-called 'Primakoff Experiment', an experimental program at the Jefferson Lab. From their first experiment in 2004, the researchers determined the lifetime of the neutral pion with more than double the precision ever recorded before. The team then carried out a second experiment in 2010 to challenge their own previous results, and further improved their precision by a factor of two. The final results from the team's second experiment is expected to be published in 2018.

It may not immediately be apparent why the precise measurement of this quantity is so important to furthering the aims of particle and nuclear physicists alike. However, it must be understood first that QCD, despite being a successful theory that entails a complete description of the strong force, is almost impossibly complex to solve exactly at a low energy scale. While it is supported by plentiful evidence, some aspects of QCD are not completely understood. For instance, the problem of quark confinement still requires quantitative analysis to be fully explained, as does a second major problem with QCD theory – known as chiral symmetry breaking.

The equations of QCD encompass certain crucial symmetries, referred to as 'chiral symmetry'. Chiral symmetry is present when two separate forms of an object are mirror images of each other, such as a left hand and a right hand. The theory suggests that chiral symmetry spontaneously 'breaks' because of the so-called 'QCD vacuum'. This symmetry breaking effect gives birth to particles known as 'Goldstone bosons'. The neutral pion is one of such Goldstone boson particles – whereby the predicted symmetry somehow ends as soon as the particles are measured experimentally. Therefore, a precise value of the lifetime of the pion could significantly help scientists to learn more about the puzzling mechanisms responsible for this symmetry breaking.

At the Jefferson Lab, Professor Gan and her team worked on the Primakoff Experiment to find the value of this important quantity by aiming a beam of gamma-rays at atomic nuclei. This set up was implemented to induce the 'Primakoff effect', a phenomenon in which the incident particles exchange a single photon with the target nuclei to produce neutral pions. As explained earlier, the neutral pion rapidly decays into two daughter photons. By taking detailed measurements of the decay processes, Professor Gan and her team acquired key lifetime measurements for these particles.

Effectively, with their measurements of the so-called Primakoff effect on various mesons (such as neutral pions), the scientists are working to vigorously test the predictions of QCD confinement theories as discussed above, with the hope of finally unveiling the true origins of QCD confinement.

Search for New Physics Beyond the Standard Model

In recent years, Professor Gan is leading a group of physicists who successfully developed the JLab Eta Factory (JEF) experiment. This is a new experiment aimed to search for dark gauge bosons and a new type of symmetry-breaking force, by measuring some very rare decays of eta. With JLab's 12 GeV energy beam, available GlueX experimental apparatus, and a future upgraded calorimeter, this experiment will offer the best data in the world of neutral rare meson decays. The team hopes to reveal new physics that could exist beyond the scope of the Standard Model.

As mentioned earlier, despite its many successes, the Standard Model still cannot explain issues such as the existence of dark matter and dark energy. It also does not explain why there is far more matter than antimatter in the Universe – another key unanswered question in this field.

These limitations have given rise to the search for new theories beyond the boundaries of what the Standard Model can offer. Professor Gan explains how the 'results from this experiment will have the potential to shed light on the … mystery of dark matter, and the asymmetry of matter-antimatter in the Universe.' Her continued research in these fields could drive contemporary physics rapidly forwards to provide explanations of the abstract phenomena that current theories cannot yet describe.

In addition to her ground-breaking work in nuclear and particle physics, Professor Gan is also actively engaged in STEM outreach work. Not only does her research aim to advance our understanding of the Universe, but she also emphasises the importance of undergraduate research. Professor Gan also enthusiastically encourages the role of women in the field, and generally aims to promote the integration of research and education.

Meet the researcher

Professor Liping Gan
Department of Physics and Physical Oceanography
University of North Carolina Wilmington
Wilmington, NC, 28403
USA

Professor Liping Gan obtained her BSc in physics at Peking University in China in 1985, and her MSc at the same institution in 1988. She then achieved her PhD in physics at the University of Manitoba, in Canada, after which she completed two post-doctoral research fellowships. She moved to the University of North Carolina, Wilmington (UNCW) in 2001, where she initially worked as an Assistant Professor, then an Associate Professor, and was ultimately promoted to her current position as a full Professor of Physics. Professor Gan joined the Executive Committee for the Southeastern Section of the American Physical Society as a Vice Chair in 2016, then Chair-Elect in 2017, and became Chair in 2018.She also served as a nuclear physics panel member for the American National Science Foundation (NSF). Her current research interests focus on QCD confinement and new physics beyond the Standard Model, which she explores by testing fundamental symmetries in precision measurements of light meson decays at Jefferson Lab (JLab). She is a spokesperson or a co-spokesperson for three high rated Jlab experiments (the PrimEx, PrimEx-eta and JEF experiments). In addition to her research, Professor Gan is a motivated STEM promoter, and has been a long-running member of various UNCW undergraduate research organisations and 'Women in Science and Engineering' boards.

CONTACT

E: ganl@uncw.edu
T: (+1) 910 962 3583
W: people.uncw.edu/ganl/

KEY COLLABORATORS

The PrimEx collaboration and GlueX collaboration at Jefferson Lab

FUNDING

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Jefferson Lab
Thomas Jefferson National Accelerator Facility

SUPERNOVA-ACCELERATED ELECTRONS TO DARK MATTER: A CAREER IN RADIO ASTRONOMY

Considering we didn't know of their existence just a century ago, our current knowledge of the structures and dynamics of galaxies is extraordinarily impressive. Among those who have enhanced our understanding of these building blocks of the Universe is **Dr Uli Klein,** a former researcher at the University of Bonn who spent 45 years as a radio astronomer. Now retired, Dr Klein is dedicated to sharing his extensive knowledge with students of astronomy and astrophysics, and with the wider public.

When Dr Uli Klein was completing his PhD at the University of Bonn in 1979, making observations using radio telescopes was a particularly challenging task, because turbulence in the Earth's atmosphere distorted any detected signals. At the time, radio astronomers tackled this issue using the 'dual-beam' technique, which involved pointing two receiving antennae at two slightly-separated points on a radio-emitting source, such as a single galaxy. By measuring the differences in the signals picked up by the two receivers, atmospheric turbulence could be cancelled out.

However, this method only worked when observing single objects. For larger patches of sky, the large variations in atmospheric turbulence meant that the received signals could not be cancelled reliably, making observations far more difficult.

A New Era for Radio Telescopes

Through the work of Dr Klein and his colleagues, the dual-beam technique was adapted to pick up clear radio signals across large objects in the sky. This improvement would allow Dr Klein to go on to dedicate his career to radio astronomy through observations of clusters of many galaxies. As Dr Klein explains, there was much to explore in the coming decades. 'The *radio window* allows the astronomer to explore a huge number of phenomena in the interstellar and intergalactic media,' he says.

Of particular interest to Dr Klein were the radio frequencies emitted by galaxies. 'My personal interest has always been focussing on the structure and evolution of galaxies, which I mainly explored using big radio telescopes,' he continues. At the time, few radio telescopes were bigger or more sophisticated than the Effelsberg telescope at the Max Planck Institute in Germany. With a diameter of 100 metres, it remains one of the largest steerable telescopes in the world since its construction in 1972.

Using his newly developed multiple-beam technique, the Effelsberg telescope was the ideal resource for Dr Klein to observe the radio wave emissions of many galaxies, situated over wide expanses in the night sky.

Exploring Synchrotron Radio Emissions

At the time, astronomers were well aware that galaxies emitted radio waves through a variety of mechanisms. One such mechanism, known as 'thermal emission', involves interstellar ionised gas clouds giving off low-energy radio waves with characteristic frequencies due to their temperature.

Thermal emission would become an important line of study to Dr Klein later in his career, but his earlier research focused on another, less-explored radio source – 'synchrotron radiation'. The mechanism of producing synchrotron radiation involves electrons being accelerated in curved paths by magnetic fields. As the direction of an electron changes, it will lose a small amount of energy through emitting radio waves. Measuring

‘The *radio window* allows the astronomer to explore a huge number of phenomena in the interstellar and intergalactic media’

synchrotron radiation would, therefore, allow astronomers to map magnetic fields on a galactic scale, giving them important insights into the behaviour and evolution of galaxies.

‘I investigated the distribution and strength of magnetic fields, both inside galaxies as well as in between them,’ Dr Klein explains. ‘To this end, we measured the intensity and polarisation properties of synchrotron radiation emitted in the interstellar and intergalactic medium, which is produced by relativistic electrons travelling close to the speed of light.’

As well as mapping these magnetic fields, Dr Klein’s work with the Effelsberg telescope also provided insights into how radio emissions were shared between synchrotron and thermal emissions. His team found that synchrotron radiation dominated, with the average galaxy rarely producing more than 20% of its observed radio waves through thermal emission. In later research, Dr Klein would further explore the origins of the relativistic electrons (those travelling near the speed of light), which give rise to synchrotron radiation.

Accelerated by Supernovae

One strange consequence of Dr Klein’s early research was that the intensity of synchrotron radiation produced by different galaxies was remarkably similar. His team concluded through these studies that supernova explosions – the final death throes of massive stars – could be responsible for accelerating electrons to similar, relativistic speeds.

However, it wasn’t until studies conducted shortly before his retirement that Dr Klein managed to produce a realistic explanation for the acceleration process and the similarities in radiation intensity. In these studies, his team observed the remnants of supernovae in violently star-forming galaxies – correlating what they found with the synchrotron radiation produced by the galaxies.

The work allowed Dr Klein and his colleagues to confirm their prediction that relativistic electrons were accelerated during supernova explosions and also revealed details about the process involved. ‘Electrons attain their energy in multiple supernova shocks,’ Dr Klein describes. ‘Supernova explosions generate expanding shells of ejected material; multiple events of this kind kick the charged particles back and forth in the interstellar medium, thereby pushing them to ever higher energies.’

This relatively simple idea of electrons being pushed to relativistic speeds was a major advance in our understanding of the origins of radio emissions in galaxies. However, other aspects of radio astronomy investigated by Dr Klein remain far more mysterious.

Mapping Dark Matter

In a sense, clouds of molecular gas and dust act as galactic skeletons, gathering in dense bands along the spiral arms of galaxies. These structures, which occupy the vast spaces between stars known as the ‘interstellar medium’, are incredibly useful to radio astronomers. The clouds contain an abundance of atomic hydrogen, which, due to quantum effects of the orbiting electron, emit a reliable source of radio waves known as the ‘hydrogen line’.

The wavelength (the distance over which a wave’s shape repeats) of

hydrogen line radio waves is approximately 21 centimetres. By measuring the shifts in this wavelength, which arise from the Doppler Effect, astronomers can measure how fast the clouds of gas are moving as they rotate around the centre of the galaxy – giving a relationship between rotation speed and distance from the centre of the galaxy known as the 'galactic rotation curve'.

Using classical calculations developed from the gravitational equations proposed by Newton, it would be reasonable to expect that the interstellar material will rotate at its fastest around the centre of the galaxy – a massive region composed with dense clusters of stars and possibly black holes.

Further away from the centre, the speed should drop off at a predictable rate, reaching its slowest speed at the edge of the galaxy. However, Dr Klein's measurements of the galactic rotation curves of many galaxies revealed that this wasn't the case at all. Rather than dropping off, the speed of interstellar gas actually remains almost perfectly constant, no matter how far it is from the galactic centre.

Clearly, a more mysterious force must be at play – originating from the gravitational influence of Dark Matter. 'From such observations, one can deduce the rotation curves of galaxies, which in turn disclose the distribution and amount of Dark Matter,' says Dr Klein. 'Dark Matter must consist of still unidentified particles, which have solely gravitational interaction.'

The composition of Dark Matter may remain a bewildering mystery, but Dr Klein and his team could still compare the galactic rotation curves they observed with Newtonian rotation models to construct models of how it must be positioned in and around galaxies. They concluded that Dark Matter must form 'haloes' around galaxies – essentially vast hemispheres that appear on either side of galactic discs – with central-density cores.

Again, Dr Klein's work has proven that radio astronomy can be used to unlock the mysteries of galactic dynamics. One day, his team's research could provide an important basis for determining what Dark Matter is really composed of.

Commitment to Communication

Having provided the world of astronomy with new revelations about the structures of galaxies for almost half a century, Dr Klein has now reached the end of an extraordinarily successful academic career. Now, he has turned his attention to inspiring a new generation of astronomers by sharing his extensive knowledge with wider audiences.

'Since my retirement, I have essentially ceased my professional research and turned to public-relation work,' he says. 'I'm giving public talks on all kinds of astronomical themes to laymen, in particular to school pupils. I'm chairing an astronomy club which utilises part of the former astronomical observatory of the University of Bonn. Here, we convey astronomical knowledge to public audiences or school classes, and give people the opportunity to perform observations with our team of experts.'

This dedication to science communication will surely set an example to other scientists, ensuring that future generations will continue to view a career in research as an exciting, realistic possibility.

Meet the researcher

Professor Dr Uli Klein
Argelander Institute for Astronomy
University of Bonn
Bonn
Germany

Before his retirement, Dr Uli Klein was a professor of astronomy at the University of Bonn since 1991. In 1981, he received his PhD from the University of Bonn with a thesis project conducted at the Max Planck Institute for Radio Astronomy in Bonn. He then worked as a postdoctoral research assistant there between 1981 and 1984, before becoming a research assistant at the Radio Astronomic Institute of the University of Bonn (now Argelander-Institute for Astronomy). Between 1989 and 1990, he returned to the Max-Planck-Institute for Radio Astronomy as a staff member. At the end of his academic career, he was a Spokesman of a Research Unit of the German Research Foundation, before retiring in 2017. Dr Klein's research interests are focussed on the evolution of galaxies and clusters of galaxies, and on image processing.

CONTACT

E: uklein@astro.uni-bonn.de
W: https://astro.uni-bonn.de/~uklein

FUNDING

Deutsche Forschungsgemeinschaft

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INVESTIGATING OUR GALAXY'S LARGEST STAR PRODUCTION FACTORIES TO REVEAL STELLAR AND PLANETARY ORIGINS

Star forming regions are dense complexes of young and newly forming stellar clusters, which drive the evolution of galaxies. **Dr Jeremy Drake**, a Senior Astrophysicist at the Smithsonian Astrophysical Observatory, and his collaborators analyse X-ray, optical and infrared radiation emitted from these star production factories to assay their contents and probe the physics of star and planet formation.

Star forming regions (SFRs) are highly active regions of galaxies, and are made up of between a hundred and millions of young stars. In more massive regions, supernova explosions occur – the violent death throes of massive stars – causing matter to be energetically expelled across the region and into the larger host galaxy. Stellar winds generated by newly formed massive stars also inject matter and energy into SFRs and beyond. These regions of the cosmos are therefore crucial places to understand, driving galaxy evolution and giving birth to all the stars and planets in the Universe.

Typical methods for studying very young stars involve the detection of infra-red (IR) and visible light, using Earth-based telescopes. However, these types of radiation cannot penetrate through the dense interstellar gas and dust clouds often found in and around SFRs, or separate out the young stars from the myriad foreground and background objects. To enable the visualisation of star clusters that are hidden within these clouds, scientists have hit on their X-ray properties as powerful tracers. Very young stars have much more energetic magnetic dynamos than older stars like the Sun, and this magnetism generates extreme heat at the stellar surface that radiates as X-rays.

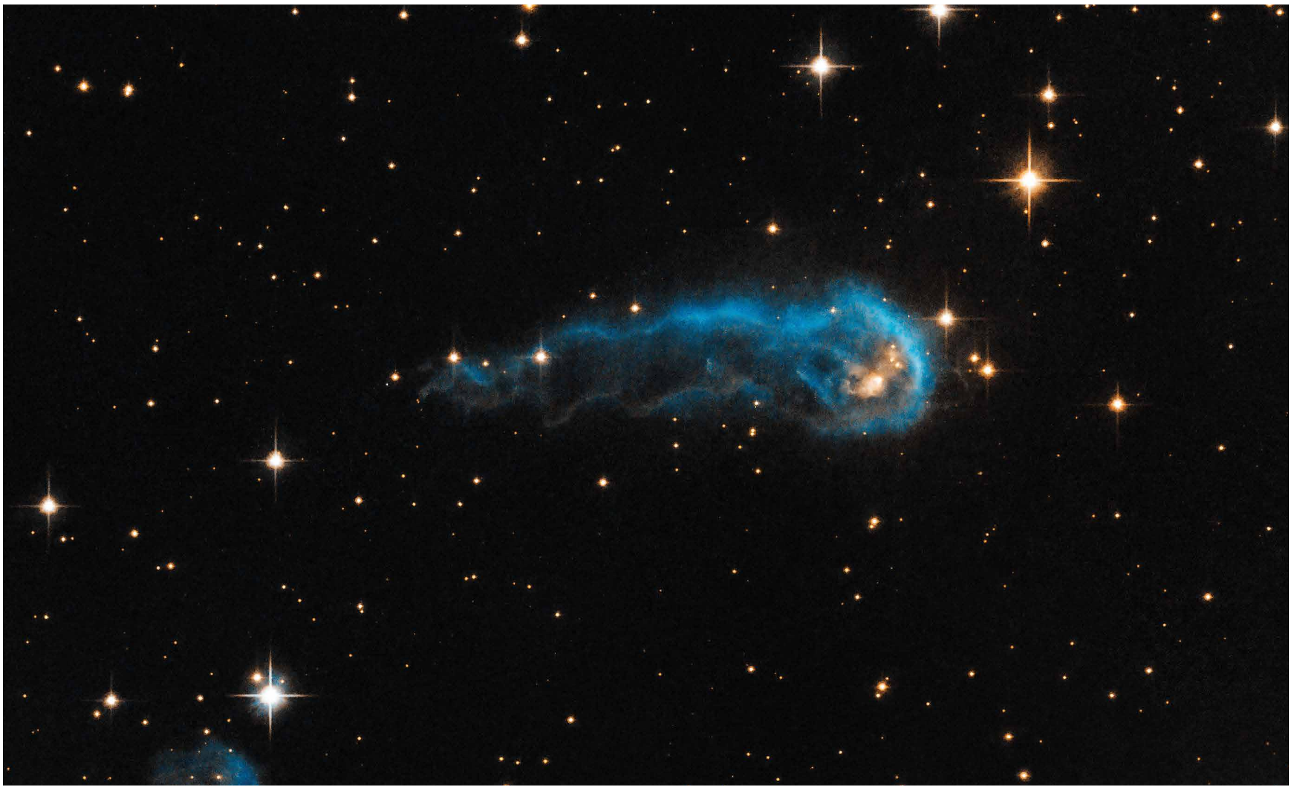
X-ray emissions cannot be detected using terrestrial telescopes, as they are filtered out by the Earth's atmosphere. To circumvent this problem, scientists use NASA's Chandra X-ray Observatory – a telescope that orbits almost 140,000 kilometres above the Earth's atmosphere. Chandra has been specifically designed to distinguish and detect the X-ray emission from energetic cosmic sources, including young stars, supermassive black holes, and the diffuse X-rays from high-energy astronomical events, such as supernova.

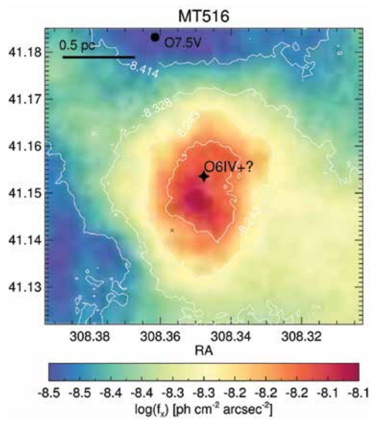
One large SFR of particular interest is the Cygnus X complex, a region made up of hundreds of thousands of young stars lying 4,600 light years from Earth. The central region within the Cygnus-X complex is called Cygnus OB2 – a so-called 'OB association', as it contains many O- and B-type stars. O-type stars are between 15 and 100 times the mass of our Sun, and have surface temperatures of between 30,000 and 55,000°C (the Sun, by comparison, has a surface temperature of around 5,500°C). B-type stars are smaller, at 2–16 times the mass of our Sun, with surface

temperatures ranging between 10,000 and 30,000°C.

The high-energy radiation emitted from these O- and B-type stars is believed to trigger the formation of new stars, by ionising nearby dust clouds, compressing them and causing them to collapse. Another way that these massive stars might trigger star formation is when they die, in supernova explosions, and the resulting shockwaves may cause clouds to compress and collapse.

As one of the largest SFRs visible from the northern hemisphere, and the closest truly massive SFR, Cygnus OB2 offers a plethora of information on the processes behind star and planet formation. However, the region is concealed behind a large blanket of dust, referred to as the Cygnus Rift. This restricts our ability to visualise and analyse the hidden star cluster using classical IR and visible light observations.





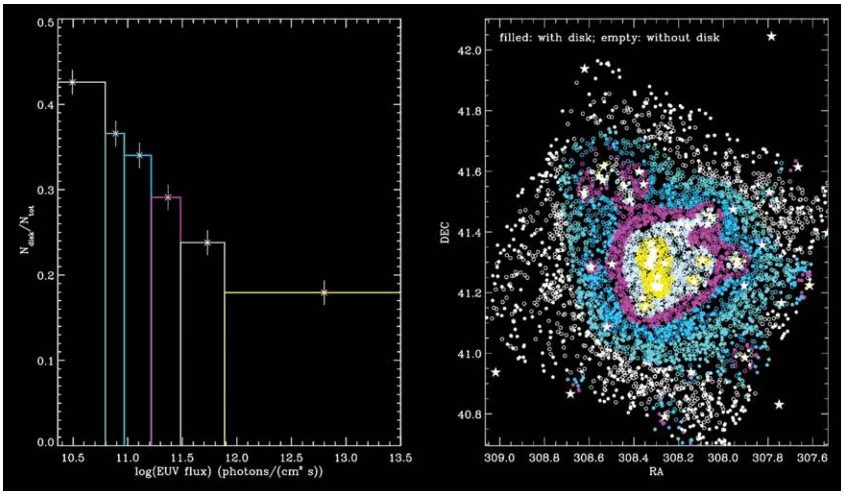
Dr Drake and his international team of astronomers use X-rays to unveil the hidden young stars of Cygnus OB2, allowing them to be studied in more detail. When asked what initially drew him to this field of research, Dr Drake describes that he became fascinated by how 'a comparatively minor aspect of the workings of a star – its magnetic dynamo and related X-ray emission – draws together such diverse aspects of astrophysics and ultimately has a strong bearing on something as profoundly important as planet formation and evolution, and the origin and evolution of life'.

Surveying Cygnus OB2 with the Chandra X-ray Observatory

The Chandra Cygnus OB2 Survey is an imaging spectroscopy project undertaken using the Advanced CCD Imaging Spectrometer – an instrument capable of measuring both the energy and position of incoming X-rays, housed on board the Chandra X-ray Observatory. Alongside his colleagues, Dr Drake analyses data from this survey, in the hope of answering key questions about the formation, growth and clustering mechanisms of stars in SFRs.

The Cygnus X region is known to have formed following the gravitational collapse of a giant molecular cloud. Models simulating this suggest that following the collapse, an initial burst of star formation occurs. The subsequent perturbation of gas clouds can then cause further waves of star formation. Scientists had previously estimated that the central region of Cygnus OB2 was two million years old, but Dr Nick Wright from Keele University, a member of Dr Drake's team, uncovered evidence that supports the presence of regions at least five million years old that are likely to have led the initial star formation. The Chandra survey allows researchers to create false-colour stellar density diagrams, where the age variation across different regions can be visualised as a colour gradient. Dr Drake and his team use these results to reconstruct how the star formation in Cygnus OB2 might have proceeded.

Another aim of the Chandra survey is to uncover the statistical distribution of stars with different masses, to probe the origins of massive star formation. Currently, there are two proposed mechanisms by which a massive star can form – either following a large gravitational collapse event as described above, or during ultra-dense clustering of newly forming stars during which objects can gravitationally merge to gain more and more mass. The team is also using data from Chandra to map the mass surface density of stars within Cygnus OB2 to understand if this SFR is undergoing an evolutionary clustering process, or if the region is continuously expanding. They found that, unlike other massive SFRs studied to date, Cygnus OB2 was never a gravitationally-bound region and has always been a loose association.



Probing Protoplanetary Disks and Circumstellar Envelopes

Most stars in the Universe are formed in stellar clusters within larger structures such as an OB association – our own solar system was probably formed in such a region. The energy of the radiation emitted from the massive O- and B-type stars in such an association can have a profound effect not only on the star formation process itself, but also on the evolution of protoplanetary disks – rings comprising solid and gaseous matter that surround a newly-formed star. One major puzzle is whether this exposure can cause significant gaseous photoevaporation – a process where the high-energy radiation dissipates the gas in the disk, potentially preventing planets from forming.

Using Chandra, team member Dr Mario Guarcello from the Palermo Astronomical Observatory identified the proportion of young Sun-like stars that still possess a protoplanetary disk in Cygnus OB2. The team found that protoplanetary disks were more depleted in regions of intense UV emission. In particular, they measured a greater level of depletion near O stars in regions of intense high-energy UV radiation. Owing to its massive stellar content, the intense UV radiation fields make Cygnus OB2 a hostile environment for protoplanetary disks.

A young star, its protoplanetary disk and any remaining circumstellar envelope of gas remaining from its formation each possess a unique spectroscopic signature (a specific pattern of radiation of different energies). By measuring the signatures of the radiation emitted from different stellar sources, Dr Drake's team categorised each one to describe the evolutionary progress of their protoplanetary disk and envelope. The majority of stars have no disks or envelopes left at all. Of those with some remaining circumstellar material, they found that most possess partially or completely depleted envelopes but have complete inner disks. The team also discovered that a small proportion of stars possess disks that are still growing.

After identifying the evolutionary progress of protoplanetary disks along with their location in the region, the team were then able to trace some of the region's history. The stars clustered to the centre tended to be bereft of disks and circumstellar gas, but are surrounded by an annular over-density of protoplanetary disks. They found smaller localised regions containing recently formed stars in the outer vicinity of Cygnus OB2. The team could conclude from these findings that OB associations do indeed trigger star formation.

A Region Bathed in X-Rays

Identifying the sources and processes that lead to the emission of X-ray radiation is complex, with multiple competing processes all contributing to the X-rays picked up by the detector. Diffuse X-ray radiation is theoretically expected in SFRs because massive stars drive streams of charged particles that get heated to millions of degrees in turbulent collisions. Using the mosaic of Chandra X-ray observations, team member Dr Facundo Albacete-Colombo from the Universidad Nacional de Río Negro in Argentina constructed a map of the diffuse X-ray signal. The map revealed the large-scale diffuse emission from powerful stellar winds as predicted, and the interactions of these winds with the interstellar medium. As a bonus, the team discovered that evolved massive stars can produce bright halo-like X-ray diffuse emission structures that had never been seen before.

Future Work

The European Space Agency's Gaia satellite is currently mapping the galaxy and will provide additional information on the 3D positions and movements of stars within the Cygnus OB2 region of the Cygnus X complex. Once stellar motion has been resolved, the mechanisms underlying the formation of the stellar association and its various sub-clusters should become more apparent. 'This will give us important clues for how the region and its stars formed, and allow us to predict its future,' says Dr Wright, thus enabling the team to make accurate predictions on the future evolution of the region. 'Observations from the ground by the Atacama Large Millimeter Array should also give us new key insights into the evolution of the protoplanetary disks in the Association, and a greater understanding of planet formation in the more violent parts of the Universe,' adds Dr Drake.

Dr Drake's team has revealed some of the best-kept secrets of the Universe's most violent regions. Detecting and analysing X-ray radiation has allowed the team to visualise hidden young stars within our galaxy, bringing to light some of the more elusive aspects of star and planet formation.

Meet the researchers

Dr Jeremy Drake

Dr Jeremy Drake graduated with a D.Phil degree from Oxford University, and was subsequently awarded a NATO Postdoctoral Fellowship to work at the University of Texas, USA. A further postdoctoral term and then staff scientist position at the University of California, Berkeley, was followed by a move to the Smithsonian Astrophysical Observatory to work on NASA's Chandra X-ray Observatory. Dr Drake's research interests include the high-energy aspects of star and planet formation, stellar evolution, and planetary radiation environments.

E: jdrake@cfa.harvard.edu

Dr Nick Wright

Dr Nick Wright obtained a PhD from University College London before taking up a research position at the Harvard-Smithsonian Centre for Astrophysics in Cambridge, Massachusetts, and then a Royal Astronomical Society fellowship at the University of Hertfordshire, UK. He is currently an Ernest Rutherford Fellow at Keele University, UK, where he studies the structure and dynamics of star forming regions and young star clusters.

Dr Juan Facundo Albacete Colombo

Dr Juan Facundo Albacete Colombo obtained a PhD from the University of La Plata (Argentina) and subsequently was a Marie Curie post-Doctoral Fellow at the Osservatorio Astronomico di Palermo (Italy). Since 2007, he has been a staff member of the National Council of Research (CONICET) at the University of Rio Negro in Argentina. His studies mainly focus on the X-ray properties of young low mass and high-mass stars in Galactic star forming regions and their impacts on the local interstellar medium. If he ever hangs up the astrophysics gloves, he will be a sailor.

Dr Vinay Kashyap

Dr Vinay Kashyap obtained a PhD in Astronomy & Astrophysics at the University of Chicago. He subsequently carried out postdoctoral research there and later at the Smithsonian Astrophysical Observatory in Cambridge, Massachusetts. He is currently an Astrophysicist at the SAO, where he studies solar and stellar coronal plasma and astro-statistical techniques. He is also a Calibration Scientist at the Chandra X-ray Center, working on the X-ray imaging capabilities of the Chandra X-ray Observatory.

Dr Mario Guarcello

Dr Mario Giuseppe Guarcello obtained his PhD in physics at the University of Palermo, Italy, with a thesis on the star formation in the Eagle Nebula. In 2010 he moved to Cambridge, Massachusetts, USA, as a Postdoctoral Research Fellow at the Harvard-Smithsonian Center for Astrophysics for a collaboration on the Chandra Cygnus OB2 Legacy Project. He is currently a postdoctoral researcher at the INAF - Osservatorio Astronomico di Palermo. His research is mainly focused on star formation and star forming regions, the evolution of protoplanetary disks, and the properties and variability in pre-Main Sequence stars.

Dr Ettore Flaccomio

Dr Ettore Flaccomio obtained a PhD in physics at the University of Palermo in Italy, with a thesis on the X-ray activity of young Pre-Main Sequence stars. During the course of his research he has spent extended periods as a visiting scientist at the Smithsonian Astrophysical Observatory in Cambridge, Massachusetts. He currently holds an Astronomer position at the Italian 'Instituto Nazionale di Astrofisica' (INAF), working at the Observatory of Palermo. His main scientific interests are the formation and early evolution of young stars with particular reference to the relation between magnetic activity, mass accretion, and circumstellar disks.

INVESTIGATING COSMIC SNOWBALLS

Professor David Jewitt and his team at UCLA explore the nature of comets. These fleeting visitors to our cosmic shore are important sources of information, and can help to reveal the origin and evolution of the solar system. Most recently, Professor Jewitt's team have explained the unusual activity of some of the most distant comets in the solar system.

Comets play a vivid historical role in the human psyche, often being interpreted as portents of impending doom. In the era of modern science, we realise that comets are simply icy leftovers, frozen in time since the solar system's formation about 4.6 billion years ago.

Far from bringing us doom and disaster, comets offer scientists unparalleled opportunities to learn about the earliest periods of the solar system's evolution. At the same time, they are some of the most challenging objects to study and remain some of the least well understood.

What Are Comets and Where Do They Originate?

Comets are composed of a central core or 'nucleus' of rock, dust, water ice and various frozen gases such as carbon monoxide, carbon dioxide and assorted hydrocarbons, which coalesced together at ultra-low temperatures in the outer parts of the protoplanetary disk. The distinctive tails that we are all familiar with are an optical distraction, produced when ice in the nucleus is heated by the Sun, releasing gas (outgassing) and ejecting dust into a distended, expanding cloud called the coma.

Comets come from two very different sources within the solar system – one providing short-period objects (with orbital periods of less than 200 years), and the other supplying long-period objects (greater than 200 years). The nearest store of cometary precursors, containing billions of nuclei larger than a kilometre across, is called the Kuiper Belt. This is a fat disk of objects encircling the Sun with an inner edge at Neptune's orbit – approximately 7.5 billion kilometres from the Sun, or 30 AU – and reaching out to at least several thousand AU. Pluto resides in this region and is now recognised as large Kuiper Belt object.

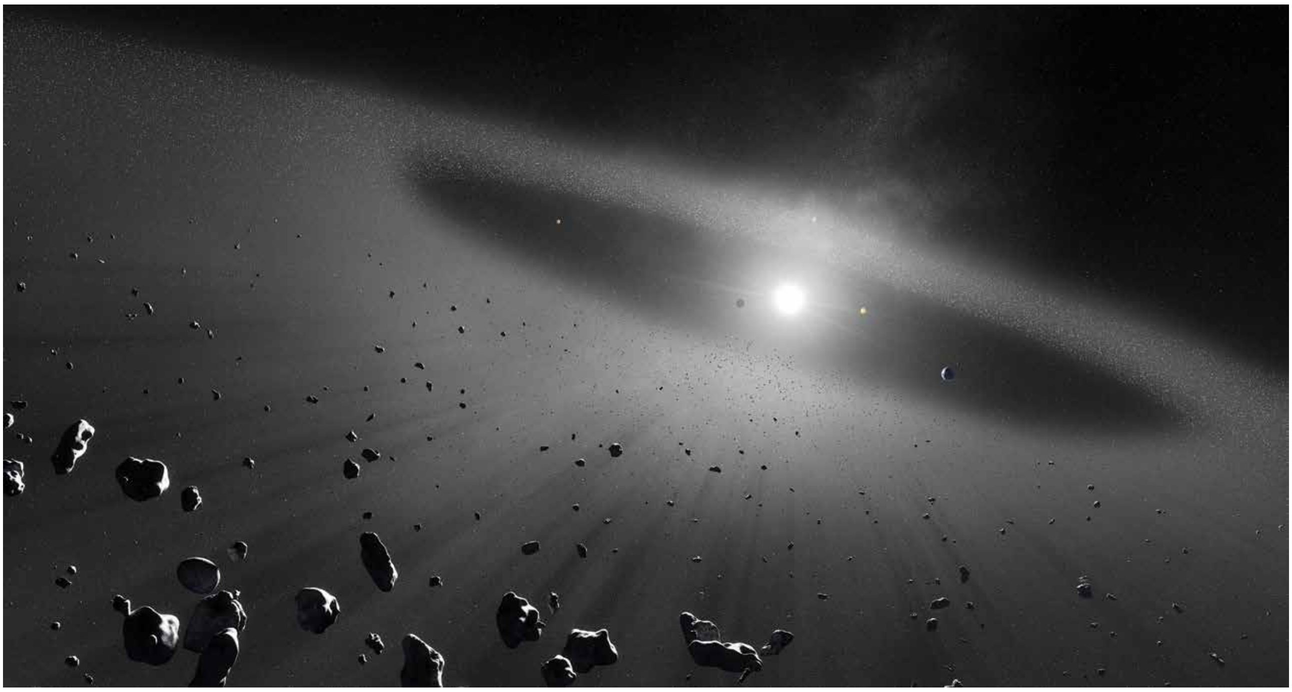
The Kuiper belt was discovered by Professor David Jewitt and his former student Jane Luu in 1992. 'The year 1992 marked the beginning of an intense period in which almost everything we did produced a discovery, starting with the mapping of Kuiper Belt structure,' he recalls. 'We found that the belt is thick, more like a doughnut than a sheet of paper, providing evidence of an unexpectedly violent past.'

Subsequent work has shown that some of the Kuiper belt objects formed in-place, while others were probably formed nearer the Sun and then scattered outwards by the gravity of the growing planets. The complex dynamical history of the solar system is imprinted in the orbits of the Kuiper belt objects.

Centaurs and the Kuiper Belt

Since then, Professor Jewitt's research has helped to illuminate numerous mysteries relating to cometary bodies and their behaviour. He investigates comet-like objects called Centaurs, and probes their unexpected behaviour when they are far from the Sun. Centaurs are recent escapees from the Kuiper Belt, on their way either to near-Sun destruction or to an icy death, when ejected from the solar system by the gravity of the gas giants – Jupiter, Saturn, Uranus and Neptune.

‘Specifically, I am interested in comets that show activity where water ice does not sublimate because it is too cold.’



The mechanism driving outgassing from comets is called sublimation, in which ice transforms directly into a gas, bypassing the liquid phase. Dust particles trapped in the ice are dragged out by the rush of gas and then swept away by the pressure of sunlight, giving rise to the characteristic tail. Sublimation of water ice begins at the orbit of Jupiter (at 5 AU) and grows stronger the smaller the distance to the Sun.

Centaurs orbit beyond Jupiter and so they are too cold for the dominant water ice to sublimate. Surprisingly, however, even in these distant objects, cometary activity is sometimes observed, with far-away Centaurs ejecting material in the form of a tail and coma. Professor Jewitt suggests that various other processes are at play that may cause trapped gases to be released. Ices that are more volatile than water ice may play a role. It is also likely that crystallisation, in which water molecules suddenly snap into an ordered arrangement after previously existing as a disordered jumble, allows Centaurs to show activity even as far out as Saturn (10 AU).

The Oort Cloud

While the Kuiper Belt is the main source of short-period comets, the long-period comets come from a completely different region called the Oort Cloud. First proposed by the Dutch astronomer Jan Oort, this is a diaphanous spherical region of vast extent surrounding the Sun. The Oort cloud extends to 50,000 AU (7.5 trillion km – almost a lightyear) or more, with an outer edge carved by the eroding effects of passing stars.

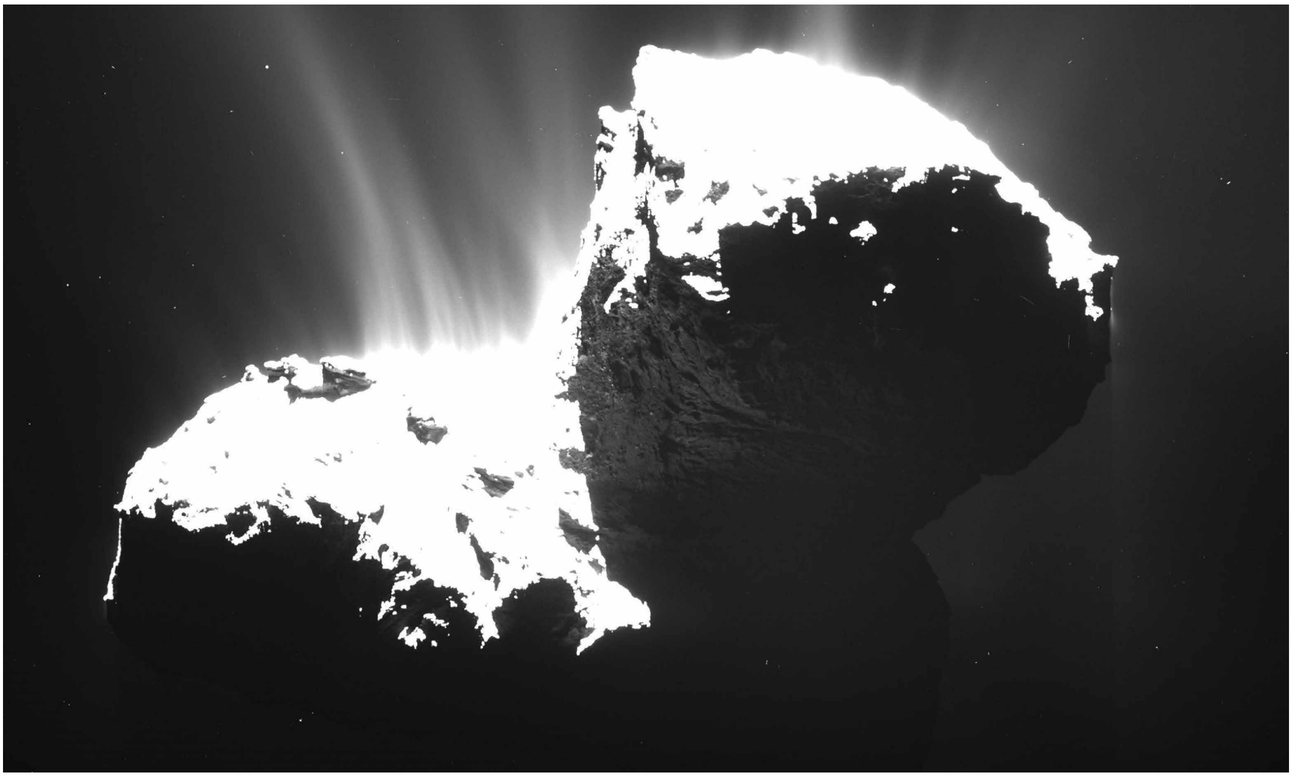
The Oort cloud is so large that, even with a trillion constituent members, no two comets ever collide. Also, these comets could not have formed there, because the density of matter in the Oort cloud is far too low. Instead, the Oort cloud comets coalesced in the vicinity of the growing giant planets and were ejected by them too fast to be captured in the Kuiper belt, but too slow to completely escape the gravity of the Sun. Simulations suggest that for every comet in the Oort cloud, another 90 to 99 were ejected to the interstellar medium, never to return.

The orbits of Oort cloud comets are disturbed by galactic tidal forces and gravitational effects from nearby stars, some of which occasionally pass through the cloud. This causes them to move inwards towards the inner solar system where Earth and the other rocky planets reside. These inward-scattered objects are the long-period comets such as C/2011 W3 (Lovejoy, see cover picture).

Cold Comets: How Do They Work?

As Professor Jewitt has observed, cometary tails are seen in distant regions of the solar system that are far too distant and cold for the sublimation of water ice to occur. So, what exactly is happening? What internal processes are being kick-started to induce sublimation-like behaviour, giving these far-away comets their characteristic tail and coma?

As previously mentioned, one mechanism that might explain this behaviour is crystallisation. Solid materials can exist in two forms – crystalline and amorphous. Window glass, for example, is amorphous,



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meaning that the molecules of silicon dioxide in the glass are jumbled together in no particular order.

At the high temperatures found on Earth, water ice exists only in its crystalline form, in which the molecules of water are packed together in orderly, hexagonal crystals. This means that the ice in your home freezer and ice on the roads on a cold winter's day is always crystalline. But at the low temperatures found in space, ice tends to grow in an amorphous form.

However, amorphous ice is unstable, meaning that it will spontaneously crystallise once the temperature rises above a critical value. When this happens, energy is released and gas molecules that were trapped in the amorphous ice are rapidly expelled. The result is, in effect, a mini-explosion. Since Centaurs are merely inward-drifting Kuiper belt objects, Professor Jewitt concludes that the Kuiper Belt must also be rich in amorphous ice. This is important, because it would set severe constraints on the thermal evolution of Kuiper belt objects. Even if warmed to only −190°C, ice in the Kuiper belt would have long-since crystallised.

Extreme Comets

Recently, Professor Jewitt and his colleagues examined a comet that is so far from the Sun, and so cold (−213°C), that even crystallisation is impossible. The long-period comet, C/2017 K2 (Pan-STARRS), is currently about 2.4 billion kilometres from Earth, and was active even when well beyond the orbit of Uranus (at 20 AU). No other inbound comet has been seen to be outgassing at such large distances.

Since crystallisation is impossible so far out, another process must drive the activity. Sublimating 'supervolatile' ices, such as carbon monoxide, carbon dioxide and nitrogen, provide a potential explanation. Professor Jewitt found that an exposed ice patch on the comet of 10 square kilometres would produce the outgassing that his team observed. Such a patch would occupy only about 1% of the surface of the nucleus, thought to be about 9 kilometres in radius. The survival of supervolatile ice is only possible because of the comet's vast distance from the Sun. Although now extremely faint, comet C/2017 K2 (Pan-STARRS) will make its closest approach to the Sun in 2022, and could then be a spectacular object.

An even more extreme object with the ungainly name 1I/2017 U1/'Oumuamua passed Earth in late 2017. It holds the distinction of being the first interstellar object ever detected passing through the solar system, and likely originated as a comet ejected from the protoplanetary disk of another star. Professor Jewitt calculated that the solar system contains, at any instant, 10,000 similar interstellar objects. He also estimated that, in the Milky Way galaxy, there are between 10 and 100 trillion trillion such bodies, all of which have escaped detection until now because of their faintness.

Curiously, although this object has spent billions of years drifting between the stars with a temperature only 10 degrees above absolute zero, Professor Jewitt and collaborators observed neither a coma nor a tail. The reasons for this remain a mystery for future study.

Meet the researcher

Professor David Jewitt
Department of Earth, Planetary & Space Sciences
Institute for Planets & Exoplanets
University of California, Los Angeles
Los Angeles, CA
USA

Born in England, David Jewitt was an undergraduate at University College London before moving to the California Institute of Technology (Caltech) in Los Angeles, where he received his PhD in 1983. He was an Assistant Professor at the Massachusetts Institute of Technology (MIT), before moving to the University of Hawaii, where he first took a position as Associate Professor, before being promoted to full Professor. He finally moved back to Los Angeles in 2009, where he began his current position as Distinguished Professor of Astronomy at the University of California, Los Angeles. He has been awarded The Shaw Prize for Astronomy and The Kavli Prize for Astrophysics, and is a fellow of various institutions, including University College London, the American Academy of Arts and Sciences and the National Academy of Sciences. Professor Jewitt's particular research interests include solar system formation, the Trans-Neptunian solar system, physical properties of comets, Centaurs, irregular satellites, Trojans, Active Asteroids and the sub-millimeter properties of comets & young stars.

CONTACT

E: jewitt@ucla.edu
W: http://www2.ess.ucla.edu/~jewitt

KEY COLLABORATORS

Bin Yang, European Southern Observatory
Chad Trujillo, Northern Arizona University
Harold Weaver, Johns Hopkins University
Henry Hsieh, Planetary Science Institute
Jane Luu, Massachusetts Institute of Technology
Jessica Agarwal, Max Planck Institute
Jing Li, UCLA
Man-To Hui, UCLA
Max Mutchler, Space Telescope Science Institute
Scott Sheppard, Carnegie Institution for Science

UCLA
Earth, Planetary, and Space Sciences

A RARE UNIVERSE? THE MULTIVERSE DEBATE THROUGH THE LENS OF PHILOSOPHY

How did we get here? How could a universe with such simple physical laws have created something as complex as us? These questions are so fundamental that even after millennia, neither scientists nor philosophers have reached a universally satisfying answer. **Dr Simon Friederich,** a philosopher at the University of Groningen, focuses his attention on one particular suggested response to the mystery of our existence: that it can be explained by the hypothetical existence of many universes beyond our own. But like any worthy philosopher, he is aware of the limits of our ability to determine the truth in such fundamental matters.

From the most imperceptible motions of particles to the pulls of distant galaxies, every conceivable event in our universe is ultimately dictated by laws and constants that appear fundamental and unchangeable. If the masses of some of the lightest fundamental particles – the electron and the lightest quarks – had been remotely different, stable atomic nuclei could not have formed. If the force of gravity were even slightly weaker than it is, galaxies and even stars may never have coalesced, while if it were stronger, stars would have been smaller and more short-lived.

Tampering with other fundamental constants, including the energy density of the early universe and the cosmological constant, would have similarly catastrophic consequences. Logically speaking, it would seem that with so many of these values in play, the chances of anything as complex or intricate as life being allowed to emerge should be astronomically small. For philosophers and physicists alike, our very existence has long been one of the universe's greatest mysteries.

The Fine-tuning Conundrum

Dr Simon Friederich of the University of Groningen is well aware of the problems that thinkers face when trying to solve this conundrum. 'According to many physicists, the laws and constants in our universe seem fine-tuned for life,' he explains. Attempts at explaining this fine-tuning have included divine intervention, as well as the speculative idea of an elegant 'theory of everything', as searched for by Einstein. However, such speculative approaches are rarely satisfying for scientists or philosophers. Dr Friederich is more intrigued by a different suggestion: 'Might the proper reaction to fine-tuning be to infer that we live in a multiverse: a collection of real universes with different laws and constants?'

The idea behind the suggested multiverse conclusion is that out of a vast number of universes where the conditions don't allow observers like us to exist, our universe has hit the jackpot. The idea is, according to Dr Friederich, that 'if there are many universes with different laws and constants, it is only to be expected that there is at least one with the right ones for life.' The chances

of life emerging in a given universe may still be miniscule, but not zero – the consequences of which we see in our universe. With this multiverse response, it might appear that the fine-tuning that allows us to exist is not so mysterious after all. However, as any philosopher will tell you, even ideas that seem satisfying at first are rarely unopposed. This case is no exception.

The Lucky Gambler

To understand the opposition that some philosophers have to the multiverse argument, Dr Friederich invites us to imagine walking into a casino, sitting down at a table, and observing a gambler at play. Incredibly, the gambler

wins the very first game you witness – naturally causing you to question the circumstances that could have brought about such an extraordinary event. You might conclude that the gambler must have played many games before you first walked in. But as statisticians point out, you'd be wrong. Why?

Games of chance are typically independent from each other, which in this case means that the gambler would have had the same chance of winning, no matter how many games they had played beforehand. Had there been many such games, they would not have increased the gambler's chance of winning *this* game at all. If we can exclude that the game you witnessed was manipulated or was otherwise special, there is only one adequate reaction to your extraordinary observation: that you really were just very lucky to see it. Dr Friederich explains how this reasoning can be extended to oppose the idea of using a multiverse to explain the finely-tuned nature of our own universe. 'Some philosophers argue that the inference of multiple universes commits the "inverse gambler's fallacy": inferring from one remarkable outcome that there are likely many similar events with less remarkable outcomes,' he says. Without any way for us to measure the laws and constants of universes beyond our own, we could, therefore, be following the same flawed reasoning that led us to believe that the gambler had played many games before we came to sit at their table. 'Consequently, postulating many other universes does not make it any more likely for this universe to have the right conditions for life.'

Our Lucky Planet

In a recent study, Dr Friederich discusses this objection against the inference from fine-tuning to a multiverse, using the analogy of life emerging on planets within our own galaxy. He notes that scientists are not concerned about why precisely Earth happened to be hospitable to life. It is satisfying enough to conclude that the Earth is the right distance from the Sun; that it is the right size to support a stable atmosphere; that the right chemicals were present on its surface, among other factors. Under these conditions, life naturally came to be. On other planets, however, we know for a fact that this isn't the case.

In recent years, astronomers have observed a great number of planets and studied their properties. From small, icy worlds in our own solar system to hot gas giants in others, we are now aware of thousands of planets that, for a wide variety of reasons, are completely inhospitable to life. From observing so many of these planets, therefore, we have empirical evidence that the conditions on our planet that allowed us to exist are quite rare. So should we be surprised that we find ourselves on *this* exceptional planet, observing other planets which are, much more commonly, lifeless? Of course not, Dr Friederich argues. But there are two coherent responses to Earth's life-friendliness: we can either regard it as accounted for by our observations being biased towards observing life-friendly conditions, simply because without them we could not have existed in the first place; or we can regard them as a lucky coincidence for which there is no further explanation.

Naturally, Dr Friederich extends this analogy to the multiverse. In our universe, the laws and constants that appear finely tuned are analogous to the exceptional conditions we see on

Earth, while other universes can be compared to the many life-hostile planets we have observed. And if there are two coherent responses to Earth's fine-tuning for life (regard it as accounted for by the existence of many other life-hostile planets, or accept it as a lucky coincidence), then there are also two coherent responses to our universe's fine-tuning for life (regard it as accounted for by the existence of many other universes, or accept it as a lucky coincidence). But if these responses are indeed both coherent, it may ultimately be impossible to decide whether the inference from fine-tuning to a multiverse commits the inverse gambler's fallacy or not.

Not Leaving Things to Chance

In his latest research, Dr Friederich has worked towards developing an alternative, more modest, argument from fine-tuning for a multiverse against which the inverse gambler's fallacy charge cannot be raised. At the root of his new argument is the idea that the considerations according to which life requires fine-tuning partly undermine the central advantage that single-universe theories usually have over multiverse theory: that they make more specific empirical predictions.

Multiverse theories propose that there are different universes with vastly different conditions. This reduces their ability to make measurable predictions. But, as Dr Friederich explains, 'if we can predict the laws and constants from the fact alone that there is life, the predictive success of single-universe theories is no longer very impressive in comparison.' The fact that life requires fine-tuning may therefore make it a bit more rational to believe in a multiverse after all. According to Dr Friederich, his new fine-tuning argument for the multiverse is preferable to the old one because it is immune to the inverse gambler's fallacy charge.

A Theory in Need of Evidence

In further recent work, Dr Friederich explores the perhaps insurmountable difficulties that scientists and philosophers face when trying to make specific multiverse proposals empirically testable. He notes that if we want to make predictions about the nature of a multiverse, we need to have an idea of what an observer would find in universes that are very different from ours. 'The most widely used strategy to make predictions from multiverse theories is to interpret a multiverse theory as predicting what typical multiverse inhabitants will observe,' Dr Friederich explains. 'Some researchers have suggested that we should subject this "typicality principle" to an empirical test, but this idea is a non-starter.'

Since the candidate multiverse scenarios suggested by physicists are extremely vast and varied, several auxiliary assumptions must be made to make them testable. In particular, a so-called cosmic measure must be chosen as well as a physical proxy for observer number in any specific multiverse region. But, according to Dr Friederich, 'the use of a cosmic measure and an observer proxy is very problematic because those can be chosen more or less freely by scientists to make predictions that conform to their theoretical preferences.' So, while the inference from fine-tuning to a multiverse would not necessarily commit the inverse gambler's fallacy, without independent empirical evidence for some concrete multiverse scenarios, any further ideas about the multiverse would ultimately be distorted by our own ideas about what other universes should look like.

If any observations come along that suggest the existence of universes beyond our own, Dr Friederich will surely be at the forefront of those answering the philosophical questions that arise. Until then, he will focus on expanding his ideas to reflect on and inform current scientific and philosophical practices. He also hopes to bring his ideas to the public in detail: 'I will combine all the threads of my thinking on this topic in a book that will hopefully appear not so far in the future.'

Meet the researcher

Dr Simon Friederich
University College Groningen
Faculty of Philosophy
University of Groningen
The Netherlands

Dr Simon Friederich completed two PhDs, the first of which was in in theoretical physics from the University of Heidelberg in 2011, and the second in philosophy from the University of Bonn in 2014. Combining these two interests, he went on to become assistant professor of philosophy of science at University of Groningen, where he is also a member of the Young Academy Groningen. He is also an external member of the Munich Centre for Mathematical Philosophy. Through his work, Dr Friederich has now explored a wide variety of scientific fields through the scope of philosophy, including interpretations of quantum mechanics, and the status of mathematical language.

CONTACT

E: s.m.friederich@rug.nl
W: http://simonfriederich.eu/
@simonfriederich

FUNDING

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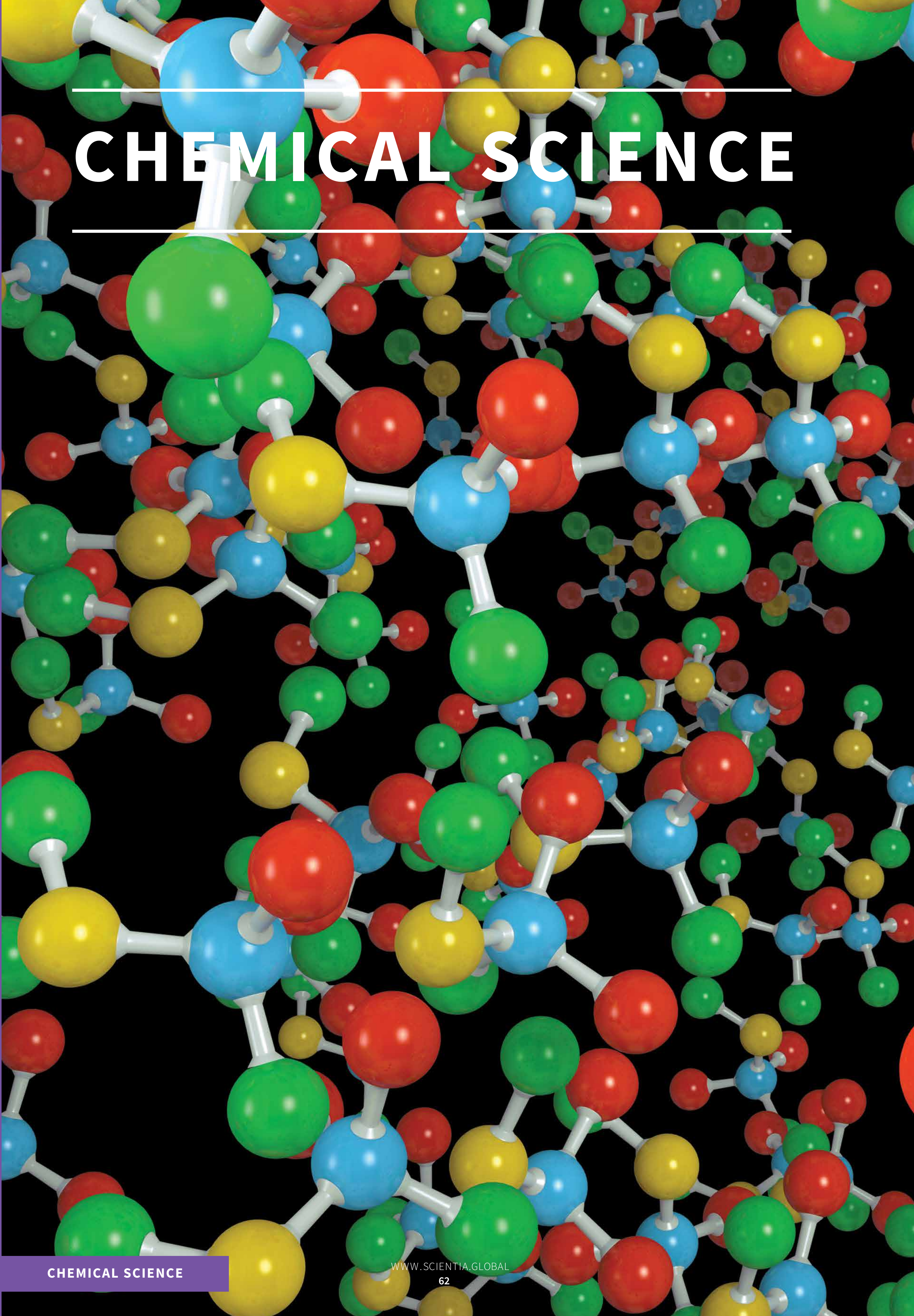
CHEMICAL SCIENCE



FINDING SOLUTIONS THROUGH CHEMICAL SCIENCE

Though often eclipsed by its trendier siblings – physics and biology – in the public sphere, chemical science is absolutely essential to our modern lives. From medicines to batteries, and from smartphone screens to food preservation, countless aspects of our day-to-day existence are direct products of chemical research.

In the future, chemical science will continue to help us solve problems and develop new technologies, in fields such as renewable energy, carbon sequestration, pharmaceuticals for antibiotic-resistant bacteria and water desalination.

Therefore, in this section of the edition, we celebrate the chemical scientists who are pioneering new discoveries and technological innovations that will enrich our lives even further. To open this section, we have had the pleasure of speaking with Dr Anne Hultgren, Executive Director and CEO of the Arnold and Mabel Beckman Foundation. In particular, Dr Hultgren tells us how the Foundation supports researchers whose creative and interdisciplinary research will lead to new tools for scientific discovery in the chemical and life sciences.

Next, we meet Dr Wieland Steinchen and Professor Gert Bange, from the Center for Synthetic Microbiology and Philipps University of Marburg, who have been developing the use of a special analytical tool known as 'Hydrogen-Deuterium Exchange Mass Spectrometry' to understand protein chemistry in bacteria. The team's insights may prove useful in the prevention and treatment of bacterial infections.

Keeping with the theme of analytical chemistry, we next introduce Dr Simon Humphrey and Sam Dunning at the University of Texas at Austin, who have created a new type of chemical sensor that can distinguish between normal water (H_2O) and heavy water (D_2O). The team's new sensor material, which contains luminescent lanthanide atoms, could be useful in applications ranging from medical imaging to detecting leaks of radioactive waste.

In the fourth article of this section, we showcase the work of Dr YuHuang Wang and his research group at the University of Maryland, who also develop luminescent materials that can be used for analytical applications. Rather than working with lanthanide-based materials, the team develops carbon nanotubes that contain synthetically-created 'quantum defects'. These quantum defects luminesce brightly with near-infrared light. The team's new carbon nanotubes could be used as highly-selective sensors, even in complex biological systems.

Last but not least is the fascinating research of Dr Alfred Msezane at Clark Atlanta University. His team has gained remarkable insight into the behaviour of electrons in heavy atoms and molecules, such as lanthanides and fullerenes – large carbon molecules, which include spherical fullerenes and carbon nanotubes. For the first time, Dr Msezane and his colleagues have developed a robust mathematical theory to gain a fundamental understanding of how such heavy systems gain electrons to form negative ions. Their insight will prove invaluable in the field of water purification for developing countries, using heavy-ion based catalysts.

THE ARNOLD AND MABEL BECKMAN FOUNDATION

Located in Irvine, California, the Arnold and Mabel Beckman Foundation supports researchers and non-profit research institutions in making the next generation of breakthroughs in chemistry and the life sciences. Founded in 1978 by philanthropists Arnold and Mabel Beckman, the Foundation supports US institutions and young scientists whose creative, high-risk and interdisciplinary research will lead to innovations and new tools for scientific discovery. In this exclusive interview, we have had the pleasure of speaking with Dr Anne Hultgren, Executive Director and CEO of the Arnold and Mabel Beckman Foundation. Here, she tells us all about the Foundation's history, and the various ways in which it continues to accelerate the advancement of science today.

Who were Mabel and Arnold Beckman, and what inspired their passion to advance scientific research? Please describe how they came to establish the Beckman Foundation.

Arnold O. Beckman (1900–2004) and Mabel Meinzer Beckman (1900–1989) spent a lifetime together, dedicated to a career focused on advancements in science. They left a profound impact on science and society through the introduction of instrumentation that transformed the biology and chemistry laboratory from qualitative observations to the modern quantitative laboratory. Dr Beckman's inventions that merged electronic measurement techniques into analytical instrumentation opened up new fields of exploration for scientists around the world.

Arnold Beckman started his chemistry career at the early age of nine years old in Cullom, Illinois when his father built him a 'laboratory' in a shed in their backyard. His high school teachers recognised his talents and helped him to get several jobs in chemical and textile manufacturing industry. When he started college, he was already working as a consultant to several established companies to measure the chemical by-products and quality of their products. Arnold Beckman went on to study photochemistry at the University of Illinois – Urbana Champaign, and then received a PhD in chemistry at Caltech in the 1920s where he was hired as an assistant professor.

In 1934, a chance phone call from a friend started Dr Beckman on a new path, and he began his transition from academic researcher to entrepreneur and into a businessman who founded a multibillion dollar company – not at all common for scientists in those days. A former classmate from Illinois had contacted him with a problem he was facing at the Southern California Fruit Growers Association: he needed to quickly and accurately measure the acidity, or pH, of lemons in the fields to determine the optimum time to harvest for the best tasting juice.

Dr Beckman spent a month making his first glass electrode pH meter with an electronic read-out dial, and he sent the prototype to his friend. When his friend called two months later and asked him to make another because his lab mates were always borrowing the first one, Dr Beckman decided that there was a business opportunity. His company – initially National Technical Laboratories, later renamed Beckman Instruments – was founded, and he began developing scientific instruments that are still used in laboratories worldwide.

While the list of inventions is long, some notable examples are: The pH meter; the UV and IR-spectrophotometers; the oxygen analyser used in submarines, airplanes, space missions, and infant incubators; precision variable resistance dials that first enabled radar and later became essential components in any instrument with a knob; an analogue computer system used in manufacturing process controls; the ultracentrifuge that enabled protein and nucleic acid separations; and environmental oxidant recorders to measure smog composition and sources, providing the scientific foundations in the Clean Air Act.

Dr Beckman always said, 'I have done more for the advancement of science by providing analytical instruments to

‘As we like to say at the Foundation – the future looks bright – and we are confident that over the next 40 years we will continue the Beckmans’ commitment to supporting scientific research and young scientists and honour their legacy of philanthropy.’

researchers than I could have done by myself in my own laboratory.’ Along with the success of their company came much personal financial success for the Beckmans. In the 1970s, they began discussing thoughts and ideas with trusted friends about how to leave a legacy and use their wealth to help others. Dr Beckman later reflected on that decision process and recalled ‘We knew that our fortune came from selling instruments to scientists, and so we decided that we should give back to scientists.’ In 1977, they formed and personally funded the Arnold and Mabel Beckman Foundation, and started their philanthropy with their first gift to University of Illinois – Urbana Champaign in 1978.

Tell us about the innovative research institutes that were set up by the Foundation, and the types of research that are carried out in them.

The earliest gifts the Beckmans made as part of the Arnold and Mabel Beckman Foundation were to establish the five Beckman Institutes, all built around the core principle of collaboration in the sciences. The Beckmans worked very closely with each Institute in the strategy, planning, design, and construction of the buildings to make sure that the Institutes would enable their vision that the next advances in science and technology were going to occur because of increasingly interdisciplinary programmes. The results are the Institutes located at University of Illinois – Urbana Champaign, Caltech, City of Hope, Stanford, and University of California – Irvine.

The Institutes were founded based on innovations both in science and in the management of the laboratories within the host University. Most of the Institutes themselves have very few permanent staff or members; rather, they were designed to help bring groups together and provide the infrastructure and instrumentation for collaborative projects to happen. By building shared resources, this allows the researchers to access state-of-the-art instruments, and the experts dedicated to using and maintaining them, without having to build that capability within their own individual laboratory. This deliberate design allows projects to come and go through the Institutes depending on need and innovation, and this flexibility keeps the research at the forefront of science.

These institutes continue to produce ground-breaking scientific discoveries today. Please tell us about a few recent research highlights from one or more of these institutes.

We are incredibly proud of the work and progress made within the Beckman Institutes over the years, so it’s hard to pick just a few examples. The Institute at University of Illinois – Urbana Champaign is unique in the range of projects that are supported within the Institute, from nanoscale imaging capabilities to materials engineering to cognitive development programmes with longitudinal studies on mothers, infants and children.

For example, recently at UIUC, the Autonomous Materials Systems Group members Moore, Sottos, and White commercialised a new self-healing material that can respond to stresses in the environment and adapt rather than fail, while Schantz and Llano from

the Cellular and Molecular Foundations of Intelligent Behavior Group published a landmark study on the environmental factors that influence child brain development, with a particular focus on auditory system development.

The City of Hope Beckman Research Institute has for many years been a pioneer in research on personalised treatments for cancer and other devastating diseases. They continue this tradition with Dr Yanhong Shi, who recently demonstrated a technique to use induced pluripotent stem cells (iPSC) for personalised treatment of neurological diseases, including Alzheimer's, that will be moving into clinical trials in the near future.

As a final example, at the Stanford Beckman Research Center, Dr Daniel Jarosz's research in protein hereditary traits is creating a paradigm shift in our understanding of how certain traits may be influenced through prion adaptions that are passed from parent to child, rather than just through the commonly understood genetic mutation or variability.

In addition to running the centres, describe some of the other ways through which the Beckman Foundation currently supports scientific research in the US. Who is eligible to benefit from the Foundation's various programmes and awards?

The Foundation also has several grant programmes that focus on young scientists to foster the next generation of innovators and leaders in science. When Dr Beckman was asked to describe his long-term goal for the Foundation, he explained that he wants his Foundation to 'find and support the young people with innovative ideas who don't yet have the clout to get the major government research grants.'

To meet this goal, the Foundation has a trio of annual grant programmes for young scientists in chemistry and life science research. First is the Beckman Young Investigators Program for new faculty members within the first three years of a tenure-track position. These are four-year awards for junior faculty to build new research directions within their laboratories. The second programme is a Chemical Science Postdoctoral Fellowship Program, with a focus on new postdocs interested in fundamental chemistry problems and chemical instrumentation development. Our third annual programme is the Beckman Scholars Program for undergraduate institutions with a strong culture of involving undergraduates in laboratory research. The Scholars Program provides grants to support 15-month research projects in selected mentor laboratories.

In addition to these annual programmes, the Foundation also funds special initiatives when possible. As a recent example, the Foundation's Scientific Advisory Council realised that the innovations associated with Cryogenic Electron Microscopy were revolutionising the field of structural biology, but that the instrumentation cost was impeding the adoption of the technology within the US, especially for smaller research universities that had excellent programme ideas. This challenge became a perfect opportunity for the Foundation, and in 2017 we provided grants to five universities to share in the cost of acquiring new Cryo-EM instrumentation. We are hopeful that this increase in Cryo-EM capabilities will help accelerate the discoveries that this new measurement technique enables, carrying on the legacy of Dr Beckman's passion for novel methods.

Please tell us about the Arnold and Mabel Beckman Center of the National Academies of Sciences and Engineering in Irvine, California, and how it facilitates research collaborations.

The Beckmans realised that Southern California was a natural location for a West Coast location for the National Academies of Sciences and Engineering, especially given the large number of Academy members who live here, and to provide a more convenient meeting space to promote collaboration around the Pacific Rim.

They presented a concept to the Academies leadership of creating the 'Beckman Center', a versatile meeting space which would be dedicated to conferences about advances in science and technology, emphasising collaboration and multidisciplinary topics. Working with the Irvine Company, the Beckmans designed and built the Beckman Center, and donated both the building and land to the National Academies.

Today, the Beckman Center continues the original mission of hosting Academies functions and scientific programmes, including the Kavli Frontiers of Science Symposium, the Keck Futures Initiative, the Arthur M. Sackler Colloquia, and the Distinctive Voices lecture series that brings popular science talks to the general public.

Finally, please tell us about the future goals and plans for the Foundation.

The Foundation is celebrating its 40th year, from the first gift made in 1978 and over $700M in grants and support to science since. We're marking this milestone with a year-long speaker series that touches on themes revolving around the impact of the Foundation in scientific innovation, philanthropy, and partnerships with other STEM organisations in our local region.

Looking forward, we are excited to continue our grant programmes for young scientists, support the Beckman Institutes, and host our annual Beckman Symposium, where nearly 300 Beckman award winners and alumni attend a three-day event to present their newest research findings as poster or oral presentations, learn about a broad range of research topics from their peers, and discuss career tips with experts from academic and industry. We are also always exploring opportunities to work with science programmes within our hometown of Orange County, CA to inspire future scientists, and developing new special initiative programmes, like Cryo-EM, to meet the needs of the scientific community.

As we like to say at the Foundation – the future looks bright – and we are confident that over the next 40 years we will continue the Beckmans' commitment to supporting scientific research and young scientists and honour their legacy of philanthropy.

www.beckman-foundation.org

Arnold and Mabel BECKMAN FOUNDATION

BRIDGING THE GAP BETWEEN PROTEIN STRUCTURE AND DYNAMICS

Proteins are present in all living organisms. The unique functions they perform in biochemical processes are dependent on their three-dimensional structure. **Dr Wieland Steinchen** and **Professor Gert Bange**, from the Center for Synthetic Microbiology (SYNMIKRO) and the Faculty of Chemistry at the Philipps University of Marburg, aim to understand the structures and functions of several different proteins. They use a special analytical technique, known as 'Hydrogen-Deuterium Exchange Mass Spectrometry', or HDX-MS, to carry out their investigations.

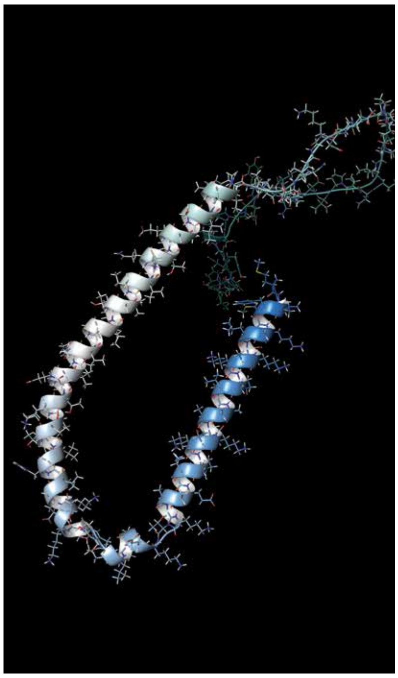
Understanding the Structure and Function of Proteins

Proteins are compounds comprising a chain of amino acids. This chain is folded up into a three-dimensional shape that gives each protein its unique set of properties. Understanding the structure, reactivity and function of proteins, and other large molecules, is vital in understanding how they will interact with other chemicals in different conditions. Many analytical techniques have been developed to ascertain this information. As a result, there are several, steadily growing libraries that provide structural and chemical information on proteins and the subunits that make them up.

However, there is always room for further contributions to this field of study. Proteins function as catalysts, transport and store useful compounds in the body, provide mechanical support to cells and tissues, help in fighting disease, generate movement, transport signals around the body, and control growth. Therefore, detailed information on protein chemistry is useful in many applications and can aid in improving, or in some cases, inhibiting their action in living organisms, including humans.

To that end, enhanced analytical techniques and equipment are being developed. In recent years, a technique known as 'Hydrogen-Deuterium Exchange Mass Spectrometry', or HDX-MS, has offered an attractive, new route for analysing the behaviour and structural features of proteins. In a nutshell, the technique monitors the exchange of hydrogen atoms from the protein with deuterium atoms in an appropriate solvent (deuterium is a version of hydrogen which, in addition to a single proton, has a neutron in its atomic nucleus). The degree to which this exchange occurs at various points along the protein is dependent on its physical structure and folding patterns. This is the parameter that is measured in HDX-MS, and this information can complement other high-resolution structural approaches.

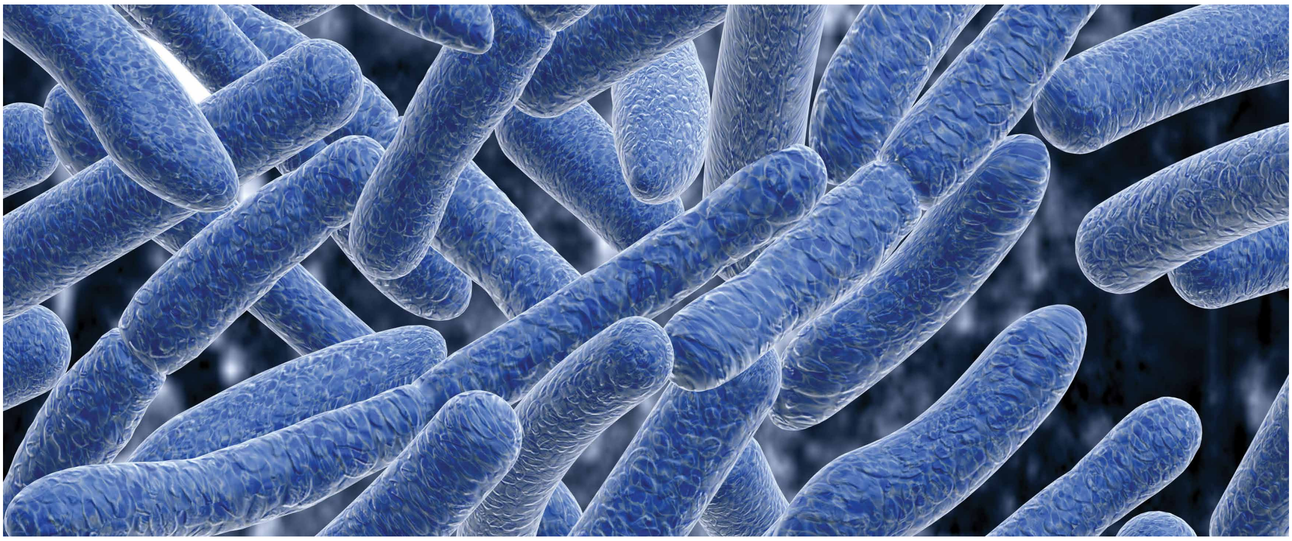
Dr Wieland Steinchen and Professor Gert Bange at the Philipps University of Marburg have become specialists in the field of HDX-MS analysis. While they too acknowledge that 'HDX-MS data are most ideally interpreted together with structural information obtained by other techniques,' they also note that, 'even in the absence of structural information, HDX-MS provides useful insights into



the dynamic and structural properties of proteins and macromolecular assemblies.'

In fact, the latter well summarises Dr Steinchen and Professor Bange's research work. They have been using the HDX-MS methodology to characterise the structure and function of numerous proteins, especially that involved in metabolism of *second messengers* or their target proteins.

‘HDX-MS data are most ideally interpreted together with structural information obtained by other techniques. However, it is important to note that even in the absence of structural information, HDX provides useful insights into the dynamic and structural properties of proteins and macromolecular assemblies.’



Second Messenger Proteins and Cellular Adaptability

The ability of living organisms to adapt to nutrient deficiencies, environmental change or external stress is critical to their survival. Biochemicals known as ‘second messengers’ play a vital role in this regard. Under certain circumstances, they transmit signals from a receptor on the surface of a cell, to proteins that can initiate cellular processes to counteract or remedy the change in conditions.

In bacteria and plants, for example, a set of second messengers known as ‘alarmones’ are integral to cellular adaptability. Alarmones are biochemicals that are produced in greater quantities in response to stress. For example, when bacteria are starved of energy, the alarmones ‘guanosine tetraphosphate’ and ‘guanosine pentaphosphate’, collectively referred to as ‘(p)ppGpp’, modify cellular processes to help the bacteria conserve energy and survive. This is a big problem in cases where bacteria have caused infection. Cellular survival strategies make the bacteria harder to kill and infection harder to treat. It can also make disease control (in hospitals, for example) incredibly difficult.

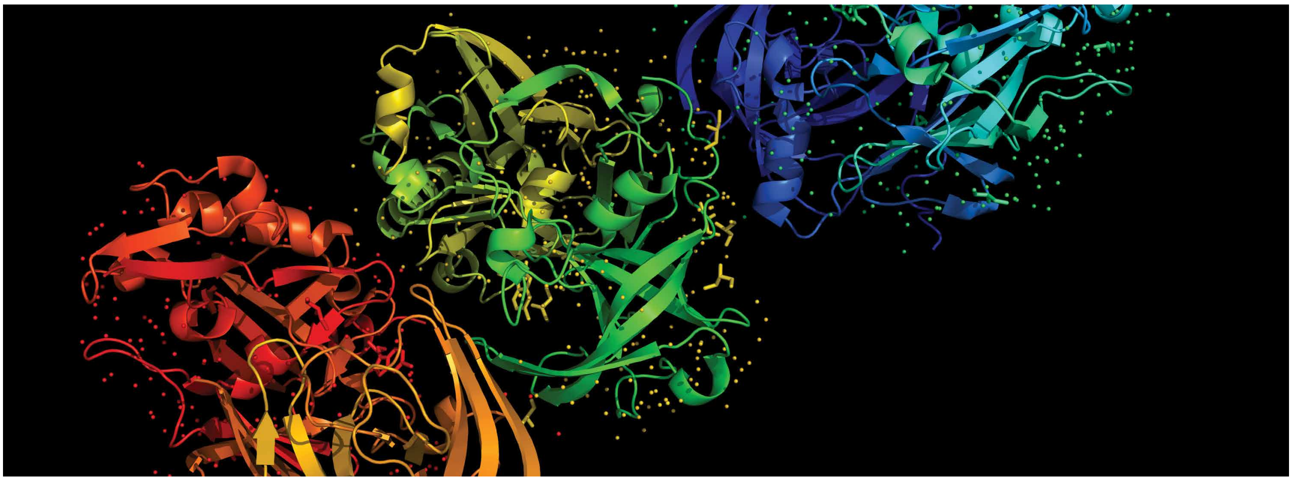
(p)ppGpp was the subject of Professor Bange and Dr Steinchen’s collaboration in 2015. Their goal was to understand the structural details of this alarmone combination and how exactly it is synthesised. Specifically, they examined the nature of a large molecule known as ‘Small Alarmone Synthetase 1’, or SAS 1, which has a central role to play in the synthesis of (p)ppGpp. As mentioned earlier, understanding the structure of large molecules is crucial to understanding its function.

Dr Steinchen and Professor Bange presented a thorough molecular description of the synthesis reaction’s catalytic mechanism. This understanding, in cases of infection, would be extremely useful in discouraging (p)ppGpp production and limiting bacterial growth. This work also laid the foundation for the team’s subsequent research into the nature of other second messenger proteins – they wanted to gain further insight into their structure, and its relationship to function, using the HDX-MS methodology.

Second Messenger Proteins and Biofilm Synthesis

In a collaboration of 2017, Professor Bange and Dr Steinchen investigated the role of second messenger proteins in the formation of so-called ‘biofilms’. Biofilms are aggregations of microorganisms, such as bacteria, which form as a defence mechanism. They do this in response to a significant environmental change. Biofilms cover surfaces and act as a protective layer. Biofilms can be both beneficial and detrimental to living organisms. Focusing on the negative effects of biofilms, they are a large contributor to disease and antibiotic resistance in humans.

Crucial to bacterial biofilm formation is the production of chemicals known as ‘extracellular polysaccharides’. And crucial to the formation of extracellular polysaccharides is a second messenger protein known as ‘cyclic dimeric GMP’, or ‘c-di-GMP’. So, an understanding of the processes behind c-di-GMP formation would help in understanding biofilm formation and how this can be discouraged in the case of treating disease.



In their research of 2017, Professor Bange, Dr Steinchen and their colleague Professor Becker from SYNMIKRO identified a class of c-di-GMP-responsive transcription factors (proteins that help turn specific genes 'on' or 'off'), which had clearly acquired the ability to sense the signalling molecule c-di-GMP. Ultimately, this results in the formation of a biofilm. Interestingly, the binding of c-di-GMP to this class of c-di-GMP-responsive transcription factors was highly reminiscent of another process the team had observed before. By drawing this comparison, they were able to gain insight into the binding of c-di-GMP to its target, thus bridging the knowledge gap between the structure and function of this particular second messenger protein.

The Role of Premature Folding States

In a recent research paper published in 2018, Dr Steinchen, Professor Bange and colleagues noted that scientists have extensive knowledge about proteins in their mature, folded states. However, it is generally unknown whether partially synthesised and folded proteins can execute biological functions too. In response to this challenge, Professor Bange and Dr Steinchen together with Professor Bibi from the Weizmann Institute (Israel) decided to take a closer look at premature folding states. They focused their research on a certain signal receptor protein found in *E. coli* bacteria known as 'FtsY' – a protein that plays a vital role in the production of other proteins found in cell membranes. As highlighted in the associated study, their goal was to investigate the underlying structural mechanism of how FtsY binds to signalling molecules that, in turn, trigger the production of other proteins.

In short, the team found that structural intermediates, which differ greatly from the mature FtsY structure, can facilitate the binding of signalling molecules. In terms of wider implications, the research highlighted how certain intermediates, even though they may be temporary in nature, can dictate biological function. And it may explain, in part, why bacteria are so adaptable and resilient under changing conditions where normal processes are affected in some way.

HDX-MS Capability at Philipps University of Marburg

Throughout many of Dr Steinchen and Professor Bange's research projects, HDX-MS has proved itself to be a most valuable tool. Indeed, even at the technique's current stage of development, it has immense potential. One reference work commented, 'while once a challenging and therefore sparingly used method, modern HDX-MS is more straightforward, rapid, and routine than in the past. As a result, the breadth of applications of the method has expanded.' And, of course, there will never be a shortage of proteins to study using the HDX-MS technique.

Considering the foregoing, and after having honed his skills in relation to the use of HDX-MS, Professor Bange, with the support of his colleague Dr Uwe Linne, developed significant HDX-MS analytical capabilities at the Philipps University of Marburg. In time, a professional, operational unit providing scientific and technical support for HDX-MS-based analytics was created, known as the 'Marburg Core Facility for Interactions, Dynamics and Biomolecular Assembly Structure', which was financially supported by the Deutsche Forschungsgemeinschaft (DFG). Dr Steinchen works as a scientist at that same facility.

Using the resources and expertise at their disposal, Dr Steinchen and Professor Bange continue to develop novel approaches to understanding protein structure and function using the HDX-MS methodology. Their current focus is on understanding how proteins contribute to cellular adaptability and resilience. As described above, this knowledge may be used in the prevention and treatment of disease.

But the team also seeks to understand the broader implications of cellular adaptability and resilience: 'We want to understand how microorganisms – which provide the greatest diversity within the biosphere – conquer every possible niche ranging from hot springs to the human gut due to their fast adaptability.' Again, understanding protein structure and dynamics is crucial to understanding the strategies that cells use to adapt to changing circumstances. In this quest, HDX-MS has been, and will be, a most invaluable analytical tool.

Meet the researchers

Dr Wieland Steinchen
Center for Synthetic Microbiology (SYNMIKRO)
& Faculty of Chemistry
The Philipps University of Marburg
Marburg, Germany

After studying pharmaceutical science at Friedrich Schiller University in Jena, Germany, Dr Wieland Steinchen undertook his doctoral studies at the Philipps University of Marburg, under the supervision of Dr Gert Bange. He received his PhD in 2017 with the doctoral thesis entitled 'Structural and Mechanistic Analysis of (p)ppGpp Synthetases'. He is now based at the university's Faculty of Chemistry and LOEWE Center for Synthetic Microbiology (SYNMIKRO), and works as staff scientist at the associated HDX-MS research facility.

CONTACT

E: wieland.steinchen@synmikro.uni-marburg.de
W: https://synmikro.com/facilities/interaction,-dynamics-und-assembly/team.html

Professor Gert Bange
Center for Synthetic Microbiology (SYNMIKRO)
& Faculty of Chemistry
The Philipps University of Marburg
Marburg, Germany

Dr Gert Bange received his PhD in biochemistry from the University of Heidelberg, Germany in 2007. After postdoctoral research at that same university, he took up a position at the Philipps University of Marburg as Independent Research Group Leader of the LOEWE Center for Synthetic Microbiology (SYNMIKRO). In 2015, Dr Bange and his colleague Dr Linne started a designated facility for HDX-MS-based analytical science at Philipps University. Dr Bange currently serves as full professor of Systems- Biochemistry at that same institution and runs a research group known as the 'Bange Lab'. He heads the core facility for interactions, dynamics and biomolecular assembly structure of the Deutsche Forschungsgemeinschaft (DFG).

CONTACT

E: gert.bange@synmikro.uni-marburg.de
W: https://synmikro.com/bange/

FUNDING

Deutsche Forschungsgemeinschaft

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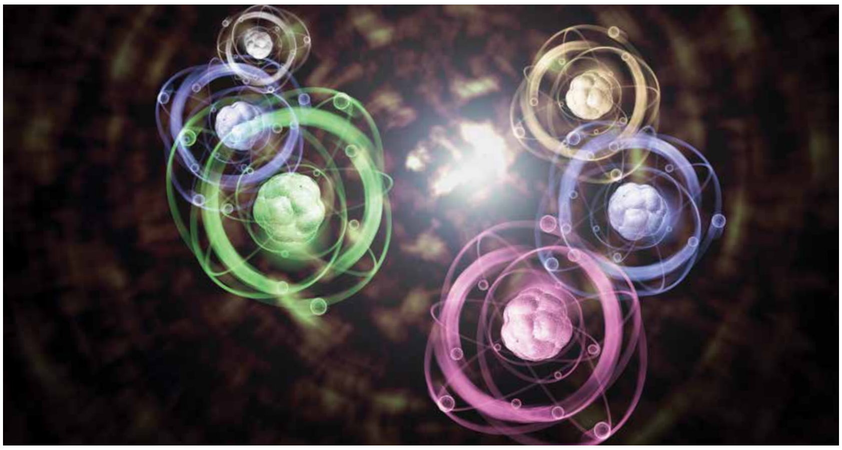
Philipps Universität Marburg

A NEW GENERATION OF CHEMICAL SENSORS

Dr Simon Humphrey and **Sam Dunning** at the University of Texas at Austin have created a new lanthanide-based chemical sensor that can identify trace levels of water in many different solvents, and can even distinguish between normal water and 'heavy water'. The team's new material could potentially be applied to medical imaging and for cleaning up chemical spills.



Lanthanides – the Ideal Photoemitters

From your schooldays, you may remember using universal indicator or litmus paper to measure pH. While these simple tests are well known and widely available, more sophisticated chemical sensors are needed to help tackle issues such as cleaning up chemical spills, remediating old industrial sites, and detecting radioactive contamination in water supplies. Although many techniques are available for these applications, very few allow for rapid on-site detection, with samples often needing to be sent away to a lab for analysis.

Now, Dr Simon Humphrey, Sam Dunning and their colleagues at the University of Texas at Austin have developed a new class of lanthanide-based materials, which could form the basis of a new generation of rapid chemical sensors that could be used for these applications.

Due to their light-emitting – or 'photoluminescent' – properties, molecules containing lanthanide (Ln) ions (charged atoms) have been increasingly explored as chemical sensors. The term 'lanthanide' refers to the group of elements with atomic numbers 57 to 71, from lanthanum (La) to lutetium (Lu). When grouped together with the chemically similar elements yttrium and scandium, you may have heard them described as 'rare earth elements', and they have applications in electronics, high-strength magnets and catalysis.

After absorbing light, lanthanide ions emit visible and infrared light at specific frequencies. This means that a solid-state sensor (for example, a dipstick) could be easily read either using the naked eye or a UV-reader to detect chemical impurities in a sample. Each type of lanthanide ion (for example europium or terbium) emits a very distinct frequency of light that is characteristic of that particular element. This means that lanthanide-based chemical sensors can be tuned to detect a specific impurity.

Exciting Lanthanides

For an element to exhibit photoluminescence, it must first become 'excited' by absorbing light energy. However, lanthanide ions are difficult to excite by directly absorbing light. In a molecule, excitation of lanthanide ions is commonly achieved by surrounding them with light-absorbing organic molecules known as 'chromophores'. A chromophore is part of a molecule that readily absorbs light, being present in dyes and in chlorophyll, giving leaves their striking green colour.

Light energy absorbed by the chromophore is transferred to the lanthanide ions in the molecule, which then re-emit light with high efficiency. This is quantified by the photoluminescence 'quantum yield', which describes the efficiency with

which absorbed light is re-emitted from a material – so a high quantum yield is desirable in making chemical sensors.

Metal-Organic Frameworks

Dr Simon Humphrey, Sam Dunning and their colleagues at the University of Texas at Austin focused on developing a stable and tuneable material that would exploit the light-emitting properties of lanthanides for creating chemical sensors. While previous research in the Humphrey lab has investigated the potential of metal-organic frameworks (MOFs) for storing gas and catalysing reactions, the team recently developed a new MOF with potential uses in medical imaging, chemical clean-up and detecting chemicals produced due to radiation exposure, and published their work in the journal *Chem* (*Chem* 2017, DOI: j.chempr.2017.02.010). Composed of a network of metal ions with co-ordinated organic ligands, MOFs are 3-dimensional porous materials made up of organic molecules and metal ions (such as lanthanide ions). MOFs containing lanthanide ions benefit from the high quantum yields of lanthanides to produce a material that can give a large photoluminescence response from a small amount of sample.

Maximising the efficiency of light emission is crucial in creating a chemical sensor that is portable and practical for use in the field, without needing large laboratory equipment off-site. The wider body of research into MOF chemistry has established a number of design principles that enable researchers to have control over the distance between the lanthanide ions in the solid material. This 'tuneability' allows the luminescence properties of the MOF to be optimised for sensing applications.

PCM-22 – a New Chemical Sensor?

While lanthanide-based MOFs have been reported as good chemical sensors for pH, explosives and temperature, many of these sensors are incompatible with a broad range of solvents, or are only stable over a small pH range. In their recent *Chem* paper, Dunning and Dr Humphrey report the synthesis of an MOF material called PCM-22, which is made up of lanthanide ions and a chromophore.

The team discovered that PCM-22, which contains controlled amounts of lanthanide ions, is able to detect trace levels of water in a variety of solvents including ethanol and acetone. These solvents had previously been incompatible with conventional chemical methods of detecting low concentrations of water. So how does their detector work?

When PCM-22 is placed in a solvent, solvent molecules (such as water) move through its pores and bind to it. Then, when UV light is shone on PCM-22, its chromophores absorb energy, which is transferred to the lanthanide ions and the material emits specific colours of visible light. The exact frequency of emitted light depends on the type of solvent molecules that are interacting with PCM-22, as its chemical environment affects its excitation and photoemission energy. In other words, the vibrations of the solvent molecules disturb the lanthanide emissions in a unique way, depending on the solvent-lanthanide combination.

Technology that employs visible light is advantageous as it can be read by the human eye, or using a standard digital camera (even on a mobile phone) in conjunction with appropriate software. The unique signatures of colour and brightness emitted by the team's new material can thus be used to identify and quantify many different chemicals. Once the material has been calibrated against known samples, a catalogue of

fingerprints for different solvents can be created, and easy-to-use ‘dipstick-style’ sensors could be made.

Most significantly, not only can PCM-22 detect low concentrations of normal water (H_2O) in a range of different solvents, but it can also distinguish between normal water and so-called ‘heavy water’ (D_2O), at levels as low as 10 parts per million.

Heavy Water

Heavy water, or deuterium oxide (D_2O), is so-called because of its composition. A typical hydrogen atom (H) has one proton in its atomic nucleus with one electron orbiting around it. A deuterium atom (D) is very similar, containing one proton with one electron, but it also has one neutron in its nucleus. Because protons and neutrons are almost of the same mass (electrons have virtually no mass), deuterium can be thought of as a ‘heavy’ hydrogen atom, being roughly twice the mass of hydrogen, but with the same chemical properties due to its single proton and single electron.

D_2O is simply a molecule of water (H_2O), which contains deuterium atoms in the place of hydrogen atoms. Once mixed together, heavy water is almost indistinguishable from normal water, because of their close chemical and physical properties.

These properties have been used by scientists to our advantage. For example, deuterium-containing solvents are used in nuclear magnetic resonance spectroscopy (NMR), which works in a similar way to hospital MRI scanners. But the similarities can also pose problems: when water comes into contact with sources of radiation, such as radioactive uranium, neutrons can be incorporated into H_2O water molecules, creating D_2O. Because of this, the presence of D_2O can be a sign that water has become contaminated by radioactive waste. But, since D_2O is so chemically similar to normal water, how can we distinguish between them?

The Many Applications of PCM-22

Distinguishing between normal and heavy water normally requires a costly test using a laboratory-based machine. However, because the frequency of light emitted by PCM-22 is dependent on the nature of the interacting solvent molecules, and since the vibrations of H_2O and D_2O molecules are different (due to their different masses), PCM-22 can distinguish between these two types of water.

‘We make the material with europium and terbium ions,’ says Dunning. ‘The europium emission is more readily quenched or “turned off” in the presence of H_2O compared to terbium. Since the vibrations in D_2O are different due to its mass, it isn’t as good at turning off the europium emission, which gives us the yellow emission colour in the presence of D_2O, versus just green for H_2O.’

Dr Humphrey and Dunning’s new class of material could change the way authorities respond to chemical spills or leaks of radioactive waste. In addition, PCM-22 has the potential to streamline some of the processes involved in medical and research imaging that rely on nuclear magnetic resonance (NMR) technology. NMR machines require heavy water to function and to work properly, and this heavy water needs to be very pure. However, heavy water can easily be contaminated with normal water from moisture in the air.

‘When you buy heavy water from a manufacturer it starts out ultrapure,’ says Dr Humphrey. ‘But as soon as you unscrew the bottle, hydrogen atoms from the air start swapping with deuterium atoms. A week later, all of the Hs have become scrambled with the Ds and it effectively ruins the heavy water. It’s an exchange that you can’t stop.’

Dipsticks coated with PCM-22 could provide a cheaper and far quicker way of assessing the purity of heavy water, with the material being sensitive enough to detect H_2O concentrations as low 10 parts per million in a D_2O solution.

With UT Austin’s Office of Technology Commercialization already beginning work to license the team’s technology to companies, it is hoped that PCM-22 sensors will be available in the near future to revolutionise the way we go about identifying different solvents including heavy water, whether it’s to clean up a chemical spill or to optimise MRI scanners.

Meet the researchers

Dr Simon Humphrey
College of Natural Sciences
University of Texas
Austin, TX
USA

Dr Simon Humphrey is an Associate Professor at the University of Texas at Austin. He obtained his PhD at the University of Cambridge in 2005 under the supervision of Paul T. Wood, in the field of magnetic and porous coordination polymer synthesis. Dr Humphrey later worked as a US Department of Energy Postdoctoral Research Associate at the Lawrence Berkeley National Laboratory (2005–2007) in the field of nanoparticle catalysis. After undertaking a Fellowship at St John's College, Cambridge in 2006, he later joined the Faculty at the University of Texas at Austin in 2009. The Humphrey group is engaged in research into porous phosphine-based frameworks as well as the reproducible preparation of noble metal nanoparticles for applications in heterogeneous catalysis.

CONTACT

E: smh@cm.utexas.edu
W: http://humphrey.cm.utexas.edu/wordpress/?page_id=40

Sam Dunning
College of Natural Sciences
University of Texas
Austin, TX
USA

Sam Dunning graduated with a Master's degree from the University of Sheffield in 2014, where he worked with Dr Michael Morris studying nickel bis(dithiolene) complexes. Upon graduating from the University of Sheffield he joined The University of Texas at Austin to undertake his PhD studies. His research in the Humphrey group centres on the synthesis of luminescent phosphine coordination materials (PCMs) for solvent identification and trace water detection. Recently his research has shifted to focus on single-crystal-to-single-crystal metal incorporation in new, pillared PCMs.

CONTACT

E: samdunning@utexas.edu
W: http://humphrey.cm.utexas.edu/wordpress/?page_id=5

FUNDING

University of Texas College of Natural Sciences
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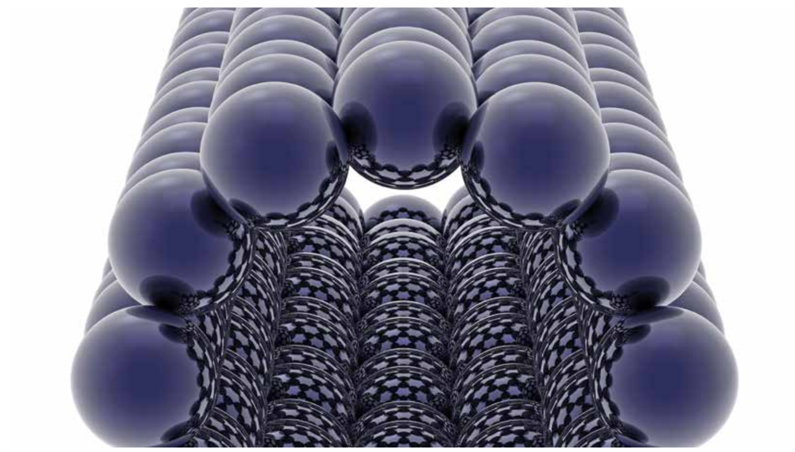
A BRIGHT FAMILY OF QUANTUM DEFECTS

Carbon nanotubes are a remarkable material – more conductive than copper and stronger than steel, yet just a billionth of a metre wide. Their application has already proven invaluable across science and engineering, but only recently have scientists looked into expanding their functionality even further as a unique source of light. **Dr YuHuang Wang** and his research group at the University of Maryland have now synthetically created 'quantum defects' in carbon nanotubes that luminesce brightly in the near infrared. This work has opened up opportunities for experiments in fields ranging from biochemistry to quantum physics.



Exploring the Properties of Carbon Nanotubes

The story of Dr Wang and his team's research may begin with graphene. Itself a fascinating material, graphene consists of single-layers of carbon atoms arranged in a honeycomb structure. When sheets of graphene are conceptually rolled up into cylinders, they create one-dimensional structures that the world of material science has become much indebted to: carbon nanotubes. Depending on the structure in which the carbon atoms are arranged within that cylinder, the resulting nanotube can have a variety of different properties. One particular result of this structural arrangement is the determination of whether the nanotube is a conductor or a semiconductor.

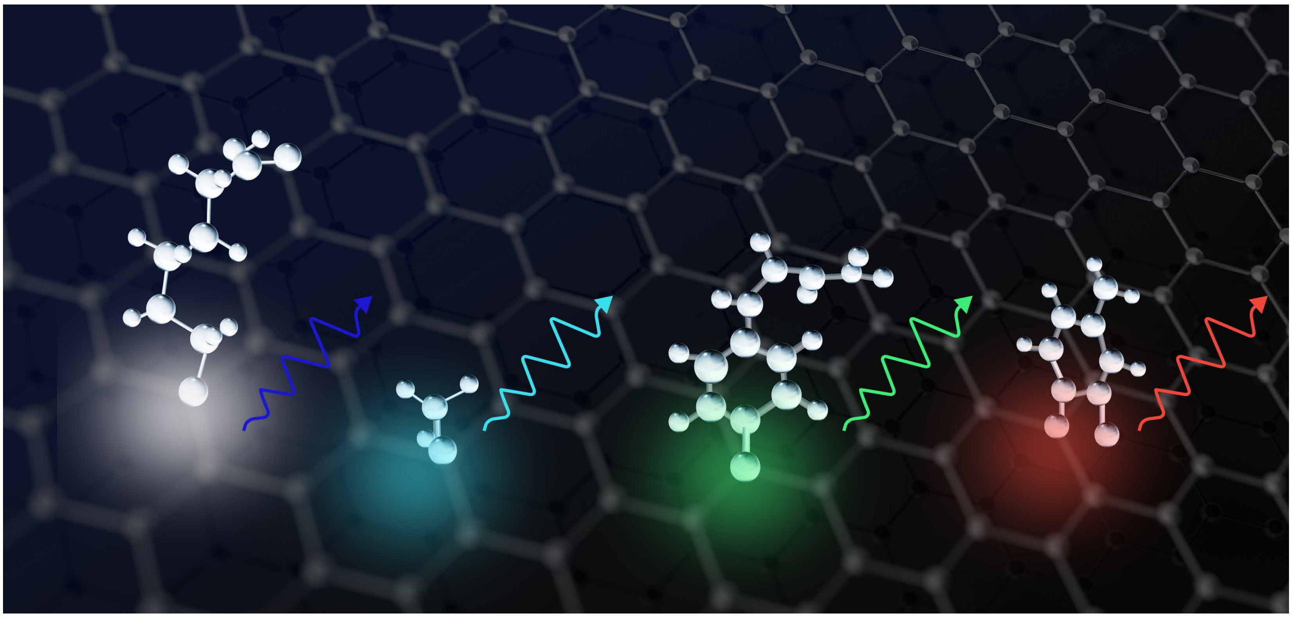
To test this distinction, a scientist can cause a nanotube to absorb a packet of light energy, called a 'photon', which excites an electron in the nanotube to a higher energy level. If the nanotube is a conductor, another electron will immediately come along to fill the place where the excited electron had been. However, in semiconducting nanotubes, the electron will leave behind a 'hole'. The excited electron and this corresponding hole, together known as an 'exciton', can travel down the nanotube as a quasi-particle. Depending on the other properties of the semiconducting nanotube, the excited electron will either recombine with the hole by losing the excess energy as heat (known as a 'dark' state) or by emitting a photon (a 'bright' state).

Introducing Quantum Defects

One problem that Dr Wang and his colleagues initially faced was that dark states occur at lower energy levels than bright states. That means for unmodified carbon nanotubes, dark states occur far more frequently, and that photon emission from excitons is particularly inefficient. However, by attaching groups of molecules to the walls of nanotubes through chemical bonding, bright emissions can be made to occur far more efficiently. These molecular groups create 'quantum defects' that have a lower energy level than the dark states, allowing the excitons to be trapped there and emit light.

'One may picture the semiconductor host as an ocean, whereas the quantum defects create potential wells or islands,' Dr Wang explains. The excitons are channelled to the potential well where the energy of the bright state is driven below that of the dark, allowing emission from the excitons to occur efficiently. 'We found that by pushing the potential well deeper, we can efficiently harvest the so-called dark excitons, which were theoretically predicted but had been

‘As with the islands in a sea, these quantum defects serve as the focus points where interesting new chemistry and physics may occur’



experimentally inaccessible,’ adds Dr Wang. Overall, 28-times more photons could be produced by nanotubes with quantum defects than by regular carbon nanotubes.

After Dr Wang’s initial experiments, this improvement in photon emission, or ‘photoluminescence’, has already introduced a range of useful applications for scientists. Importantly, the nanotubes can be used as pH sensors. Depending on whether the surrounding environment is an acid, which contains an excess of protons, or a base, which is proton-deficient, the molecular structure of certain quantum defects will change in predictable ways. These structural changes subsequently vary the intensity and peak position of the quantum defect’s photoluminescence, depending on the acidity or basicity of the surrounding environment, allowing scientists to accurately measure pH at molecular scales.

The photoluminescence of the quantum defects also changes depending on the temperature of their surroundings, allowing scientists to use the nanotubes as nano-thermometers. These early experiments demonstrate how carbon nanotubes can be modified for use as sensors with high chemical selectivity even in complex biological systems. However, Dr Wang’s team is conducting further, more intricate studies to further improve the practicality of these defect sensors.

Tuning Molecular Defects

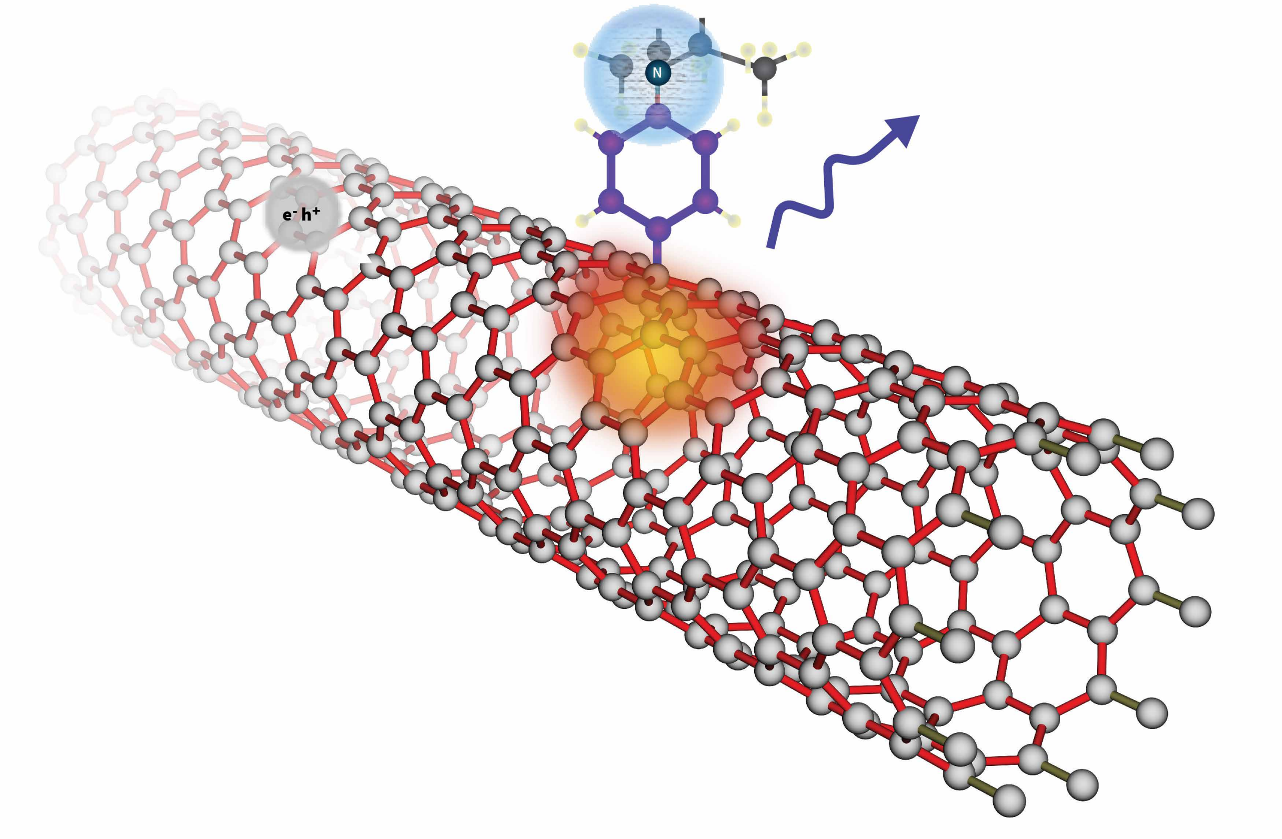
Dr Wang and his colleagues have found that a variety of different defects can be created by chemically bonding molecular groups to the surfaces of semiconducting carbon nanotubes. By precisely monitoring these chemical reactions, the nature of the subsequent photoluminescence can be made to vary widely.

In each of the functionalised nanotubes they have produced, the frequencies (or energies) of the photons emitted by excitons that are trapped by these defects entirely depend upon the unique molecular structure of the defect. This is an incredibly useful result, as it means that scientists can alter carbon nanotubes after they have been synthesised to produce whichever type of photoluminescence that is required.

In other words, Dr Wang’s team has created a ‘tuneable’ quantum emitter – a much desired tool among scientists wishing to control photoluminescence at a molecular scale.

Using Dr Wang’s molecularly-tuneable quantum emitters, a biologist, for example, could use multiple nanotubes to directly image different parts of a complex biological system, or monitor a chemical change that occurs locally. On the other hand, a physicist would be able to produce individual photons of precisely known frequencies for use in quantum physics experiments. As Dr Wang describes, ‘in one direction, we are exploring the use of these organic colour centres as single photon sources for quantum information applications. In another, we are interested in probing chemical reactions at the single molecule level.’

Overall, Dr Wang and his team have produced over 50 distinct quantum emitters with the same nanotube host structure, giving scientists a wide range of distinct, tuneable types of photoluminescence to choose from.



Precision Molecular Engineering

In their most recent studies, Dr Wang and his colleagues worked towards improving the efficiency and precision with which photon-emitting carbon nanotubes can be synthesised. In previous studies, extreme conditions were required for defects to bond to the nanotubes. However, Dr Wang's team discovered that the process could be made far more efficient, which would be important for scientists wishing to synthesise tuneable nanotubes in their own labs.

To do this, the team exploited the effect of 'resonance' on their carbon nanotubes. As with many physical systems, from bridges to individual atoms, carbon nanotubes have a natural frequency at which they vibrate. When driven by an external force featuring the same frequency, the amplitude of the vibrations will greatly increase – an effect known as resonance.

For carbon nanotubes, this resonant frequency is on the same scale as the frequencies of visible light. When driven to resonance by a visible light photon (a process called 'optical resonance'), electrons in the carbon nanotube become excited, which may heat the material through a process known as the 'photothermal effect'. Under these conditions, molecular defects can chemically bond to nanotube surfaces around 154 times faster than without light. Under such controlled conditions, scientists can engineer quantum defects into their nanotubes far more precisely and efficiently.

Dr Wang and his colleagues also use optical resonance to selectively choose carbon nanotubes with particular structures to incorporate the molecular defects. As discussed earlier, carbon nanotubes can have a wide variety of arrangements of carbon atoms composing their surfaces. The distinct structure of each nanotube is described by a symmetry property known as their 'chirality'. Nanotubes with different chiralities will exhibit slightly different properties – and among these is their optical resonance.

With this in mind, Dr Wang's team subjected a mixture of carbon nanotubes made of two different chiralities to a single frequency of visible light and reacted them with a particular molecular group to create a quantum defect. Since this light only causes the nanotubes of one chirality to optically resonate, only they react with the molecules to form photoluminescent defects, while the nanotubes of the other chirality were excluded from the reaction. This result reveals a wide range of potential applications in nanoscale engineering, including the ability to 'write' such fluorescent features in carbon nanotubes on a molecular scale.

Dr Wang is optimistic that their work will have an impact on the world of nanotechnology. 'Quantum defects may open up an entirely new dimension to materials engineering, to chemically probe trapped excitons, and to harvest the energy of dark excitons as light,' he believes. 'Our work has triggered many exciting advances which are opening new research fronts in nanochemistry, photophysics, quantum theory, materials engineering, optoelectronics, and biological imaging.'

Meet the researcher

Dr YuHuang Wang
Department of Chemistry and Biochemistry
University of Maryland
College Park, MD
USA

Dr YuHuang Wang completed his PhD in chemistry at Rice University in 2005. He was one of the last graduate students of the Nobel Prize winning chemist Richard E. Smalley, who he had first read about while growing up in rural China. Dr Wang has since brought about a range of important developments in nanotechnology, including 'cloning' of carbon nanotubes and helping to create the first conductive rival of Kevlar. Dr Wang has been working at the University of Maryland since 2008, where he became Professor of the Department of Chemistry and Biochemistry in 2017. He is a world leader in his field through his work with quantum defects in carbon nanotubes, and was awarded the NSF CAREER Award in Chemistry for 2011–2016.

CONTACT

E: yhw@umd.edu
T: (+1) 301 405 3368
W: www2.chem.umd.edu/groups/wang/

KEY COLLABORATORS

Lyndsey Rae Powell, University of Maryland
Mijin Kim, University of Maryland
Hyejin Kwon, University of Maryland
Yanmei Piao, University of Maryland
George C Schatz, Northwestern University
Stephen Doorn, Los Alamos National Laboratory
Daniel Heller, Memorial Sloan Kettering Cancer Center
Ming Zheng, National Institute of Standards and Technology

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UNIVERSITY OF MARYLAND

NEGATIVE ION FORMATION IN COMPLEX HEAVY SYSTEMS

When an electron is absorbed by a heavy atom or molecule, a heavy, negatively-charged ion is formed. These negative ions can be used for a wide array of useful applications, from organic solar cells to water purification. However, the electron absorption process for heavy particles is a complex many-body process, making it difficult for physicists to understand how the ions form. **Dr Alfred Msezane** at Clark Atlanta University has developed a robust mathematical theory to gain a fundamental understanding of negative ion formation in such heavy systems for the first time.

Among the most famous recently-discovered heavy molecules are fullerenes – complex arrangements of carbon atoms that form hollow, ball-shaped structures. Perhaps the most well-known fullerene molecule is C_{60}, or 'buckminsterfullerene'. This almost perfectly spherical molecule of 60 carbon atoms has proved remarkably useful in a variety of fields, particularly nanotechnology. Many other varieties of fullerene have also been fabricated. These molecules contain widely varying numbers of carbon atoms, often with more complex, less spherical shapes than C_{60}.

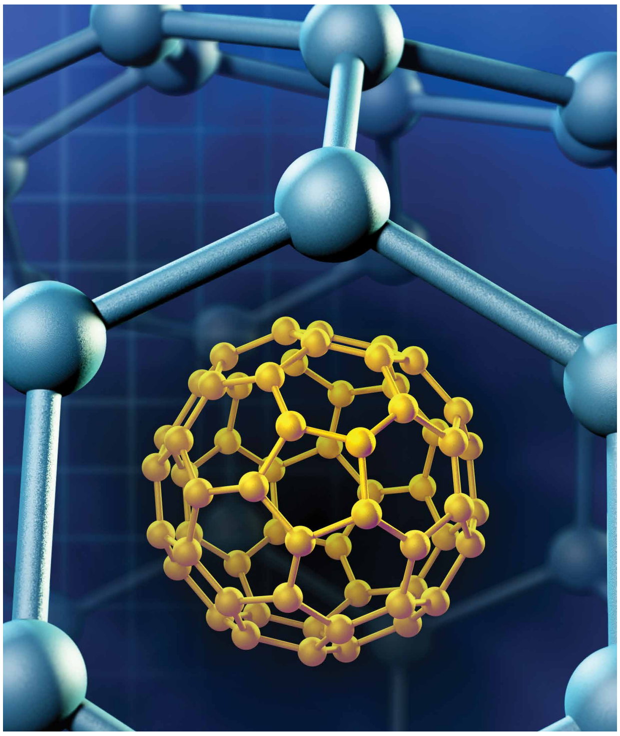
Another newly-explored area of chemistry involves lanthanide and actinide atoms. Occupying the bottom rows of the periodic table, these elements contain large numbers of protons and neutrons in their nuclei, making them some of the heaviest and most complex atoms ever discovered.

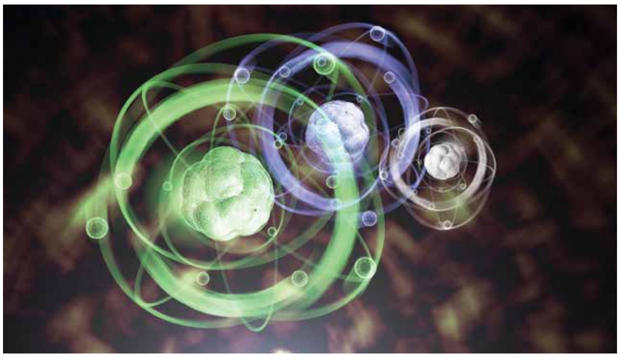
Chemical reactions involving such heavy atoms and fullerenes have become a widely studied area in modern chemistry and chemical physics. Until very recently, the interactions of both types of systems with other particles, particularly electrons, have been notoriously difficult to understand, largely due to the complexity of the processes involved. In discovering how these interactions can take place, scientists hope to unlock new, useful properties of heavy atoms and fullerenes for use in experiments and wider applications.

Recently, scientists have begun to carefully explore how low-energy electrons can be made to collide with fullerenes and heavy atoms to form large, negatively-charged ions. An understanding of this process would give researchers a greater knowledge of how chemical reactions involving these heavy systems take place. This insight would benefit developments in applications including the production of materials for creating efficient organic solar cells and methods to efficiently transport medicine throughout the human body.

For Dr Alfred Msezane and his team at Clark Atlanta University, perhaps the single most important application is the development of methods for inexpensive water purification. Heavy negative ions can act as catalysts in a reaction that transforms water into hydrogen peroxide – an important chemical in the purification process. The ability to produce heavy negative ions inexpensively would make it significantly easier for people in the developing world to source drinkable water, helping to prevent disease.

However, the electron absorption process is much harder to understand when larger complex atoms and molecules are involved. Because of their large size, these systems are already home to large numbers of electrons, which interact with each other through a variety of mechanisms. These interactions are remarkably complex, making it incredibly difficult for scientists to predict what exactly will happen when another electron is introduced into the system. Through both theory and experiment, Dr Msezane and his team are working towards gaining a fundamental understanding of the mechanisms underlying the formation of heavy, negatively-charged ions for the first time.





A Robust Mathematical Framework

One of the most challenging problems in atomic and molecular physics when exploring negative ion formation in heavy complex atoms and fullerene molecules is determining accurate and reliable values for the 'electron affinity' of the atoms and molecules involved. This term describes a fundamentally important quantity in atomic and molecular physics: the amount of energy released when an extra electron is added to an isolated gaseous atom or molecule, turning it into a negatively-charged ion.

However, as Dr Msezane describes, the complexity of heavy atoms and molecules has meant that accurate and reliable values for the electron affinity have long eluded researchers in the past. 'Indeed, the published literature abounds in incorrect electron affinities for the lanthanide and actinide atoms,' he says. 'Also, theoretical electron affinities for the fullerenes are available for only the near-spherical fullerenes. Calculating their electron affinities using conventional theoretical methods is a formidable task due to the presence of the large and diverse intricate configurations.'

In his research, Dr Msezane acknowledges the pressing need to obtain robust, accurate and reliable values for the electron affinities of heavy systems. Ultimately, these values are key to understanding how the interactions that transform heavy particles into negatively-charged ions work. Without a fundamental understanding of the physics at play in the determination of reliable electron affinities, producing heavy negative ions is not particularly feasible, making applications from organic solar cell production to water purification incredibly difficult.

To obtain more robust electron affinity values, Dr Msezane and his colleagues have adapted existing mathematical theory to reliably predict the interactions of low-energy electrons with heavy complex systems. 'The crucial electron-electron correlations and the vital core polarisation interactions are embedded in our novel and robust "Regge pole" methodology,' he explains. 'This allows us to gain a fundamental theoretical understanding of the mechanism underlying negative ion formation in low-energy electron collisions with complex heavy atoms and fullerene molecules, leading to the formation of stable negative ions.' Consequently, reliable electron affinity values can be extracted.

Essentially, the Regge pole methodology Dr Msezane describes is composed of a set of equations that model the behaviours of large systems of electrons, each of which has its own influence over the properties of the system as a whole. Importantly, the model describes what happens to an incident, low-energy electron as it collides with the larger system.

As the incident electron approaches the system, it initially travels in a straight path. However, the repulsive forces between the incident electron and the system cause the electron to deviate, or 'scatter' from its original path – potentially becoming trapped by the system. The Regge pole methodology describes how the angle of this scattering will vary, depending on a quantum property of the electron known as its complex angular momentum and its energy. This scattering and the interactions between electrons in the system give rise to two fundamentally important quantities, both of which are vital to exploring the mechanism involved in negative ion formation.

Total Cross-Sections & Binding Energies

The first of these quantities is named the electron elastic scattering 'total cross-section'. The term describes a quantum mechanical cross-sectional area surrounding an electron system which, if entered by an incident electron, will scatter the electron to some degree. Calculations of the total cross-section reveal the second fundamental quantity, known as the negative ion 'binding energy'. This value represents the minimum energy required to form a stable negative ion of the system, namely the incident electron attached to the complex heavy atom or the fullerene molecule.

Together, the two quantities form the basis of Dr Msezane's objective to obtain the accurate and reliable electron affinity values. 'We have extracted reliable ground state binding energies of formed negative ions from our calculated electron elastic scattering total cross-sections for the fullerenes that matched excellently the measured electron affinities; this is a theoretical feat that has never been achieved before,' he says. 'And these calculated ground state negative ion binding energies correspond to the electron affinities of the heavy atoms and the fullerene molecules.'

A strong motivation for extracting theoretical electron affinity values using the Regge pole methodology in this way is that Regge poles are generalised bound states; therefore, they rigorously determine negative ions binding energies. Thus, calculated binding energies of the negative ions formed during the collisions correspond to the electron affinities of the systems, leading to a direct comparison with experimentally measured electron affinities. Where previous measurements of electron affinities suffered due to the complexity of heavy atoms and fullerene molecules, resulting in long-standing unreliability of published values, Dr Msezane's research offers the first concise method to test and guide both measurements and other theoretical calculations of this quantity. 'Indeed, the Regge pole methodology requires no assistance from experiment or other theory to achieve the remarkable results for the heavy atoms and fullerene molecules,' he states.

Patterns of Resonances in Negative Ion Formation

Dr Msezane's current focus is to directly measure experimentally the quantities his team has explored theoretically, by observing the characteristic oscillatory patterns, or 'resonance structures' in the electron scattering total cross-sections that characterise negative ion formation in low-energy electron collisions with heavy systems. These resonance structures, which yield the important negative ion binding energies, allow for a far more comprehensive examination of negative ion formation than previous studies have achieved.

'Our immediate objective is to identify and delineate the resonance structures in the electron elastic total cross-sections for the considered systems and determine negative ion binding energies,' says Dr Msezane. One particularly important feature of these resonance structures is the range of energies over which their oscillations will occur – a quantity that characterises the formation of each different heavy negative ion.

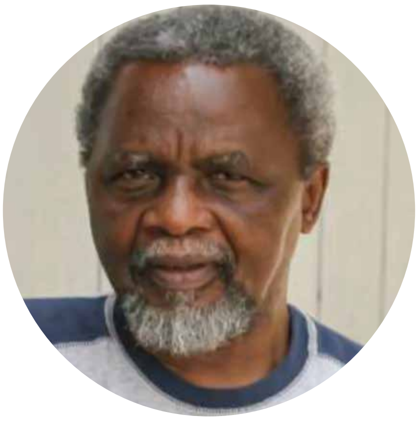
In recent studies, Dr Msezane and his colleagues found that resonance structures in the total cross-sections of heavy systems generally occur over extremely narrow ranges in energy, giving rise to dramatically sharp resonance peaks. Mathematical analysis of the shape and size of these peaks has ultimately allowed the researchers to accurately extract definitive electron affinities of both fullerene molecules and heavy atoms for the first time.

Already, the available experimental values for electron affinity for the fullerene molecules agree remarkably with the values that Dr Msezane has calculated through his theoretical Regge pole methodology. 'Indeed, the methodology requires no assistance whatsoever from either experiment or other theory to achieve the unprecedented feat,' he says. His team's future work now promises significant advances in our ability to understand and fabricate negatively-charged ions from heavy systems, allowing for a diverse range of applications.

Improving Understanding & Solving Societal Issues

Dr Msezane's research has brought about important advances in the field of atomic and molecular physics. This increased level of understanding could open up many new avenues for research in fields encompassed by both physics and chemistry. However, the advantages of producing heavy, negatively-charged ions stretch far beyond academic advances alone. 'Understanding chemical reactions involving negative ions also has importance and utility in terrestrial and stellar atmospheres, organic solar cells, drug delivery, device fabrication and nanocatalysis,' Dr Msezane says. 'Our findings also allow for multi-functionalisation of heavy negative ions including in catalysis for inexpensive water purification in developing countries as well as in the oxidation of methane to methanol without carbon dioxide emission.'

With further studies into these areas, Dr Msezane's research could soon provide solutions to some of the most pressing issues in global society, from poverty and disease to climate change.



Meet the researcher

Dr Alfred Msezane
Department of Physics
Clark Atlanta University
Atlanta, GA
USA

Dr Alfred Msezane is a Professor of Physics and the Founding Director of the Centre for Theoretical Studies of Physical Systems at Clark Atlanta University. In a career spanning five decades, beginning in his native country of South Africa, he has published almost 400 research papers and supported scores of graduate and undergraduate students through his mentoring. Among many prestigious honours, including Fellow of the Royal Society of Chemistry, Institute of Physics, American Physical Society and American Association for the Advancement of Science, he is an appointed Member of Europe-Africa Foundation for Science & Technology, as well as a member of the Advisory Commission of the UNESCO-UNISA Africa Chair in Nanosciences and Nanotechnology. Dr Msezane's primary research interests, among his extensive research, involve gaining a fundamental understanding of the electron attachment mechanism in heavy and complex atoms and fullerenes, leading to stable negative ion formation.

CONTACT

E: amsezane@cau.edu

KEY COLLABORATORS

Dr Zineb Felfli, Clark Atlanta University

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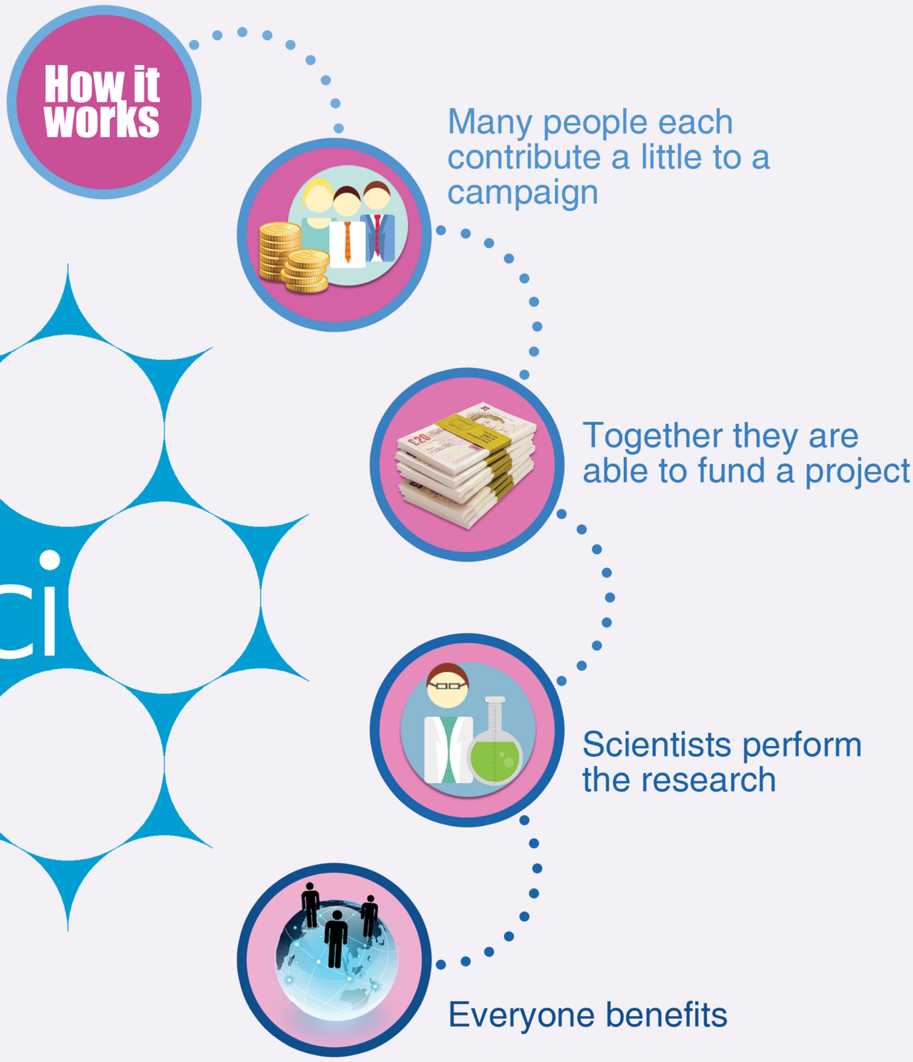

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