

chemistry

March 2018

in Australia

Very cool: cryo-EM and the chemistry Nobel laureates

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- Analytical chemistry goes outback
- What do scientific instruments find inside musical ones?
- Collaborations between countries of the Federation of Asian Chemical Societies

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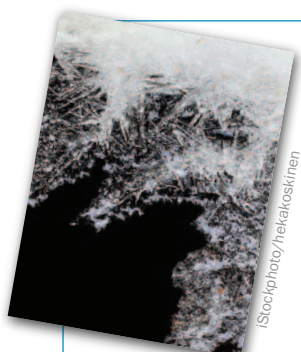
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cover story

A cool visualisation breakthrough: the 2017 Nobel Prize in Chemistry. Part 2

Last year's three Nobel laureates in chemistry each had unique approaches and contributions to their prize-winning work.

22 Desert tales from a wandering analytical chemist

Picture a large Brahman cow, on a scorching day in remote Central Australia, blocking the road and looking decidedly menacing. The ute driver at the scene, Alf Larcher, explains that it's all part of the job.

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Researchers at the Fraunhofer Institute for Integrated Circuits are examining musical instruments using scientific ones.

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From the President

I am writing this in late December 2017. As part of our most recent Board meeting and Assembly meeting, we held the annual RACI Awards night. This is one of the important meetings for our Institute and highlights the great chemistry contributions by our members. I congratulate all the award winners for 2017 (see p. 30), and would urge all members to look out for potential awardees in 2018.

At our Board meeting and Assembly in late November, it was essentially agreed that the success of the RACI National Congress celebrating the RACI Centenary meant that these congresses would continue to be held every five years. The next one has been proposed for 2022, then every five years thereafter. This timing fits well with the Pacificchem conferences held every five years ending in 0 or 5, and allows for a couple of Divisional meetings in between for more devoted and focused conferences.

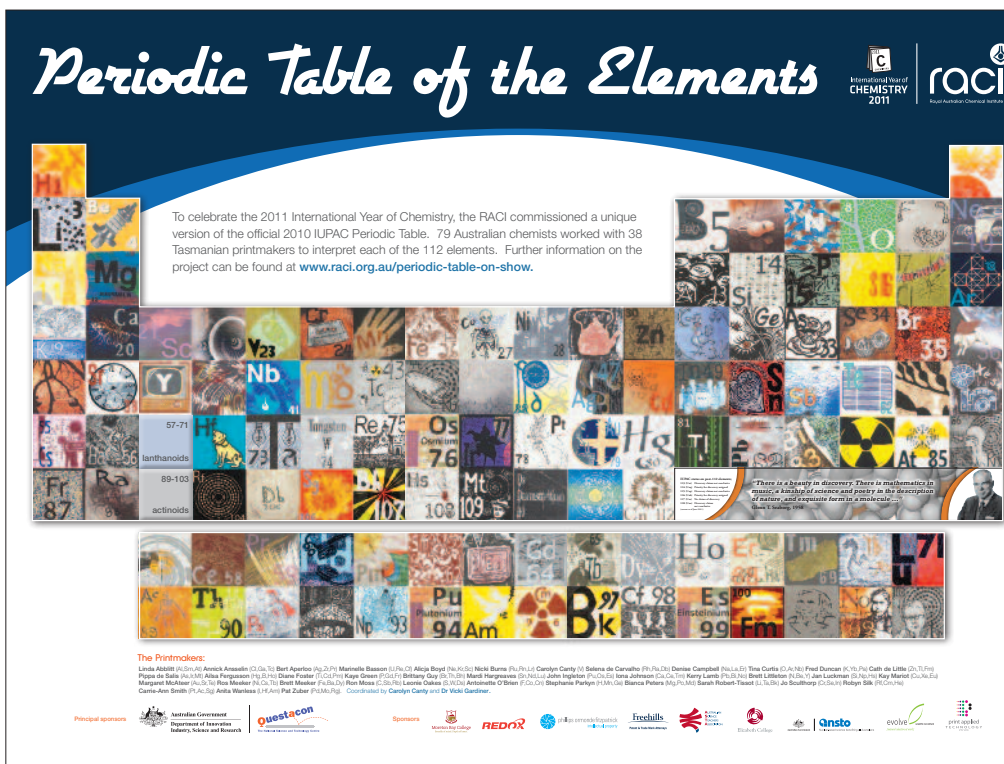
In keeping with a range of chemistry celebrations in recent years, including the International Year of Chemistry in 2011 (recognised by the United Nations) and our RACI Centenary in 2017, it was recently announced that 2019 will celebrate the International Year of the Periodic Table of the Chemical Elements. This proposal was supported by UNESCO and will celebrate the 150th anniversary of the establishment of the periodic table by Dmitri Mendeleev. The periodic table is probably seen as an emblem of chemistry by almost everyone worldwide and is one of the most astonishing and significant achievements in science. It is almost taken for granted these days that elements abide by periodic trends and enable a somewhat predictability about chemical behaviour. When I think about the construction and development of the table of elements, it still astounds me that someone in 1869 could build

up a chart from the approximately 90 elements at hand that could predict missing elements and their properties. The periodic table of the chemical elements is not just a great scientific discovery; it is a thing of beauty. 2019 should be another great year of celebration for this remarkable achievement.

As I enter my second year as President of the RACI, I look forward to working with all members to strengthen chemistry in Australia. If you have any issues that you would like to bring to my (and the Board's) attention, then please feel free to contact us. The RACI can only grow with support and ideas from its members, and that is why we exist ... for the members.



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Isaac Newton drawings discovered

A drawing thought to have been scratched by a young Isaac Newton into the walls of his childhood home has been discovered at the National Trust's Woolsthorpe Manor in Lincolnshire, UK.

As part of a series of scientific investigations into the home of Britain's most famous scientist, conservators using cutting-edge light technology have discovered a picture of a windmill next to the fireplace in the 17th-century manor's downstairs hall. The drawing is thought to have been inspired by the building of a mill nearby during Newton's childhood.

The discovery adds a new layer of understanding to Newton's life at Woolsthorpe, where he was born into a yeoman farming family in 1642, and where he returned in 1665 at the peak of his scientific studies. It was here that Newton undertook his 'crucial experiment' – splitting white light using a prism – and observed an apple fall from a tree, inspiring his law of universal gravitation.

Using reflectance transformation imaging (RTI), a technique that uses light to capture the shape and colour of a surface not visible to the naked eye, conservator Chris Pickup from Nottingham Trent University was able to survey the walls of the manor in painstaking detail to discover this previously unseen wall drawing, believed to have been carved into the wall around 350 years ago.

Chris Pickup said: 'It's amazing to be using light, which Newton understood better than anyone before him, to discover more about his time at Woolsthorpe. I hope that by using this technique

we're able to find out more about Newton as man and boy and shine a light on how his extraordinary mind worked.'

Newton was well known for sketching and making notes on the walls of his rooms as he developed his scientific and mechanical knowledge. Several sketches, thought to be his, had previously been uncovered by tenants removing old wallpaper in the 1920s and 30s.

William Stukeley, a friend of Newton and his biographer wrote that: 'the walls, & ceilings were full of drawings, which he had made with charcole. There were birds, beasts, men, ships, plants, mathematical figures, circles, & triangles.'

The conservation charity will continue its investigations in 2018, using thermal imaging to sense tiny differences in the thickness of plaster and paint that have covered the walls since Newton's death, which they hope could reveal more

sketches left by the young genius.

Jim Grevatte, Illuminating Newton Programme Manager at Woolsthorpe Manor, said: 'The young Newton was fascinated by mechanical objects and the forces that made them work. Paper was expensive, and the walls of the house would have been repainted regularly, so using them as a sketchpad as he explored the world around him would have made sense.

'This discovery could be just the tip of the iceberg in terms of the drawings waiting to be uncovered, and it's fitting that we're using cutting edge science inspired by Newton's work to reveal more about his childhood and his thinking.'

Find out more and view an interactive image of the graffiti at www.nationaltrust.org.uk/woolsthorpe-manor.

National Trust



Woolsthorpe Manor – the birthplace of Sir Isaac Newton.

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Botanical Resources Australia joins Sumitomo Chemical Group



Botanical Resources Australia

The Botanical Resources Australia (BRA) group of companies has become subsidiaries of Sumitomo Chemical Co., Ltd. of Japan. The acquisition of shares was unanimously endorsed by the BRA Board of Directors late last year.

Pyrethrins are insecticidal compounds extracted from the pyrethrum flower (pictured), which have the same basic chemical structure as synthetic pyrethroids. They are widely and commonly used in insecticides for household, vector control, pest control management and crop protection.

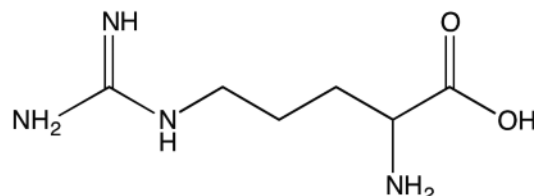
Since its establishment in 1996, the BRA Group has been producing pyrethrins in Tasmania. The Sumitomo Chemical Group has also been engaging in the production and sales of pyrethrins and is aiming to apply know-how of the BRA Group across its group. Sumitomo considers that this acquisition will enable the company to form a more stable supply system for pyrethrins by utilising production bases for pyrethrum subject to different climate conditions.

Commenting on the sale, the Founder of BRA, Ian Folder, stated: 'Sumitomo Chemical's vision and continued investment in their insect control solutions will prove a major boon to BRA, our people, our growers, our customers, and the Tasmanian economy. I am extremely proud of what we at BRA have developed – we are one of the major producers of pyrethrins and foresee tremendous upside for BRA's ongoing business.'

Commenting on the acquisition of BRA, Mr Ray Nishimoto, Representative Director & Senior Managing Executive Officer, President of Health & Crop Sciences Sector said: 'We have already had a longstanding strategic relationship with BRA, and this acquisition will provide further significant value to Sumitomo Chemical through BRA's advanced plant-breeding program, agricultural know-how, and proprietary manufacturing expertise, which will enhance our strategic position in the insect control business both in environmental health and crop protection uses.'

Botanical Resources Australia and Sumitomo Chemical

Highly charged molecules behave paradoxically



According to the Lund study, cell-penetrating peptides rich in arginine (pictured) are 'promising candidates for intracellular drug delivery'.

Chemistry researchers have determined how certain small biomolecules attach to one another. The researchers' study also overturns the standard picture – particles with the same electrical charge appear to be drawn together and not vice versa. The results may be important for the development of new drugs.

A number of chemistry researchers from several institutions including Lund University in Sweden, have managed to identify a new mechanism that makes certain charged biomolecules attach to each other (doi: 10.1073/pnas.1712078114). The biomolecules in the present study serve as models for antibacterial peptides; that is, protein-like molecules that fulfil important functions in the body.

'Antibacterial peptides are important for our immune system. If we can figure out how they work, it may be of value in the development of new drugs', said Mikael Lund, chemistry researcher at Lund University.

The present study combines theoretical computer models with experiments. The researchers were very surprised when the data indicated that the small biomolecules were drawn to each other even though they had the same electrical charge. Nevertheless, the results were later confirmed by experiments.

'We were very surprised. These biomolecules have a high electrical charge, and the expectation was therefore that this would make them push each other away', said Lund.

Instead, the biomolecules in this study demonstrated apparently paradoxical behaviour. And the explanation for this lies at the atomic level. More specifically, it is about how certain atoms bind together at the ends of the molecular chain. The researchers' study can be described as atomic level detective work, which involves mapping the exact structure of all the atoms of the molecule.

The knowledge of how these biomolecules assemble themselves, and how their electrical charge works, is valuable in drug development contexts. The type of biomolecule concerned in this study is considered to be a promising candidate for transporting drugs into the cells of patients, as the biomolecule has the ability to penetrate the cell casing. However, it is not yet entirely known how the biomolecule gets into the cells.

Lund University

Secrets of chemical communication between algae and bacteria



Doctoral candidate Prasad Aiyar examines the microalgae *Chlamydomonas reinhardtii*. Jan-Peter Kasper

If green algae of the species *Chlamydomonas reinhardtii* meet *Pseudomonas protegens* bacteria, their fate is sealed. The bacteria, measuring only some two micrometres, surround the algae, which are around five times larger, and attack them with a deadly toxic cocktail. The algae lose their flagella, which renders them immobile. The green single-celled organisms then become deformed and are no longer able to proliferate. The chemical mechanism underlying this extremely effective attack has now been uncovered by botanists and natural product chemists at Friedrich Schiller University, Jena (FSU) and the Leibniz Institute for Natural Product Research and Infection Biology – Hans Knöll Institute (HKI), Germany.

It is a gruesome spectacle that meets the eyes of Prasad Aiyar as he looks down the microscope. The doctoral candidate from India, examines the species *Chlamydomonas reinhardtii* on a microscope slide. The oval-shaped microalgae, a good 10 micrometres in size, have two flagella with which they busily swim around – that is, until Aiyar uses a pipette to add a drop of a bacterial solution. The even smaller bacteria gather together into swarms, which surround the algae. Just 90 seconds later, the algae are motionless and when one looks more closely, one can see that their flagella have fallen off.

The Jena researchers have discovered why these bacteria have such a devastating effect on the green algae. It seems that a chemical substance plays a central role in the process, as the teams under Professor Maria Mittag and Dr Severin Sasso, FSU, and Professor Christian Hertweck, HKI, report in *Nature Communications* (doi: 10.1038/s41467-017-01547-8).

Orfamide A is a cyclical lipopeptide that the bacteria release, together with other chemical compounds. 'Our results indicate that orfamide A affects channels in the cell membrane, which leads to these channels opening', explained Sasso. 'This leads to an influx of calcium ions from the environment into the cell interior of the algae.' A rapid change in the concentration of calcium ions is a common alarm signal for many cell types, which regulates a large number of metabolic pathways.

'To be able to observe the change in the level of calcium in the cell, we introduced the gene for a photoprotein into the green algae, which causes bioluminescence if the calcium level increases. This enables us to measure the amount of calcium with the help of the luminescence', explained Mittag.

In some cases, the changes in the calcium led to changes in the direction of movement, for example after light perception. In other cases, for example after the bacterial attack, they caused the loss of the flagella.

In addition, the teams were able to show that the bacteria can tap the algae and use them as a nutrient source if they are lacking in nutrients. 'We have evidence that other substances from the toxic cocktail released by the bacteria also play a role in this', said Mittag. Her team, in cooperation with the teams of Hertweck and Sasso, now also wants to track down these substances, in order to gain a precise understanding of this chemical communication between algae and bacteria.

Numerous research groups have dedicated their efforts to studying the 'chemical language' between microorganisms and their environment as part of the Collaborative Research Centre, ChemBioSys. Microbial species communities occur in virtually every habitat on Earth. 'In these communities, both the species composition and the interrelations between individual organisms of one or more species are regulated by chemical mediators', said Hertweck.

The aim of the interdisciplinary research partnership is to explain the fundamental control mechanisms in complex biosystems, which affect all life on Earth. 'We want to understand the mechanisms through which the microbial community structures are formed and their diversity maintained.' They are important, because essentials of life – not least for human beings – depend on them, for example food or air.

This is also true of microalgae such as *Chlamydomonas reinhardtii*. Such photosynthetic microorganisms (phytoplankton) make a contribution of about 50% towards fixing the greenhouse gas carbon dioxide and, as a by-product of photosynthesis, they supply the oxygen that is essential for our survival. In addition, microalgae, which are found in fresh water, wet soils or seas and oceans, represent an important base for food chains, especially in aquatic systems. For example, zooplankton in the oceans feed on the algae and together they provide food for crustaceans, which in turn are eaten by fish, before these are eaten by bigger fish or caught by humans. 'In view of the huge significance of microalgae for human life, we still know astonishingly little about the fundamental elements and the interactions in their microscopic world', said Mittag.

Friedrich Schiller University Jena



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Call for nanosafety standards body

Academics at the University of Sydney have called for the establishment of a national standards body to monitor the safety of nanomaterials commonly found in food, house paint, supplements and cosmetics sold in Australia.

Some of these products, such as colloidal silver and titanium dioxide, are restricted or under review in the European Union but freely available in the Australian market. Nanomaterials are engineered particles smaller than 100 nanometres in size – about a thousand times smaller than the width of a human hair.

Associate Professor Wojciech Chrzanowski from the Faculty of Pharmacy and Sydney Nano said: 'Human bodies are well evolved to deal with most nanoparticles if our cells are healthy. What we don't fully understand is what impact they have on cells that are under stress or in people with suppressed immune systems, such as chemotherapy patients or people living with HIV.'

Chrzanowski is an adviser on nanosafety to the World Health Organization. He said that the revolution in nanotechnology has been overwhelmingly positive for human health, particularly in improved drug delivery. However, the science is developing faster than our regulatory oversight.

'There are new nanoparticles being synthesised every day and the truth is we don't know exactly what impact they can have on human health', Chrzanowski said.

'We are calling for the establishment of Nanosafety Australia to work with existing regulatory bodies to ensure that we fully understand any risks we face from introducing nanomaterials into our diet and environment.'

Dr Laurence Macia, an immunologist at the University of Sydney's School of Medical Sciences, is looking at the impact of the nanomaterial titanium dioxide on gut microbia and how this can affect the human immune system.

Macia said: 'Titanium dioxide is found in toothpaste, icing and in coatings for chewing gum and other sweets, such as Mentos. It's even a recommended additive in at least one recipe on the MasterChef website.'

'There is a debate in the EU about this already. France and Germany have removed some products that contain nanomaterials, such as titanium dioxide, and it is a requirement products are labelled to show they have nanomaterials, but there isn't even a discussion in Australia.'

Professor Susan Pond, director of the University of Sydney Nano Institute, said: 'Nanotechnology is delivering profoundly positive changes for health and medicine, including new ways to diagnose diseases early. Nanotechnology is also allowing us to deliver medicines precisely to target cells and to produce implantable medical devices for a wide range of clinical indications, including heart disease, hearing loss, intractable wounds and arthritis.'

'However, we must also ensure we fully understand the impacts new technology has on society. That is the essential mission of Sydney Nano: to discover, develop and harness nanotechnology for the benefit of humanity.'

University of Sydney

Milestone gallery redevelopment to nurture STEM skills in 0–5 year olds

Ground Up: Building Big Ideas, Together – a screen-free space where future innovators can develop foundational science, engineering and coding skills – is now open.

Part of a \$6 million milestone gallery redevelopment at Scienceworks, Victoria, Ground Up is a new permanent exhibition created to immerse children in an imaginative world of sensory discovery and construction-play and ignite engagement with science, technology, engineering and maths (STEM).

Building on the early childhood ‘learn through play’ standard set by the Pauline Gandel Children’s Gallery at Melbourne Museum, it is part of a suite of new experiences being developed at Scienceworks. Each is aimed at engaging and preparing the next generation for a future in which an increasing number of jobs will rely on STEM skills of problem solving, hypothesising, experimenting and investigating.

Research shows girls as young as four already have a gender bias in thinking about future careers, with girls less likely to want to aspire to science and technology-based careers. So while the exhibition welcomes both boys and girls, a key part of its development was trying to combat this trend and ensure that the space made science accessible to girls.

To combat this, Ground Up has placed emphasis on collaboration, used gender-neutral colours and has a female ambassador Dot – who will pop up throughout the space.

Lynley Marshall, CEO, Museums Victoria, said Ground Up is a cutting-edge fusion of early learning education and design: ‘Ground Up: Building Big Ideas, Together is the first of a suite of new initiatives at Scienceworks aimed at igniting a passion for science, technology, engineering and maths in young Victorians. Children are innate problem solvers, so we’re thrilled to be opening a space that will encourage and build foundational STEM skills from such an early age.’

So what will children experience in the new gallery?

Upon entry, young children and adults will encounter a space that is entirely screen-free. In a world where more and more ‘technology’ means ‘digital’, this space will allow children to build foundational skills in engineering and coding using simple machines and real materials, rather than devices or touch screens.

They will be greeted by a seven-metre tall Kinetic Sculpture that introduces the concept of working machines.

By testing and tinkering, this is a space with open-ended and instruction-free experiences that encourage the development of problem-solving skills (not rote learning), emphasising that there is no one ‘right’ way of doing something.

Ground Up is divided into three broad age and activity zones, each of which develop skills and provide experiences designed for targeted stages of development.



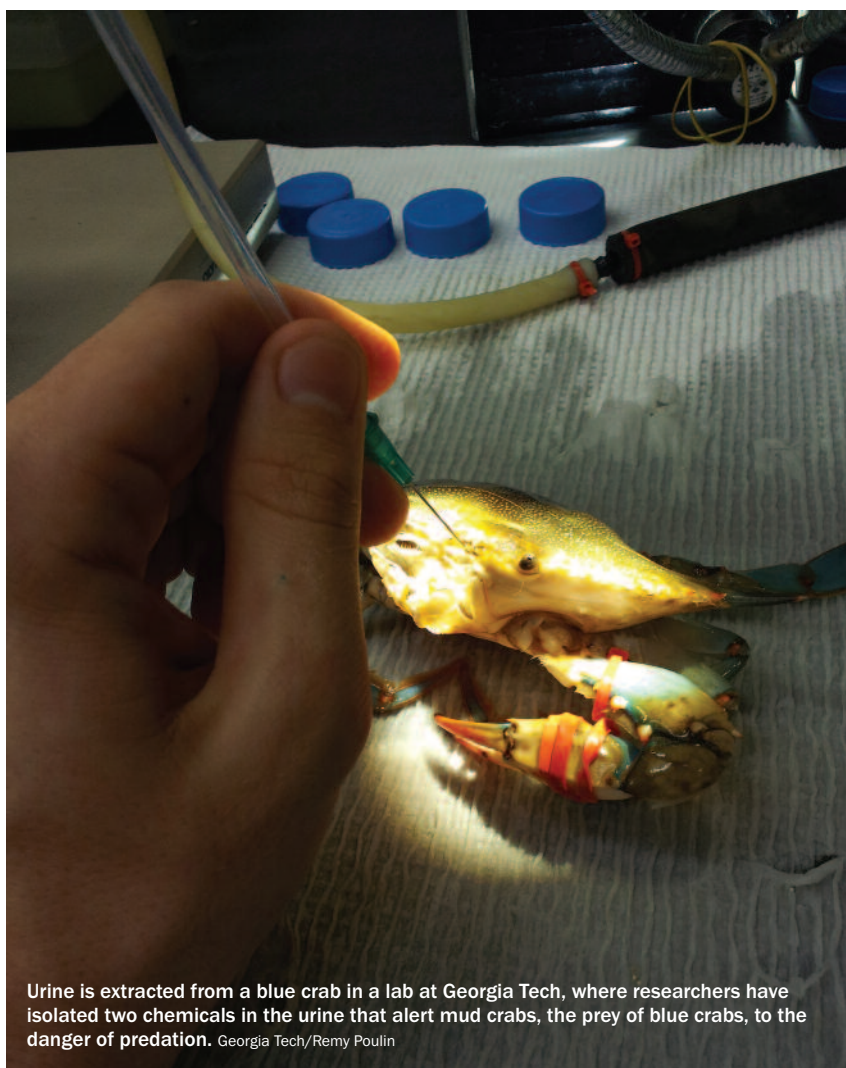
- Baby Landscape: enclosed with a rolling mount to create a safe area for babies and crawlers, it features nooks and mounds for climbing, a moving overhead light display and spinners to enable our youngest scientists to investigate how different materials move.
- Tinkering Zone: for toddlers to three year olds to engage in open-ended activities that encourage them to experiment and test their ideas.
- Collaborative Zone: designed for 3–5 year olds, is an active, physical space where children use communication and social skills to solve problems and achieve goals.

The new gallery has been created with close community and sector consultation. For two years, Museums Victoria collaborated with more than 5000 children and adults, including early childhood education specialists, additional needs experts, teachers and visitors to Little Kids Day In events at Scienceworks.

Ground Up: Building Big Ideas, Together will be part of Museums Victoria’s autism-friendly museum project, with social stories available online in early 2018.

ScienceWorks

‘Hide or get eaten’, urine chemicals tell mud crabs



Urine is extracted from a blue crab in a lab at Georgia Tech, where researchers have isolated two chemicals in the urine that alert mud crabs, the prey of blue crabs, to the danger of predation. Georgia Tech/Remy Poulin

Pssst, mud crabs, time to hide because blue crabs are coming to eat you! That's the warning the prey get from the predators' urine when it spikes with high concentrations of two chemicals, which researchers have identified in a new study.

Beyond decoding crab-eat-crab alarm triggers, pinpointing these compounds for the first time opens new doors to understanding how chemicals invisibly regulate marine wildlife. Insights from the study by researchers at the Georgia Institute of Technology, USA, could someday contribute to better management of crab and oyster fisheries, and help specify which pollutants upset them.

In coastal marshes, these urinary alarm chemicals, trigonelline and homarine, help to regulate the ecological balance of who eats how many of whom – and not just crabs.

Blue crabs eat mud crabs. Blue crabs also eat a few oysters, but mud crabs eat a lot more oysters than they do. When blue crabs are going after mud crabs, the mud crabs hide and stay still, so far fewer oysters get eaten than usual.

Humans are part of the food chain, too, eating oysters as well as blue crabs that boil up a bright orange. The blue refers to the colour of markings on their appendages before they're cooked. Thus, the blue crab urinary chemicals influence seafood availability for people, as well.

The fact that blue crab urine scares mud crabs was already known. Mud crabs duck and cover when exposed to samples taken in the field and in the lab, even if the mud crabs can't see the blue crabs. Metabolites in blue crab urine trigger the mud crabs' reaction, which also makes them stop foraging for food themselves.

'Mud crabs react most strongly when blue crabs have already eaten other mud crabs', said Julia Kubanek, who co-led the study with fellow Georgia Tech professor Marc Weissburg.

'A change in the chemical balance in blue crab urine tells mud crabs that blue crabs just ate their cousins.'

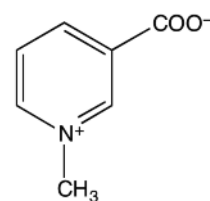
Figuring out the two specific chemicals, trigonelline and homarine, that set off the alarm system, out of myriad candidate molecules, is new and has been a challenging research achievement.

The results are published in *Proceedings of the National Academies of Science* (doi: 10.1073/pnas.1713901115).

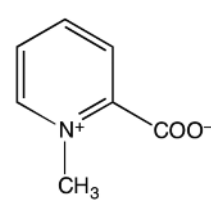
Trigonelline has been studied, albeit loosely, in some diseases, and is known as one of the ingredients in coffee beans that, upon roasting, breaks down into other compounds that give coffee its aroma. Homarine is very similar to trigonelline, and, though apparently less studied, it's also common.

Often, in the past, researchers trying to narrow down such chemicals have started out by separating them out in arduous laboratory procedures then testing them one at a time to see if any of them worked. There was a good chance of turning up nothing.

The Georgia Tech researchers went after all the chemicals at one time, by using mass spectrometry and NMR spectroscopy.



trigonelline



homarine

The researchers discovered spikes in about a dozen metabolites after blue crabs ate mud crabs. They tested the urine chemicals that spiked on the mud crabs, and trigonelline and homarine distinctly made them crouch.

'Trigonelline scares the mud crabs a little bit more', Kubanek said.

More specifically, high concentrations of either of the two did the trick. 'It's clear that there was a dose-dependent response', said Weissburg.

'Mud crabs have evolved to hone in on that elevated dose ... They detect chemicals with sensors on their claws, antennae and even the walking legs. The compounds we isolated are pretty simple, which suggests they might be easily detectable in a variety of places on a crab. This redundancy is good because it increases the likelihood that the mud crabs get the message and not get eaten.'

Evolution preserved the mud crabs with the duck-and-cover reaction to the two chemicals, which also influenced the ecological balance, in part by pushing blue crabs to look for more of their food elsewhere. But it influenced other animal populations as well.

'These chemicals are staggeringly important', Weissburg said. 'The scent from a blue crab potentially affects a large number of mud crabs, all of which stop eating oysters, and that helps preserve the oyster populations.'

All of that also impacts food sources for marine birds and mammals: Just by the effects of two chemicals, and there are so many more chemical signals around. 'It's hard for us to appreciate the richness of this chemical landscape', Weissburg said.

Identifying such metabolites and their effects is the latest chapter in constructing the catalogue of life molecules. 'Everyone knows about the human genome project, identifying genomes; then came transcriptomes (molecules that transcribe genes)', Kubanek said. 'Now we're pretty far along with proteomics (identifying proteins), but we're just now figuring out metabolomes.'

Georgia Institute of Technology

Colour printing on rewritable paper

A new strategy to produce rewritable paper that can print long-lasting yet erasable multi-colour images is demonstrated in *Nature Communications* (doi: 10.1038/s41467-017-02452-w).

Reusable paper holds environmental and cost benefits over its disposable counterpart, but its absence from the everyday marketplace stems from an existing inability to print multi-coloured, long-lasting images that are also erasable.

Chinese researchers Qiang Zhao, Wei Huang and colleagues have designed a paper and ink combination that allows them to print multi-colour images that last for more than six months, but that can also be erased on demand. The inks consist of metal salts dissolved in water, and the paper is modified to contain molecules that interact with these metals. Inkjet printing of a pattern or text causes the paper to change colour as a new compound forms. The colour adopted depends on the metal salts used, and as a broad range of these are available, a wide colour palette can be printed. Owing to the reversible nature of the chemical bonds, coating the paper with a specific substance will then break those bonds and erase the image.

The authors note that the paper can only be rewritten up to eight times before the colours will start to fade, but propose that their lost-cost strategy could bring us closer to realising commercially viable rewritable paper.

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First direct proof of ozone hole recovery



ozone depletion decreasing, but that the decrease is caused by the decline in CFCs.

The change in ozone levels above Antarctica from the beginning to the end of southern winter – early July to mid-September – was computed daily from microwave limb sounder (MLS) measurements every year from 2005 to 2016.

The researchers found ozone loss is decreasing, but they needed to know whether a decrease

For the first time, scientists have shown through direct satellite observations of the ozone hole that levels of ozone-destroying chlorine are declining, resulting in less ozone depletion.

A study in *Geophysical Research Letters* (doi: 10.1002/2017GL074830) shows the decline in chlorine, resulting from an international ban on chlorofluorocarbons (CFCs), has resulted in about 20% less ozone depletion during the Antarctic winter than there was in 2005, the first year that measurements of chlorine and ozone during the Antarctic winter were made by NASA's Aura satellite.

CFCs are long-lived and eventually rise into the stratosphere, where they are broken apart by the sun's ultraviolet radiation, releasing chlorine atoms that go on to destroy ozone molecules.

This study is the first to use measurements of the chemical composition inside the ozone hole to confirm that not only is


in CFCs was responsible. When ozone destruction is ongoing, chlorine is found in many molecular forms, most of which are not measured. But after chlorine has destroyed nearly all the available ozone, it reacts instead with methane to form hydrochloric acid, a gas measured by MLS.

Nitrous oxide is a long-lived gas that behaves just like CFCs in much of the stratosphere. The CFCs are declining at the surface but nitrous oxide is not. If CFCs in the stratosphere are decreasing, then over time, less chlorine should be measured for a given value of nitrous oxide. By comparing MLS measurements of hydrochloric acid and nitrous oxide each year, the researchers determined that the total chlorine levels were declining on average by about 0.8% annually.

The 20% decrease in ozone depletion during the winter months from 2005 to 2016 as determined from MLS ozone measurements was expected. 'This is very close to what our model predicts we should see for this amount of chlorine decline', said Susan Strahan, an atmospheric scientist at NASA's Goddard Space Flight Center and lead author of the study. 'This gives us confidence that the decrease in ozone depletion through mid-September shown by MLS data is due to declining levels of chlorine coming from CFCs. But we're not yet seeing a clear decrease in the size of the ozone hole because that's controlled mainly by temperature after mid-September, which varies a lot from year to year.'

Looking forward, the Antarctic ozone hole should continue to recover gradually as CFCs leave the atmosphere, but complete recovery will take decades.

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Scaling to new heights with gecko-inspired adhesive

Some animals, such as geckos, can easily climb up walls and across ceilings. But currently, no material exists that allows everyday people to scale walls or transverse ceilings as effortlessly. Now, scientists report in *ACS Applied Materials and Interfaces* (doi: 10.1021/acsami.7b09526) a dry adhesive that could someday make it easier to defy gravity.

Geckos can scale walls because of their unique toe pads that help them quickly attach and detach from surfaces. Interestingly, gecko toe pads are covered with bristle-like layers of the stiff material keratin. The bristle-like structure of the keratin in a toe pad helps it to stick – each pad is covered with microscopic pillars, which then branch out at the tips into even smaller structures. Scientists have manufactured dry adhesives with similar properties, but they haven't been as sticky as gecko toes. And some methods involve the use of layers, but the first layer is usually damaged as successive ones are applied. Other methods are not easily scaled up. Hemant Kumar Raut, Hong Yee Low and colleagues from Singapore University of Technology and Design wanted to create a dry adhesive that was ultra-sticky but also simple to fabricate in large batches.

The researchers made a dry adhesive with stiff polycarbonate using a nanoimprinting technique to build web-like layers. This method is cost-effective, easy to perform and scalable. To prevent damage to the first layer, the team used a sacrificial layer, which was dissolved away after the second layer was applied. In repetitive attachment and detachment tests, only a 20% decline in stickiness occurred after 50 cycles. This level of adhesion lasted for up to 200 cycles. The researchers say that their film's adhesion was comparable to that of a gecko. The team also placed the adhesive film on the feet of a miniature robot, which moved with ease up a 30° incline.

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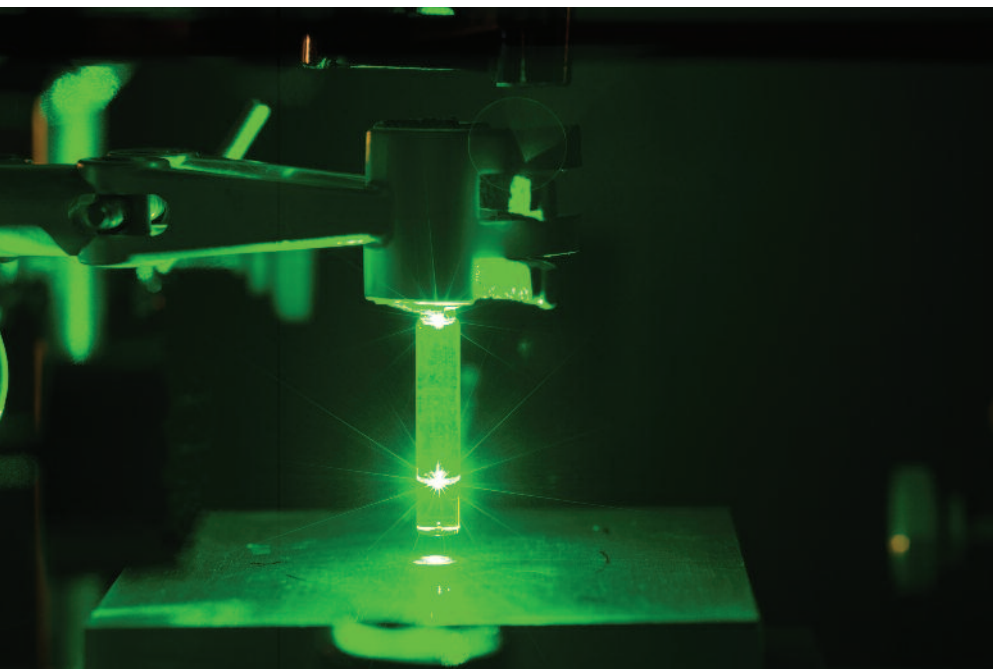
- In agriculture, farmers will be able to screen their crops for infestation and see the results immediately, in many cases a week before any problems are visible to the human eye. Rather than routinely treating crops, they will be able to treat them just where needed.
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Light colour controls thermal reactivity



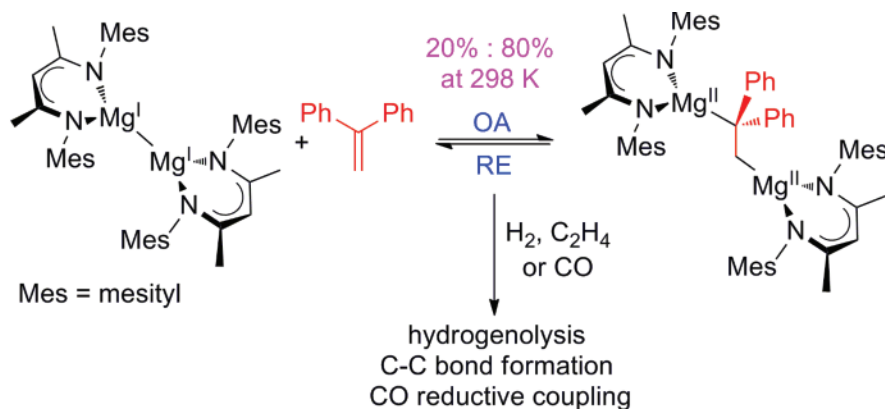
Precise control of chemical reactivity by external stimuli such as light is critical to the design of adaptive and 'on demand' reprogrammable materials. A key frontier in the realm of reaction control is the development of reaction manifolds that

can switch reversibly between thermal and photochemical bond-forming processes. Yet no reaction manifolds are currently available in which the thermal reactivity of molecules can be completely halted by exposure to light. Researchers

from the Queensland University of Technology, the Karlsruhe Institute of Technology, Germany, and Ghent University, Belgium, have pioneered exactly such a manifold based on the photopolymerisation of powerful coupling agents called 1,2,4-triazoline-3,5-diones (TADs) under green light irradiation (Houck H.A., Du Prez F. E., Barner-Kowollik C. *Nat. Commun.* 2017, **8**, 1869). The team demonstrated via trapping experiments that polymerisation results in quantitative photodeactivation of TAD reactivity, thereby providing a defined on/off switch for the thermal reactivity of these coupling agents. This finding allowed the team to design an unprecedented reaction manifold using light as a gate to switch between a thermally and a photochemically induced addition reaction, thus enabling a remotely controlled switchable reaction output. The ability to precisely regulate reaction pathways with different colours of light opens design opportunities for novel photoresists, potentially enabling sub-diffraction 3D laser lithography.

Reversible magnesium(I) redox chemistry

Over the last decade or so, the chemistry of compounds containing p-block elements in low oxidation states has been revolutionised by the realisation that such species can exhibit novel transition-metal-like properties and reactivity patterns, including reversible redox chemistry. The team of Professor Cameron Jones at Monash University has extended such redox chemistry to the s-block for the first time (Boutland A.J., Carroll A., Lamsfus C.A., Stasch A., Maron L., Jones C. *J. Am. Chem. Soc.* 2017, **139**, 18 190–3). Remarkably, the 'oxidative insertion' of 1,1-diphenylethylene into the Mg–Mg bond of magnesium(I) dimers was shown to be readily and rapidly reversible at room temperature, via 'reductive elimination' of the ethylene substrate.

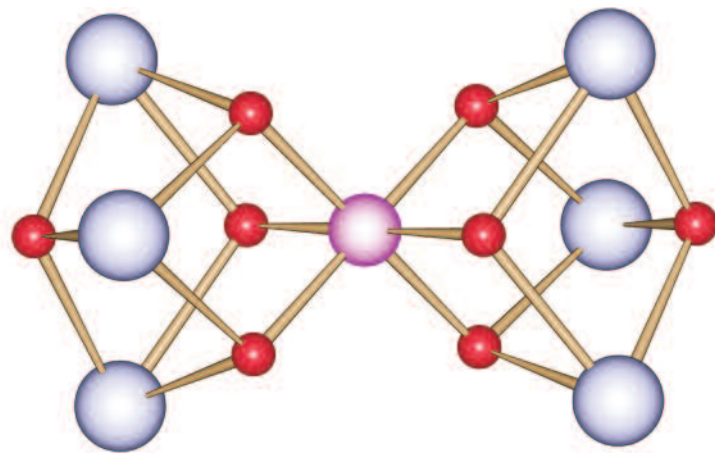


Spectroscopic and computational studies showed the insertion reaction to be close to thermo-neutral and essentially barrierless. The 1,2-dimagnesioethane products of these reactions were highly activated magnesium alkyls and showed unprecedented uncatalysed reactivity

towards H₂, CO and ethylene. These results highlight the potential for use of magnesium(I) dimers in oxidative addition-based or reductive elimination-based catalytic processes, which are so far unknown for these species.

Single-molecule toroidal magnets

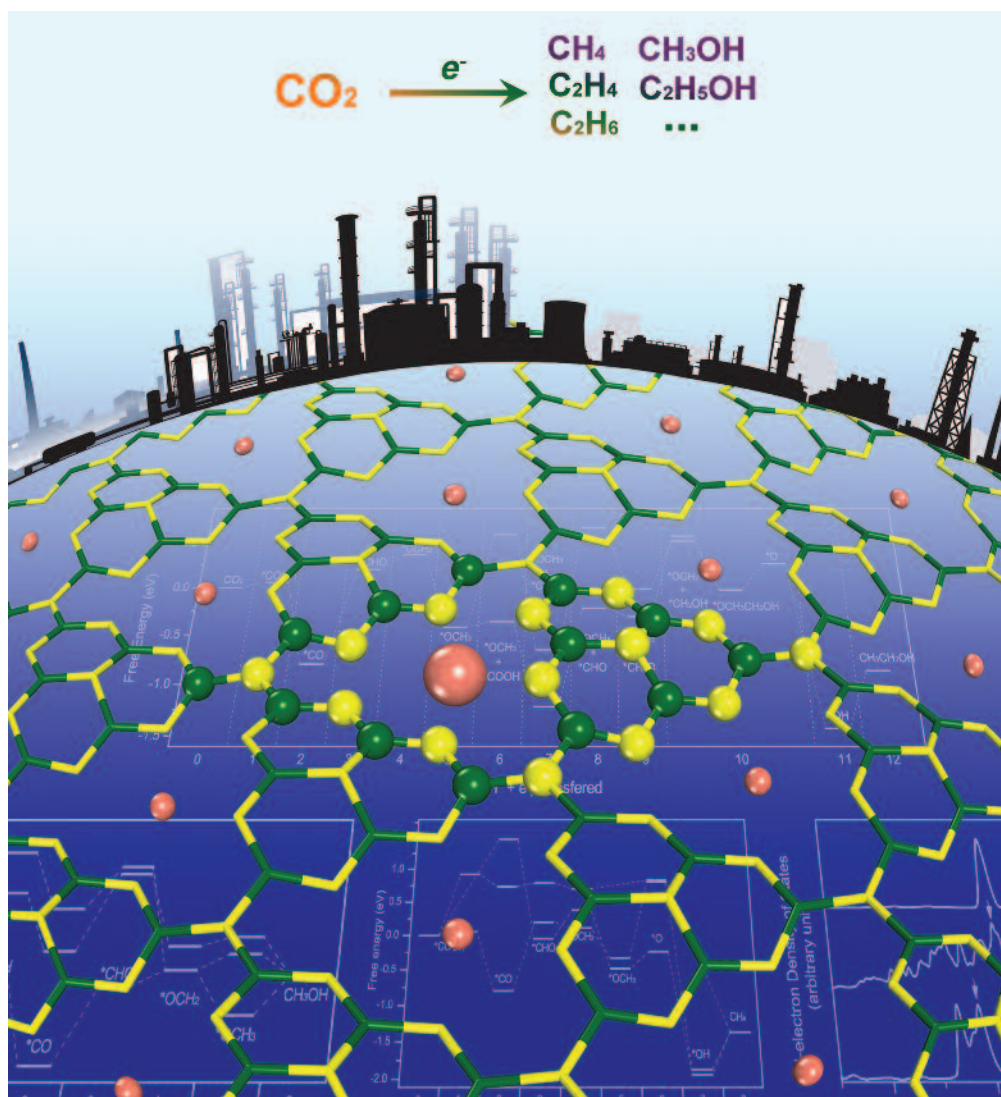
Fifty-year RACI member Professor Keith Murray and a team of international inorganic chemists from Monash University, the Indian Institute of Technology Bombay, India, Manchester Metropolitan University, UK, Karlsruhe Institute of Technology, Germany, and Institut Néel, France, have published the first examples of 3d–4f single-molecule toroidal (SMT) species (Vignesh K.R., Langley S.K., Swain A., Moubaraki B., Damjanović M., Wernsdorfer W., Rajaraman G., Murray K.S. *Angew. Chem. Int. Ed.* 2018, **57**, 779–84). Toroidal magnetism is well recognised in triangular dysprosium(III) clusters in which the f-block local moments are arranged in a vortex fashion around the ring. Following on from their recent report in *Nature Communications* (2017, **8**, 1023), which described ferrotoroidicity in a $\{\text{Cr}^{\text{III}}\text{Dy}^{\text{III}}_6\}$ coordination complex made up of two parallel Dy_3 triangles linked by a Cr^{III} ion with



con-rotation (rotation in the same direction) of Dy_3 moments, the group has reported non-Dy analogues of Tb, Ho and Er in the latest work. Squid magnetometry, including the use of microsquids on single crystals down to 0.03 K, was used to elucidate slow magnetisation reversal, while ab initio calculations were used to yield the first predictions of SMT behaviour in the Tb and Ho analogues.

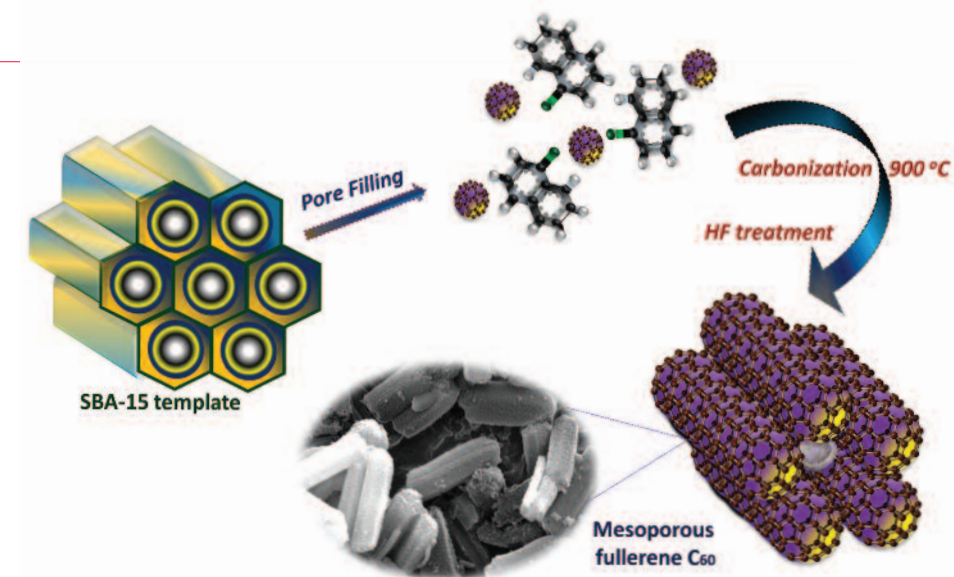
Molecular scaffolding to boost electrocatalytic CO_2 reduction

A major impediment to electrocatalytic CO_2 reduction to produce liquid fuels and other valuable chemicals is the lack of electrocatalysts with both high efficiency and good selectivity. Professor Shizhang Qiao and co-workers at the University of Adelaide have proposed a new strategy to develop electrocatalysts with high CO_2 reduction selectivity towards hydrocarbons or alcohols (Jiao Y., Zheng Y., Chen P., Jaroniec M., Qiao S.-Z. *J. Am. Chem. Soc.* 2017, **139**, 18 093–100). The strategy – applying molecular scaffolding to coordinate metal active centres – was proposed based on comprehensive density functional theory (DFT) calculations and was validated by experiments. As a proof of principle, graphitic carbon nitride ($\text{g-C}_3\text{N}_4$) was used as a molecular scaffold for Cu to modify the electronic structure of Cu in the resultant $\text{Cu-C}_3\text{N}_4$ complex and to optimise the adsorption behaviour of key reaction intermediates on the $\text{Cu-C}_3\text{N}_4$ surface. This strategy greatly improved CO_2 activation and led to more facile CO_2 reduction to desired products. Strikingly, in contrast to elementary Cu surfaces, the $\text{Cu-C}_3\text{N}_4$ complex produced significant amounts of C_2 products such as $\text{C}_2\text{H}_5\text{OH}$, C_2H_4 and C_2H_6 . This behaviour was attributed to a dual active-centre mechanism in which the Cu atoms and $\text{g-C}_3\text{N}_4$ scaffold act synergistically in the catalytic process.



Holey buckyballs

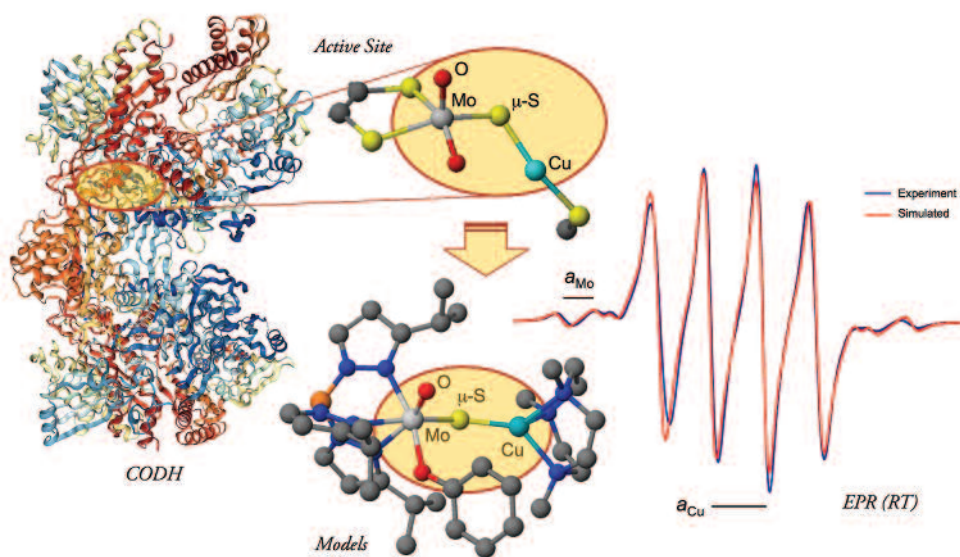
A team of researchers led by Professor Ajayan Vinu of the University of Newcastle has successfully created the world's first highly crystalline mesoporous C_{60} -fullerene, a new class of material with promising energy-related applications (Benzigar M.R., Joseph S., Ilbeygi H., Park D.-H., Sarkar S., Chandra G., Umapathy S., Srinivasan S., Talapaneni S.N., Vinu A. *Angew. Chem. Int. Ed.* 2018, **57**, 569–73). The material was made possible by the judicious choice of 1-chloronaphthalene solvent, in which C_{60} is highly soluble. This allowed the C_{60} molecules to be uniformly dispersed at high density in the nanochannels of an SBA-15 mesoporous silica template. The high density of encapsulated C_{60} enabled cross-linking of the fullerene molecules at high temperature (900°C) to generate a mesoporous material with ordered



porosity and crystalline pore walls. The highly crystalline mesoporous C_{60} exhibited a uniform rod-shaped morphology with a high specific surface area of $680 \text{ m}^2 \text{ g}^{-1}$ and tuneable pore diameters. The new material performed well as a supercapacitor electrode and as an electrocatalyst for oxygen reduction with a high selectivity for H_2O_2

production and high methanol tolerance, which could be exploited in fuel cells. The synthesis strategy employed in this work could be extended to fabricate other novel porous fullerenes and has the potential to revolutionise the field of fullerene-based materials and energy technologies.

Shedding light on carbon monoxide dehydrogenase

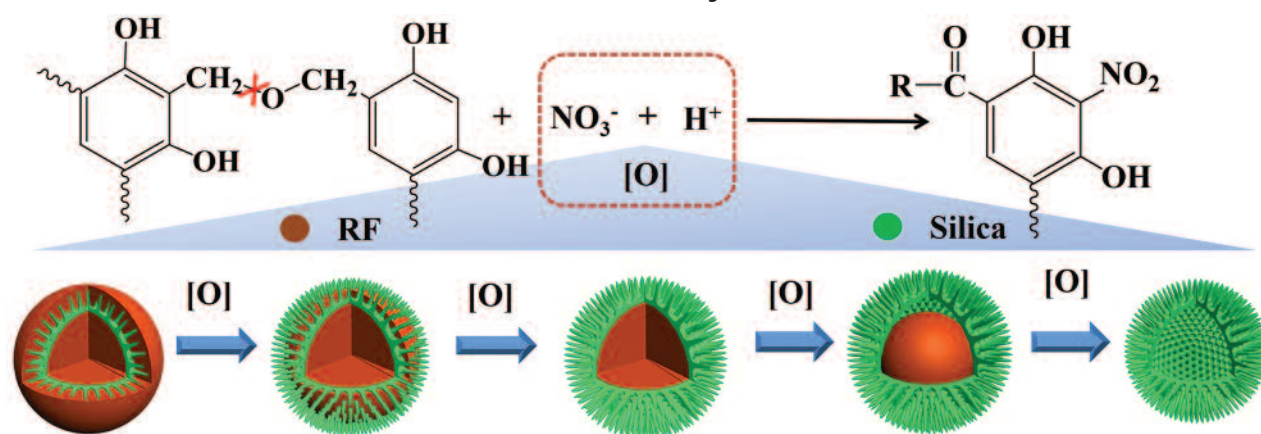


The soil bacterium *Oligotropha carboxidovorans* derives its carbon and energy from the conversion of CO to CO_2 by a carbon monoxide dehydrogenase (CODH) enzyme containing a biologically unique heterobimetallic $[(\text{molybdopterin})\text{MoO}_2(\mu\text{-S})\text{CuS}_{\text{cys}}]$ active

site. Organisms and reactions of this type are essential to the global carbon cycle and the maintenance of safe CO levels in the aerobic biosphere. The first chemical models to feature an $\text{MoO}(\mu\text{-S})\text{Cu}$ core closely related to that of CODH and to display the unique spectroscopic and

chemical (cyanolytic) properties of the enzyme have been prepared and structurally and spectroscopically characterised by Dr Craig Gourlay and co-workers at the University of Melbourne and La Trobe University (Gourlay C., Nielsen D.J., Evans D.J., White J.M., Young C.G. *Chem. Sci.* 2018, <https://doi.org/10.1039/c7sc04239f>). The extremely unstable $d^1\text{-}d^{10} \text{Mo}^{\text{V}}\text{Cu}^{\text{I}}$ complexes exhibit unprecedented electron paramagnetic resonance (EPR) spectra showing strong coupling to both Mo and Cu, with the four-line spectral components indicative of electron delocalisation from Mo^{V} onto the neighbouring Cu^{I} atom. The magnitude of the coupling depends on the bridge geometry; its observation and analysis informs the interpretation of enzyme EPR spectra as well as understanding of the electronic structure, intermetallic cooperativity, mechanism of action and electron-transfer regeneration pathways of the enzyme active site.

Intricate nanoarchitectures from chemically resistant resins



Three dimensionally cross-linked resoles are highly chemically resistant resins produced by base-catalysed phenol-formaldehyde condensation. Calcination is thus generally used to break down resole-type resins, which significantly limits the diversity of nanostructured materials that can be derived from these resins. Recently, Professor Chengzhong Yu and co-workers at the University of Queensland have developed an oxidative dissolution approach using nitrates and protons for the first time to dissolve resoles (Zhang M., Song H., Yang Y., Huang X., Liu Y., Liu C., Yu C. *Angew. Chem. Int. Ed.* 2018, **57**, 654–8). They demonstrated that the dibenzyl ether bond in the

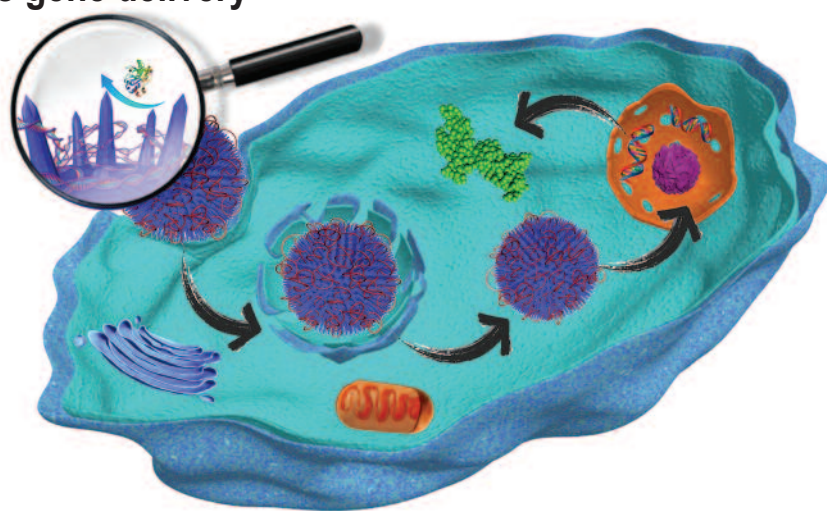
resorcinol-formaldehyde (RF) resole-type resin is preferentially cleaved by simply choosing metal nitrate solutions to achieve oxidative conditions, leading to oxidised products with carbonyl and nitro groups. Taking advantage of the facile oxidative dissolution, they successfully constructed a series of RF/silica nanocomposites with rough surface topology and versatile core-shell architectures. With a better understanding of the oxidative dissolution process, the predictable and controllable synthesis of various resole-based nanostructures should be possible.

Designer nanotopography boosts gene delivery

The key challenge for cellular delivery of genetic material lies in the development of advanced delivery vehicles to package and transport nuclei acids into the cell efficiently. Unlike small-molecular drugs and therapeutic proteins, plasmid DNA molecules possess unique rope-like structures with numerous loops. Professor Chengzhong Yu at the University of Queensland has developed silica nanoparticles with a designer nanotopography – a spiky surface similar to that of a rambutan – which exploit this feature of DNA and demonstrate superior gene-delivery performance to previous gene-delivery systems (Song H., Yu M., Lu Y., Gu Z., Yang Y., Zhang M., Fu J., Yu C. *J. Am. Chem. Soc.* 2017, **139**, 18 247–54). Silica hollow spheres were engineered with spiky, semi-spherical and flower-like nanotopographies for comparison. The spiky surface provides a laterally continuous porous space to

accommodate the rope-like DNA molecules, thus leading to enhanced loading capability and efficient DNA protection from nuclease degradation. Compared with a commercial transfection agent, the rambutan-like nanoparticles achieved a similar transfection rate but

much better enzyme stability, with no significant transfection decay after nuclease treatment. The designer nanotopography concept provides rational design of gene-delivery systems and holds great promise for gene therapy and vaccines.



Compiled by David Huang MRACI CChem (david.huang@adelaide.edu.au). This section showcases the very best research carried out primarily in Australia. RACI members whose recent work has been published in high-impact journals (e.g. *Nature*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Chem. Sci.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.

A cool visualisation breakthrough

The 2017 Nobel Prize in Chemistry. Part 2

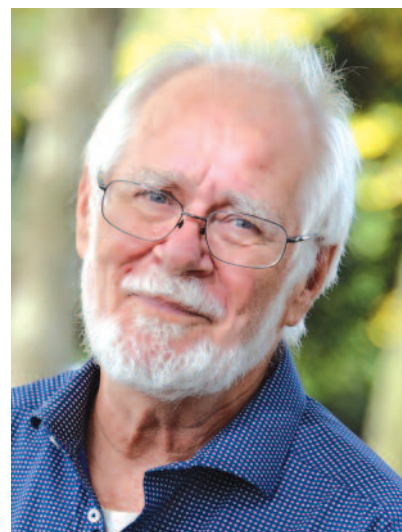
BY **DAVE SAMMUT** AND **CHANTELLE CRAIG**

Last year's three Nobel laureates in chemistry each had unique approaches and contributions to their prize-winning work.

The 2017 Nobel Prize in Chemistry was jointly awarded to three researchers for their convergent work in cryo-electron microscopy. With breakthroughs as recently as 2013, this technology is already revolutionising the high-resolution structure determination of biomolecules in solution. Working separately over decades, Jacques Dubochet (University of Lausanne, Switzerland), Joachim Frank (Columbia University, New York) and Richard Henderson (MRC Laboratory of Molecular Biology, Cambridge, UK) developed critical aspects of this technology.

The first article in this series (February issue, p. 20) examined the basic technology and the fundamental problems that needed to be solved to make this analytical technique work. In this article, we will examine the individual approaches and contributions made by each of the researchers.

Jacques Dubochet



Félix Imhof ©UNIL/CC BY-SA 4.0

Swiss biophysicist Dr Jacques Dubochet commenced his physics studies in 1962 at what is now called the École Polytechnique Fédérale de Lausanne. Graduating in 1967, he went on to obtain a Certificate of Molecular Biology at the University of Geneva, then began his study in the electron

Illustration: ©Martin Högborn/The Royal Swedish Academy of Sciences

microscopy (EM) of DNA. He completed his thesis in biophysics in 1973, through the University of Geneva and University of Basel.

The physical conditions of EM are punishing for biological samples. For a long time, it was widely considered that the dehydrating effects of the vacuum and the radiation-induced damage to the materials from the intensive, high-energy electron beams required to achieve contrast against the background made EM impractical for any but 'dead' samples.

Staining was extensively used from the 1940s to increase the differentiation against background. Biological samples were embedded in a thin amorphous film of a heavy metal salt, generating a 'cast' around the object. The cast would scatter electrons more strongly than the encapsulated material (increasing contrast, and creating a negative image), was more resistant to electron damage, and would retard the vaporisation of water from the sample. This was sufficient to provide information about the morphology of bacteria and viruses, but for single molecules or molecular complexes it only gave information about the envelope of the covered particles, and the resolution was limited to the granularity of the stain.

From the mid-1970s, Richard Henderson (discussed below) and Nigel Unwin developed a new preparation method to enable EM studies of unstained protein crystals at room temperature. They replaced water with a glucose solution to preserve the samples under vacuum, and used this method to study intact protein crystals.

However, it was Dubochet who generated the critical breakthrough in enabling analysis of liquid samples. Back in the 1950s, Humberto Fernández-Morán had already begun exploring the possibility of freezing samples and preparing thin sections for cryo-EM. It was expected that

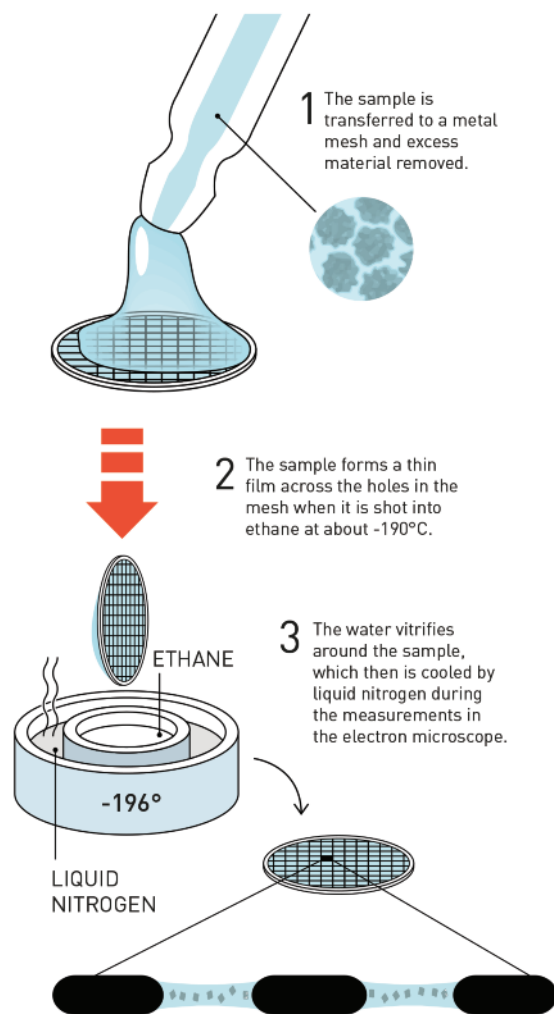
extreme cooling would both reduce water evaporation and protect biological samples from damage. But crystalline ice strongly diffracts electrons, and its formation may change the specimen structure.

Dubochet's technique involved the rapid freezing of samples using ethane (which was in turn cooled by liquid nitrogen). When cooled in this way, water solidifies in its liquid form as a glassy material called 'vitrified water' – which is now believed to be the dominant form of water throughout the universe. In this state, the supercooled liquid water preserves the biomolecules in their natural shape, even under vacuum.

It is notable that this work built on earlier studies by Kenneth Taylor and Robert Glaeser, but the technology at the time did not allow studies below -120°C , which is above the transition temperature from vitrified water to crystalline ice. Nonetheless, Taylor and Glaeser offered important contributions for specimen handling at cryogenic temperatures.

So in 1981, Dubochet and Alasdair McDowell presented a method for the formation of thin-film non-crystalline samples on a specimen grid, ready for EM analysis. The sample was sprayed on a carbon film mounted on a grid, then rapidly immersed in liquid ethane or propane at about -190°C . At cryogenic temperatures, the vitrified water allowed nearly uniform absorption of electrons, yielding impressive contrast. These samples could be maintained for long periods provided temperatures were maintained below -160°C .

With this technique now widely adopted, samples can be made sufficiently thin to allow rapid vitrification, freezing movement for 'snapshot' of activity at a given moment in time. By careful collection of multiple samples, 'movies' of action can be constructed to develop detailed understanding of the activity in biological processes.



Dubochet's vitrification method.

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But cryo-EM is not only about static structures. Because sample preparation for cryo-EM involves instant cooling of a solution, the contents of the solution can be systematically varied; integral membrane proteins may be studied in a near-native environment; and the particles may be trapped in structural sub-states or even in action, for example, while an enzyme catalyses a chemical reaction. The data may offer functional information: structural changes may be monitored and free-energy landscapes determined. (bit.ly/2y8zlnm)

Aged 65, Dubochet is now retired, and is an honorary professor at the University of Lausanne.

Joachim Frank



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Born in Germany, Dr Joachim Frank is a Professor of Biochemistry and Molecular Biophysics and of Biological Sciences at Columbia University, and Distinguished Professor of the State University of New York at Albany. He received his diploma in physics at the University of Munich, and conducted his doctoral research at the Max Planck Institute for Biochemistry, Martinsried and at the Technical University of Munich.

Frank's postdoctoral research at the Cavendish Laboratory in Cambridge, UK, and in the USA, addressed problems with electron optics and image processing. He joined the Wadsworth Center in Albany, New York, in 1975, and developed the

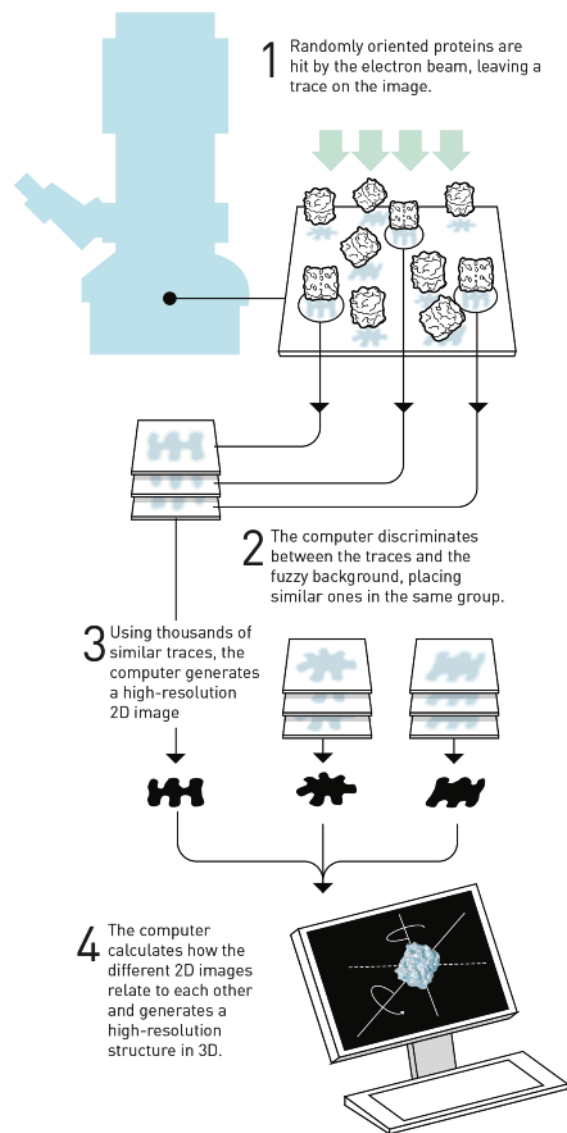
single-particle reconstruction approach.

Biological samples are rarely structurally uniform and may contain impurities. So a major problem with studies of unstained, non-crystalline, asymmetrical and randomly oriented particles in solution is, according to a 1975 paper by Frank, 'the alignment of features that are only faintly visible on a noisy background'. (bit.ly/2AAr1VK)

Frank and colleagues began studies of this issue in the 1970s and, by using studies of negatively stained glutamine synthetase, determined that it would be possible to average images of many sensitive particles to eventually construct high-resolution data, provided that the particles were uniform.

In 1981, Frank and Marin van Heel then extended this to present a method for non-uniform particles, which sorted the particle images into classes based on their orientation and structural features. By applying multivariate statistical analysis to sort the vector clusters, these clusters were then each assumed to represent a 2D projection of a particle with specific orientation and structural properties. It was then assumed that the particles within each cluster were sufficiently similar to allow averaging, increasing the signal to noise ratio.

In translating these 2D structures into 3D visualisations, Frank developed critical mathematical tools. Most



Frank's image analysis for 3D structures.

©Johan Jarnestad/The Royal Swedish Academy of Sciences

particularly, Frank and Michael Radermacher's Random Conical Tilt method combined the earlier general ideas with the application of a

Monash researchers use cryo-EM to reveal structure of important drug target

Monash University researchers have used cryo-EM to reveal the structure of an important drug target, opening the way for improved treatments of chronic diseases such as osteoporosis, diabetes and obesity.

Treatments for such chronic diseases all target Class B G protein-coupled-receptors; however, there are large gaps in our knowledge of how these receptors function. In part, this stems from their small size.

The structure solved by Monash Institute of Pharmaceutical Sciences researchers and their collaborators is that of the calcitonin receptor, a receptor targeted by treatments for hypercalcemia and Paget's disease (a bone disorder). The

breakthrough is significant not just because of the additional knowledge it reveals, but also because of the method used to uncover it.

This is the first time that a cryo-electron microscope has been used to reveal the structure of a G protein-coupled-receptor, and the first time that the full-length structure of a receptor in this class has been solved.

The research has been published in *Nature* and was conducted in collaboration with the Max Planck Institute of Biochemistry, Germany, and the University of Michigan, Stanford University, and the Mayo Clinic in the US.

Monash University

tomographic conical tilt series. The tools have been gathered into a suite of computer programs called SPIDER and made available for ready use by the scientific community.

In a 1976 issue of *Research News* (bit.ly/2BgYIeU), US biochemist Arthur Robinson commented on Frank's work 'exploring theoretical methods for averaging data from arrays of identical objects that are not periodic': 'If such methods were to be perfected, then, in the words of one scientist, the sky would be the limit'. A 2015 post by Frank concludes: 'Well, we have reached the sky now, but the history of the single-particle techniques that brought us here goes back quite a few years'. (bit.ly/2BXVauL)

Frank is a Fellow of the American Association for the Advancement of Science and the Biophysical Society. He was elected to the National Academy of Sciences in 2006, as well as the American Academy of Arts and Sciences, and the American Academy for Microbiology. In 2014, he was awarded the Franklin Medal in Life Science.

Richard Henderson



Bengt Nyman/CC BY 2.0

Dr Richard Henderson initially studied physics at Edinburgh University, but switched to molecular biology at age

21. As a research student, he worked for the MRC Laboratory of Molecular Biology (LMB) at Cambridge, UK, where David Blow's team was using X-ray crystallography to prepare one of the first protein structure characterisations (for the enzyme chymotrypsin).

As a Helen Hay Whitney postdoctoral fellow at Yale, he developed an interest in the structure of membrane proteins. Then after returning to LMB in 1973, he commenced important work in collaboration with Nigel Unwin, developing new sample preparation methods for electron microscopy.

Henderson initially turned to EM after X-ray crystallography failed in the imaging of proteins embedded in the membrane surrounding the cell. Such proteins are often difficult to work with, because when removed from the membrane they clump up into a useless mass. In Henderson's case, he simply couldn't crystallise the selected protein for X-ray studies.

In an initial study (published in 1975), Henderson and colleagues simply worked with the enzyme while still embedded in its membrane. They were fortunate that the selected enzyme molecules happened to be regularly packed and oriented in the same direction on the membrane. The researchers prepared 2D projections of bacteriorhodopsin crystals on the purple membrane, with images of the structures and diffraction patterns. They then used Fourier transformation of the structure images to calculate phases. In a subsequent study, they tilted the specimen to collect 2D projection images from multiple directions, and from these calculated low-resolution visualisations of the general structure of the protein by using methods developed by Aaron Klug (Nobel Prize for Chemistry, 1982) and colleagues. It turned out to be the best picture of a protein ever generated by an electron microscope, with a resolution of an impressive 0.7 nanometres.

Over subsequent years, multiple aspects of the technique improved, critically including both the lenses and the cryotechnology. As noted by Professor Peter Brzezinski of Stockholm University (bit.ly/2y8zInm): 'The year 1990 marked a critical milestone when Henderson and colleagues showed for the first time that it is possible to obtain high-resolution structures of biomolecules using cryo-EM through averaging over many copies of the same object'.

In an interview following the prize announcement, Henderson called attention to the fact that the Nobel Prize can be awarded to at most three recipients, and graciously acknowledged that there were 'others who've made strong contributions who didn't quite cross the threshold'.

From dream to reality

The Swedish Academy of Sciences puts it succinctly (bit.ly/2AfEwpE):

Now the dream is reality, and we are facing an explosive development within biochemistry. There are a number of benefits that make cryo-EM so revolutionary: Dubochet's vitrification method is relatively easy to use and requires a minimal sample size. Due to the rapid cooling process, biomolecules can be frozen mid-action and researchers can take image series that capture different parts of a process. This way, they produce 'films' that reveal how proteins move and interact with other molecules.

Such is the benefit of this new technology, that its range of applications is diverse. But cryo-EM is demonstrating its power, with significant practical outcomes already achieved and more still being conceived.

Dave Sammut FRACI CChem and **Chantelle Craig** are the principals of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries. Part 1 of this article was published in the February edition.



Desert tales from a wandering analytical chemist

Picture a large Brahman cow, on a scorching day in remote Central Australia, blocking the road and looking decidedly menacing. The ute driver at the scene, **Alf Larcher**, explains that it's all part of the job.

'Do you have a manual driver's licence?' was the simple question asked of me by one of my CSIRO Energy colleagues that started my odyssey to the 'Brahman moment'. To my 'yes', they replied 'We're doing a baseline water survey in Central Australia and looking for someone to drive and take samples from bores. You'll have to do a 4WD training course – are you interested?' My reply? 'Bring it on!' The trip began with a flight from home base in Perth to the CSIRO Darwin Laboratories, picking up a 4WD field vehicle and driving several hours south to the sampling area along the Stuart

Highway (which connects Darwin to Adelaide). Before departure, much groundwork had to be completed, such as client interactions and coordination, flight and accommodation bookings, shipping of sampling gear and bottles to Darwin, and checking personal protective equipment and safety protocols. Two of us would be away for three weeks, the first two staying in motel accommodation, and the third on a cattle station in the study area.

It was a hot and humid 37°C when we arrived in Darwin, during the build-up to the summer rainy season. We whizzed straight to the CSIRO laboratories to pick up our vehicle,

and we looked around their Tropical Biodiversity Research Laboratories. One thing they are into is ants: they have a big reference specimen collection and I saw two PhD students peering through microscopes at field ant specimens and comparing them to standards.

The following day we headed back to the Stuart Highway. Named after John McDouall Stuart, the leader of the first European team to traverse the continent in 1862, the highway has a rich World War II heritage, with signposts dotted along it to indicate side roads to remains of World War II airfields, hospitals and installations. I don't think I realise the extent of Australia's internal World War II effort – more reading is required!

After several hours, we reached our motel accommodation and met the locals, including the frogs under our demountable accommodation. (We eventually became used to them – the outback has plenty of room for everyone!)

Next morning we were up early, and after a hearty breakfast and more driving we turned into a bush track and reached a big clearing where our first water bore awaited. This was a monitoring bore without an incorporated pump so we had to use our portable submersible pump attached to a long reel of flexible pipe. The pump and hosing were lowered down the bore and the stagnant water was removed. Several volumes of water were removed according to calculations using the measured water level, total well depth/diameter and pumping rate. During this pumping phase, general water quality parameters (e.g. pH, conductivity) were determined using a field tester until steady, representative water flowed from the aquifer. The water was then sampled into a set of sample bottles, each pre-prepared for the different target analytes; sometimes the samples required filtration and the addition of an appropriate preservative chemical.

After sampling, the bottles were stored to ensure stability during priority shipment back to the Perth laboratory. Samples were quickly analysed by a variety of techniques such as IC (ion chromatography), ICP-OES (inductively coupled plasma–optical emission spectroscopy) and ICP-MS (inductively coupled plasma–mass spectrometry). This ensured that the 'holding times' of the analytes were not exceeded.

By measuring the radioactivity of the water along its flow path, the age and recharge rate of the water from the source can be determined.





It was spectacular termite mound country.

measuring the radioactivity of the water along its flow path, the age and recharge rate of the water from the source can be determined. This vital information is used to manage the water resource effectively. Amazing!

With the first bore done, it was on to the next site, which was further inland. The dusty, bumpy dirt road tested all my 4WD training course skills – great fun! Some technical problems were encountered at some of the bores, but they were masterfully overcome by our pump operator and a bagful of miscellaneous tap and pipe fittings. Other than along the Western Australian coast, I haven't travelled into much of Australia's rural and remote areas. I found the sampling areas truly remarkable – even more stunning during these first glimpses due to the terrain, vegetation and wildlife.

Another set of samples was taken to determine the age of the aquifer water, which was new to me. Sampling is completed by a variety of techniques, and age is determined by analysing a suite of radioactive isotopes with varying half-lives. In short, as subsurface water moves along its hydrological path from its source, its radioactivity changes, as determined by the half-lives of the radioactive isotopes present. By

Some bores were in very remote places, which meant some fabulous four-wheel driving experiences.



We set off down one of the local one-lane bitumen roads that extend endlessly into the horizon – spectacular.

As we progressed through the target list of bores, the cohesiveness of the group grew, until we operated like a well-oiled machine. This gave us some time to look around at the wonder of our surroundings. It was spectacular termite mound country.

Each day finished with the trip back to the motel, a fuel-up and vehicle check, a quick rest and a hearty pub dinner, usually with our clients. Then it was off to our rooms (dodging our friendly frogs) and a big sleep. We sampled three to five bores a week until all the bores on the target list were completed.

With one client's samples taken, it was time to move into the next sampling area, centred on a cattle station homestead. We set off down one of the local one-lane bitumen roads that extend endlessly into the horizon – spectacular. Avoiding the three-trailer road trains coming the other way was an interesting experience!

A welcoming hand-painted sign greeted us as we drove through the front gates of the homestead. The central area of the cluster of buildings consisted of a lush green lawn area, canopied by large leafy trees full of birds and in some cases mangoes. Foals pranced about while their mothers gently grazed ... a bit of paradise possible by the utilisation of the large local aquifer. Accommodation was clean, furnished and air-conditioned, with the camp cook providing three square meals a day.

Water bores were dotted about the multi-thousand square kilometre property, being used to water the tens

of thousands of Brahman cattle grown for live export. Some bores were in very remote places, which meant some fabulous four-wheel driving experiences. The landscapes and colours were once again stunning; it was like living in a Van Gogh painting. Apart from the usual troublesome creatures, we were warned about charging water buffalo and brumby mobs, which can gallop across the road without warning. That wasn't covered in my 4WD course and luckily it didn't happen.

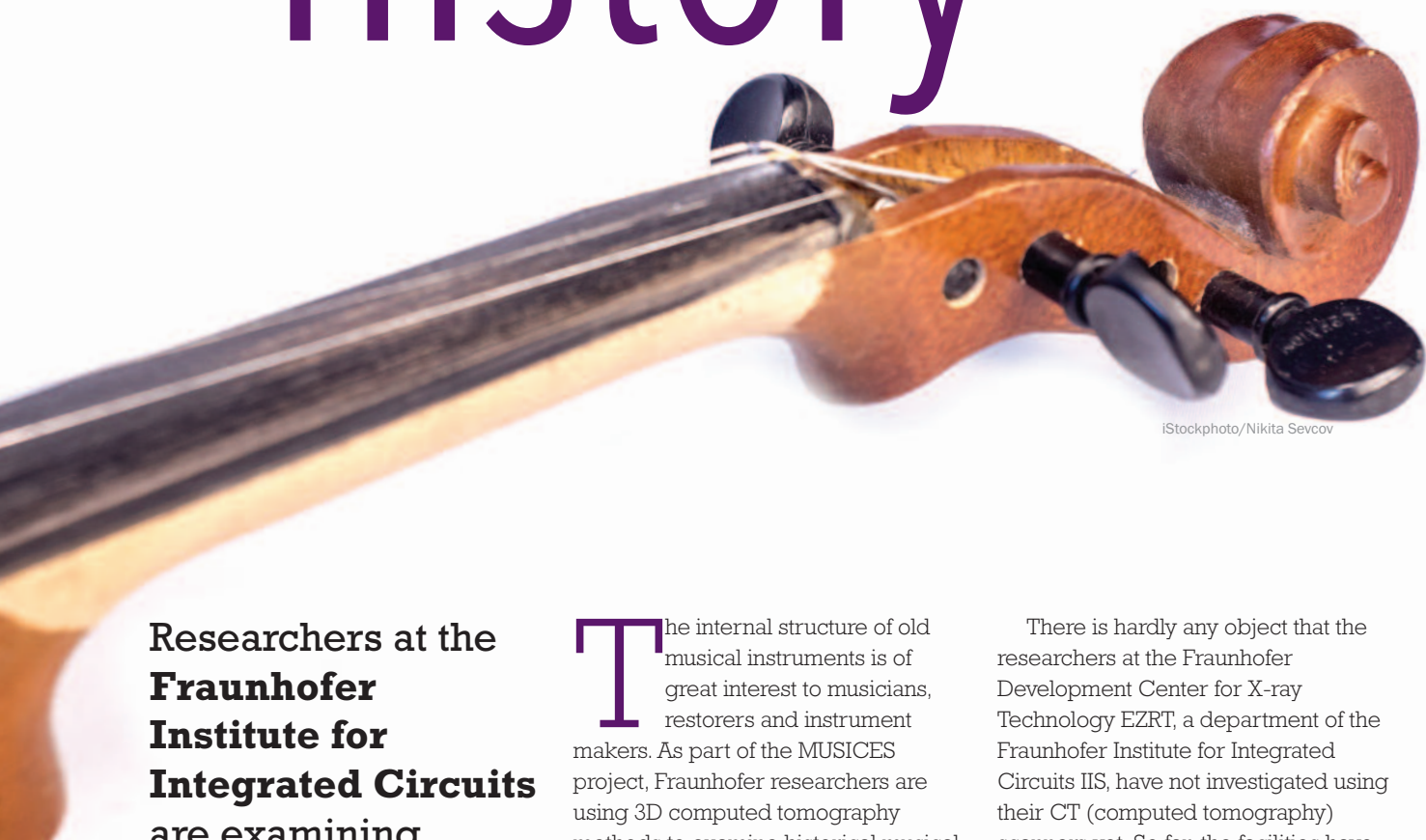
Despite what we had seen and experienced, we became impatient to get home – it had been a long trip. After a round of friendly farewells, we and our samples set off to Darwin for the flight back to Perth. It had been a successful trip.

And the Brahman cow? She turned out to be more inquisitive than menacing; after staring down the strange intruders, she trotted off.

Alf Larcher is at CSIRO Energy's National Geosequestration Laboratory.



A view into musical history



iStockphoto/Nikita Sevcov

Researchers at the Fraunhofer Institute for Integrated Circuits are examining musical instruments using scientific ones.

The internal structure of old musical instruments is of great interest to musicians, restorers and instrument makers. As part of the MUSICES project, Fraunhofer researchers are using 3D computed tomography methods to examine historical musical instruments belonging to the collection held by the Germanisches Nationalmuseum (GNM). Based on this experience, they are drawing up guidelines for obtaining the best possible images and measurement results. Until now, there has been no standard for such measurements. The results of the project will be published online.

There is hardly any object that the researchers at the Fraunhofer Development Center for X-ray Technology EZRT, a department of the Fraunhofer Institute for Integrated Circuits IIS, have not investigated using their CT (computed tomography) scanners yet. So far, the facilities have been used to analyse lightweight cast parts, rotor blades, entire cars, and landing flaps made of carbon fibre reinforced polymers, for the purposes of industrial quality control and as a non-destructive method of detecting potential defects such as hairline fissures. In the MUSICES project (see box, p. 28), the researchers in Fürth joined forces with specialists from the

The images also reveal invisible repairs, signs of damage such as cracks, delamination and woodworm attack, and structural details ...

GNM in Nürnberg and the Chair of X-ray Microscopy LRM at the University of Würzburg to take a look inside historical musical instruments, some of which are unique. Being able to examine instruments such as a violin, pianoforte, basset horn and countless others from the inside using 3D X-rays is an excellent way of evaluating their condition and determining whether, despite their age and possible deterioration due to storage conditions, they are still playable. By analysing the images, it is possible to see how the instrument was built, including its resonant parts and the materials employed. The images also reveal invisible repairs, signs of damage such as cracks, delamination and woodworm attack, and structural details, including the grain and density of the wood. The revelation of these until-now hidden areas is of tremendous value to restorers, conservators, musicians, museum educators and instrument crafters.

But we still lack standards to define the best way of using 3D CT scanning to study the condition of old musical instruments. The partners in this project are therefore developing guidelines that will enable museums throughout the world to digitalise different types of instruments and obtain images of comparable quality. It's not a trivial matter because it involves defining a large number of innumerable parameters, including radiation dose, exposure time, measuring interval and duration, the configuration of the CT scanner, and the algorithms used to reconstruct the volumes and consecutively to mine information from the 3D datasets.

Virtual online museum

This is a worthwhile effort because, as Dr Theobald Fuchs, chief scientist at Fraunhofer EZRT and MUSICES project leader explains: 'A large part of the collections of musical instruments held by museums is kept in underground storage facilities. In the case of the GNM, there simply is not enough exhibition space to showcase all 3500 of them at the same time. The CT digitalisation project will enable us to create a virtual museum in which digital facsimiles of these instruments are available to anyone with internet access.'

The team has already digitalised more than a hundred instruments dating back over several centuries – from the baroque trumpet and the mouth harmonica to the square piano. Different types of CT systems are needed to scan different-sized instruments. The square piano, for example, is X-rayed utilising a linear accelerator, which is the source of radiation in Europe's largest CT machine. The XXL X-ray environment consists of two eight-metre-tall steel scaffolding towers and a turntable with a diameter of three metres, housed in a hall covering a surface area of 400 square metres and rising to a height of 14 metres. Smaller string and wind instruments are X-rayed by using conventional apparatus. For each test, the object is placed on a turntable between the X-ray source and typically a flat-panel detector, which produces images of very high spatial resolution. A specially designed holder keeps the instrument firmly in place while the X-ray beam penetrates the rotating object. The required dose of radiation varies according to the thickness and



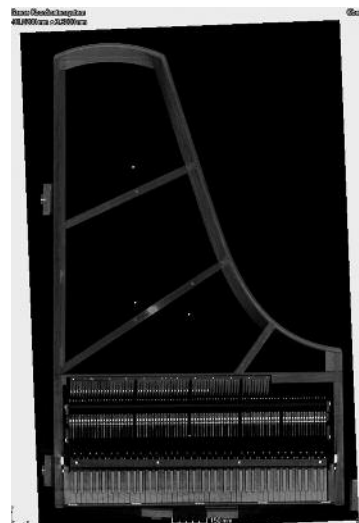
CT scan of a box-valve trumpet, viewed from the exterior. © Photo Fraunhofer EZRT



The CT scan of the interior reveals the complexity of this seemingly simple instrument. © Photo Fraunhofer EZRT



Above: X-ray image of the outer body of a pianoforte.



Right: X-ray view of the internal structure and components of a pianoforte.

© Photo Fraunhofer EZRT

density of the material. Depending on the structure and condition of the instrument, the scanning process can take several hours, during which the CT system records several thousand images, which are then stitched together to produce a three-dimensional view.

Published results will not only include the collected CT data but also detailed and comprehensible documentation of all steps in the measurement process. The examination standard defines the CT scanning parameters, and the accompanying set of guidelines provides advice on its application for different instruments.

Openly accessible metadata

Moreover, at the end of the project, all the technical parameters and metadata will be published in a database developed at the GNM. 'Ideally, we would like to be able to digitalise the museum's entire collection of historical musical instruments and place the 3D images online. Our examination standard defines the best way to go about this task', says Fuchs. 'One of the many factors that we are now able to quantify is the time needed to digitalise different instruments. For example, a complete X-ray scan of a violin at a resolution of less than

The MUSICES project at a glance

As part of the MUSICES (MUSical Instrument Computed Tomography Examination Standard) project, scans were made of more than a hundred different musical instruments of historical importance. Scientists and conservators at the GNM worked together with the Fraunhofer Development Center for X-ray Technology EZRT and the Chair of X-ray Microscopy LRM at the University of Würzburg to develop guidelines and standard procedures for the 3D computed tomography of musical instruments. The project is funded by the German Research Foundation DFG.

18th-century basset horns (with clarinets, a flute, and bassoons) at the Museum of Musical Instruments, Berlin.

Joan/CC-BY-3.0



50 microns takes up to 20 hours. This figure can be extrapolated to determine the time needed to scan an amount of x instruments. This produces a specific quantity of voluminous datasets, requiring corresponding amounts of hard disk and network capacity and special software. We have compiled a list of all these requirements.'

Another advantage of the standard is that it enables the knowledge and experience gained from scanning musical instruments to be applied to other museum collections such as telescopes and other scientific instruments or old weapons.

Thoralf Dietz is at the Fraunhofer Institute for Integrated Circuits

Collaborations in chemistry between Australia and FACS countries

It was nearly 40 years ago, on 15 August 1979, that 11 chemical societies met in Bangkok to form the Federation of Asian Chemical Societies (FACS). The objective of the Federation was to 'promote the advancement of chemistry and the interests of professional chemists in the Asia Pacific region'. The RACI has just accepted the presidency for the period 2017–19. Dave Winkler is President and Roger Stapleford is Secretary-General.

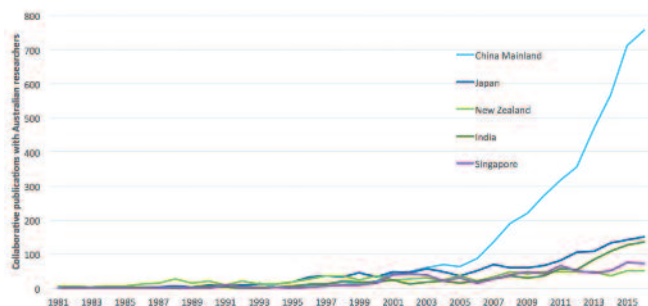
The founding societies were from Australia, Hong Kong, India, Iraq, Korea, Malaysia, The Philippines, Singapore, Sri Lanka, Indonesia and Thailand. This was a very small selection of countries from the Asia-Pacific region. Now there are 31 member societies representing countries from Mongolia in the north, Fiji in the east, New Zealand in the south and Turkey in the west.

One of the ways that the Federation sought to promote the advancement of chemistry in the region was to encourage collaboration between chemists in member countries. It established and supported a number of networks to assist chemists to understand their needs and capabilities.

Australian chemists were very active participants in these networks, and still are. In this article, we look at how these collaborations have resulted in scientific publications, and how the range of countries involved in collaborations has changed over the years.

The countries are those whose national societies are members of FACS. We analysed joint publications listed in the bibliometric database the Web of Science over the period 1981–2016.

The Web of Science covers 33 000 journals and its coverage has a distinct Anglo-Saxon bias. For example, only 185 Chinese language journals (out of approximately 10 000 such journals) are included currently. Data from the Web of Science will include research papers from the journals covered but books are only partially covered. Notwithstanding these limitations, the bibliometric data from the Web of Science gives insights into international research collaborative outputs. Plotting such data over the 1981–2006 period indicates how such collaborations

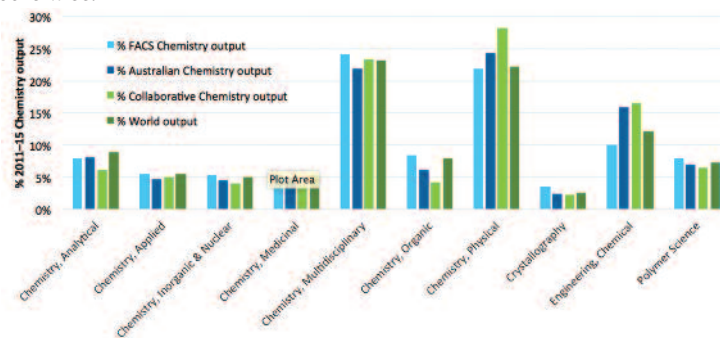


Trends in Australian chemistry collaboration with selected FACS countries 1981–2016.

have changed over time. Data for the five countries with the highest number of collaborative papers currently, namely China (Beijing), Japan, New Zealand, India and Singapore, are shown in the graph, bottom left. From negligible outputs in the early 1980s, the number of collaborative papers has grown, with those from China really increasing over the last 10 years. Those from Japan and India are also growing strongly, though less than for China, with India set to overtake Japan in the near future.

For the next set of active collaborations, namely those with South Korea, Malaysia, Russia, Hong Kong and Thailand, all show appreciable increases over the past 10 years in particular, with the strongest performers being Korea and Malaysia.

We have looked at the various subject areas of chemistry, as used by the Web of Science, to see where collaboration is strongest. The next graph shows such data 2011–15 for ten subject areas. For each subject area, we show the per cent of chemistry papers from FACS in total, of Australian chemistry overall, world chemistry output and per cent of FACS–Australia collaborative chemistry output. Of the ten subject areas, physical chemistry, chemical engineering and interdisciplinary chemistry are the most productive with physical chemistry being stronger for FACS–Australia collaboration than is the case otherwise.



Subject breakdown of Australia chemistry collaboration with all FACS countries 2011–15.

An extensive analysis of Australia–FACS chemistry collaborations is beyond the scope of this short article. Our study had a definite Australia–Asia focus. In the case of China, there were 2421 collaborative papers with Australia, suggesting a very strong collaboration, indeed the strongest for Australia. However, China also had 3144 joint publications with Japan, 1852 with Singapore and 1378 with South Korea. Therefore, care must be taken in interpreting such bibliometric data. We feel that, used with caution, it is a versatile measurement tool for gaining an understanding of international collaborations, the areas of emphasis and the changes over time.

John Webb FRACI CChem and **Tom Spurling** FRACI CChem are at the Centre for Transformative Innovation at Swinburne University of Technology, Melbourne; **Adam Finch** is Analyst, Science Impact & Policy at CSIRO, Adelaide.

2017 RACI National Award winners

Applied Research Award



Greg Qiao FRACI CChem received his PhD at the University of Queensland in 1996. He joined the University of Melbourne in 1996 and became a full professor in 2009. From 2012 to 2015, he was an Australian Research Council's (ARC) Professorial Future Fellow. He is a Fellow

of the Royal Society of Chemistry (RSC).

Qiao has published more than 230 journal papers and is a co-inventor of more than 20 patents. His key research interests are in novel macromolecular architectures; new activation methods for the RAFT process; structurally nanoengineered, antibacterial peptide polymers (SNAPPs); soft tissue engineering scaffolds; polymeric gas membranes; and chemical engineering products.

Qiao was the Chair of RACI Polymer Division from 2015 to 2016 and currently is a member of ARC College of Experts. He is an associate editor for the *Australian Journal of Chemistry* and is also on the International Advisory Boards of *Macromolecular Bioscience*, *Macromolecular Materials and Engineering* and *Ullmann's Encyclopedia of Industrial Chemistry*. Qiao received the ExxonMobil Award of Excellence for Chemical Engineering in 2015, RACI's Polymer Division Citation in 2011 and the Freehills Award in 2010.

Citation: Contributions to Chemistry and the Chemical Profession



Sam Adeloju FRACI CChem (BSc (Murdoch University), GradDipApplChem, GradDipScEd, MAppSc (Curtin University)) completed his PhD and postdoctoral studies at Deakin University, under the supervision of Alan Bond. Just four months into his postdoc, he was appointed as lecturer in chemistry at Deakin University in 1985, while also taking on the role of associate director of the Centre for Biological and Chemical Analysis. He moved to the University of Western Sydney in 1987 as a senior lecturer in chemistry and inaugural Head of Department of Chemistry. In 1988, he established the Centre for Electrochemical Research and Advanced Technology at UWS, and was its inaugural director until 2002.

Adeloju moved to Monash University in 2002 as Professorial Chair in Chemistry and Head of School of Applied Sciences and Engineering. Concurrently, he served as Campus Director of Research and Graduate Studies 2007–9, Executive Director of Australian Sustainable Industry Research Centre (not-for-profit company) 2003–9 and Acting Pro Vice Chancellor (Gippsland Campus) 2003–13. He stepped down as Head of School in 2010 and continued as a Professor of Chemistry and Director of Research Development in Science and Engineering

until 2013 when Monash discontinued its operation at the Gippsland campus. He moved to the School of Chemistry at Clayton in 2014 as Adjunct Professor of Chemistry while serving as Senior Foreign Expert under the China Talent-1000 Program 2012–16. In 2017, he was appointed Editor-in-Chief of the chemistry section of *Applied Sciences Journal* (MDPI Switzerland).

Adeloju is an internationally recognised expert in biosensing technology, nanotechnology, electroanalytical and environmental chemistry. He has published numerous papers, journals and books, speaking regularly at international conferences and conventions. He has accepted visiting professorships in chemistry at the University of Goteborg (Sweden), University of Liverpool (UK), University of Tasmania (funded by Eckart Australia), Hefei University of Technology (China), University of Kuala Lumpur (Malaysia); and he served for three years as External Advisor for Chemistry at the University of the South Pacific (Fiji).

Adeloju has devoted nearly 30 years of continuous service to the RACI. He co-established the Western Sydney section in 1989 and chaired the section for two years. He was Committee member for the Electrochemistry Division 1986–90, Secretary 1990–4 and Chair from 1994–7. He served on the RACI Council from 1994–97 and the *Chemistry in Australia* Management Committee 1997–2000. He returned to serve on the *Chemistry in Australia* Management committee in 2008 and has been chair of the committee since 2010. He also recently served as a RACI Board member from 2012 to 2015. He was awarded the RACI 2009 Applied Research Medal, the 2011 Stokes Medal from the Electrochemistry Division and the 2013 Doreen Clark Medal from the Analytical and Environmental Chemistry Division of RACI. He received his first Citation from RACI in 1997.



Suresh Bhargava

FRACI CChem is a world-renowned interdisciplinary scientist delivering research excellence that underpins significant industrial applications. As a passionate advocate for the application of technological science and engineering to

innovation, he provides consultancy and advisory services to many government and industrial bodies, including BHP Billiton, Alcoa World Alumina, Rio Tinto and Mobil Exxon. He was also a member of the independent board of directors of one of the Aditya Birla group of industries. Five of his seven patents have been adopted by the industrial partners and one has been licenced for commercialisation.

Bhargava has received many national and international awards, including the 2017 Non-Resident Indian of the Year Award by the TIMES Network, which recognised him as the most outstanding Indian academic in the Asia-Pacific region. Other notable awards include the 2016 Khwarizmi International Award (KIA) by the Government of Iran, the 2015 CHEMECA medal, the Indian National Science Academy's P.C. Ray Chair (distinguished lecture series 2014), RMIT University Vice Chancellor's Research Excellence Award (2006 and 2014), and RACI's Applied Research Award (2013) and R.K. Murphy Medal (2008). He is also an elected fellow of six learned academies, including the Australian Academy of Technological Sciences and Engineering and the National Academy of Sciences, India.

Bhargava has contributed over 410 refereed journal articles, one book, 11 book chapters and more than 200 refereed full conference papers. He has in excess of 9900 citations. Bhargava has delivered more than 50 conference keynote/plenary lectures over the last 15 years.

He has strived to create solid and

sustainable global research partnerships to improve and advance science and technology. The establishment of the Indian Institute of Chemical Technology-RMIT joint research centre is one of the best examples of his international efforts. He has also applied this innovative model to connect RMIT with Academy of Scientific and Innovative Research laboratories across India. His pioneering and entrepreneurial spirit has seen him champion innovation through the Academic Sharp Brain event at the 2017 RACI Congress, as well as discussing the missing half of innovation on ABC Radio's *Ockham's Razor*.



Helmut Hügel FRACI CChem switched from medicine to molecular science studies, receiving his PhD from the University of Melbourne. At RMIT University School of Science, he is passionately involved in teaching and research in medicinal and chemical synthesis. He has over 40 years of academic experience in research, discovery and development, mainly focused on biology oriented synthesis science, including myxobacteria metabolites to treat cancers, polyphenols for the prevention of neurological disorders, and the generation of biomaterials to sustain human function.

His personal outlook is that research makes innovative thinkers and is really relevant when it has an impact on human lives, and improving lives is the only goal that really matters.

Hügel has written more than 130 peer-reviewed publications. During the last 10 years, he has collaborated with colleagues on six ARC grants,

including synthesis of myxobacteria metabolites and analogues. In 2016, two ARC DP applications, a dementia collaborative research centre and three other grant proposals were submitted. Editorial honoraria payments, consulting fees, and miscellaneous income funds sustain his science projects.

Robert Ryan FRACI

CChem (ASTC diploma (Sydney Technical College), BSc (School of Chemistry) and MSc (School of Chemical Engineering and Industrial Chemistry) University of New South Wales) is principal consultant, VAPORFAZE (focus on innovative gas/vapour technologies to achieve pest and pesticide-free commodities).

His major career was 40 years as chief chemist, marketing manager and development manager with the Linde/BOC/CIG Industrial Gases Group, including a two-year secondment at the Welding Institute, Cambridge, UK.

In the 'insect world', Ryan is President of the Entomological Society of New South Wales, a licensed pest control operator, a government registered fumigator and a former part-time lecturer for the NSW TAFE's Pest Control Certificate Course. Ryan has experience with World Bank Fumigation Projects in China; United Nations (UNIDO) Fumigation Projects in Indonesia, Thailand and Vietnam; and Technology Transfer Fumigation Projects in the Arabian Gulf, Egypt, New Zealand, Philippines, China and Cyprus. He is currently investigating alternative global grain and commodity fumigants.

Ryan is a former NSW and National President of RACI, and a Fellow of the Australian Institute of Food Science and Technology and the Australian Marketing Institute.



Cornforth Medal



Amandeep Kaur MRACI completed her Masters studies in chemistry, with a university medal from VIT University, India, in 2012. Thereafter, she took up a research internship at ENSCCF, France, where she worked towards understanding the behaviour and biocompatibility of

transition metal-doped calcium phosphate ceramics.

Kaur completed her PhD in 2016 from the University of Sydney under the supervision of Dr Elizabeth New, during which she was awarded with the World Scholars Scholarship. Her PhD research involved the development and application of reversible and fluorescent redox sensors to understand the role of oxidative stress in biological systems. She is currently a postdoctoral research fellow at the EMBL Australia Node in Single Molecule Science and ARC Centre of Excellence in Advanced Molecular Imaging, University of New South Wales, with Dr Senthil Arumugam investigating the mechanisms underlying endosomal sorting of cargoes and lipids.

Distinguished Fellowship



Ian Rae FRACI CChem was awarded a Distinguished Fellowship. The largest single engagement of Rae's career was with Monash University, an institution that he joined in 1967 and left in 1994. His mentor Professor John Swan said that a university appointment was a platform from which to launch other involvements. Rae took him at his word, and without (he believes) interfering with his university duties, he launched into secondary school chemical education, some industrial consulting and legal work, writing for RACI (notably his trademark Letters) and dabbling in chemical history.

When Rae left university employment in 1997, through the Victoria University portal, he embarked on another career, as an adviser to the Australian Academy of Technology and Engineering, where he is a Fellow, to Australian governments and eventually to the United Nations Environment Programme. He also developed a more public face as a media adviser. As some of these activities faded, he was able to ramp up the chemical history work. In 2015, he accepted appointment as an editor of the Australian Academy of Science journal *Historical Records of Australian Science*. He is now busily entering his ninth decade, still polishing his portfolio career and writing those Letters.

Fensham Medal for Outstanding Contribution to Chemical Education

Tina Overton FRACI is Professor of Chemistry Education at Monash University and Honorary Professor at the University of Nottingham. She was previously Professor of Chemistry Education at the University of Hull, UK, and has worked in industry and in the NHS. She has taught inorganic, industrial and environmental chemistry and has designed and delivered online distance-taught and work-based programs.

Overton has published on the topics of critical thinking, context and problem-based learning, the development of problem-solving skills, work-based learning and employability. She has published learning resources that have been adopted in many institutions and has co-authored several textbooks in inorganic chemistry and skills development. She has been awarded the Royal Society of Chemistry's HE Teaching Award, Tertiary Education Award and Nyholm Prize and is a National Teaching Fellow and Senior Fellow of the Higher Education Academy.



H.G. Smith Memorial Medal



Martina Stenzel

FRACI CChem studied chemistry at the University of Bayreuth, Germany, before completing her PhD in 1999 at the Institute of Applied Macromolecular Chemistry, University of Stuttgart, Germany. She started as a postdoctoral fellow at the University of New

South Wales in 1999 and is now a full professor in the School of Chemistry as well as co-director of the Centre for Advanced Macromolecular Design.

Her research interest is focused on the synthesis of functional nanoparticles for drug delivery applications. Stenzel published more than 270 peer-reviewed papers mainly on polymer and nanoparticle design. She received a range of awards for her work, including the 2011 Le Fèvre Memorial Prize of the Australian Academy of Science.

Stenzel has served as a panel member for the Australian Research Council. She is currently the chair of the National Chemistry Committee of the Australian Academy of Science and has been active in the RACI for many years, which includes her role as Honorary Secretary and chair of the polymer division. She is currently scientific editor of the RSC flagship journal *Materials Horizons*.

Le Fèvre Memorial Prize (Australian Academy of Science and RACI)



Deanna D'Alessandro

FRACI CChem obtained her BSc in chemistry, physics and mathematics at James Cook University and received the University Medal in 2001 following Honours studies in chemistry. She completed her PhD at JCU in 2006 under the supervision of Emeritus Professor Richard Keene, receiving the 2006 RACI Cornforth Medal and a 2007 IUPAC Prize for Young Chemists. D'Alessandro undertook postdoctoral research with Professor Jeff Long at the University of California, Berkeley, from 2007 to 2009 as the Dow Chemical Company Fellow of the American–Australian Association and a Royal Commission for the Exhibition of 1851 Research Fellow. She returned to Australia in 2010 as a University of Sydney Postdoctoral Research Fellow and L'Oréal Australia for Women in Science Fellow. In 2011, she received an Australian Research Council QEII Fellowship, which allowed her to start building her own research group exploring energy-related applications of microporous materials.

D'Alessandro's research is delivering new insights into an exciting area in nanoporous molecular materials, namely, their electronic and conducting properties. These fundamental advances have enormous potential as the basis of new technologies for a diverse range of applications, including electrocatalysis, sensing and solar energy conversion. In addition to her work in the area of theoretical and experimental aspects of electron transfer, for which she has gained

international recognition, she has played a major role in the development of new nanoporous materials for the capture and conversion of greenhouse gases, particularly carbon dioxide. A common theme of her research has been a desire to tackle significant scientific challenges by probing fundamental chemical questions.

She has also been the recipient of a 2011 Tall Poppy award, a 2012 Distinguished Lectureship Award from the Chemical Society of Japan, the 2014 RACI Rennie Medal and a 2015 ChemComm Emerging Investigator Lectureship from the Royal Society of Chemistry.

Leighton Memorial Medal

Mark Humphrey

FRACI CChem joined RACI in 1982 when he was a student at the University of Adelaide and became a Fellow of the Institute in 1997.

Humphrey has been at the ANU since 1994, initially in the Department of Chemistry, and since 2009 in the Research School of Chemistry. In the past few years, he has served on the Australian Research Council's College of Experts and ERA Research Evaluation Committee. He leads major international research collaborations with France and China and has about 310 publications, mostly dealing with organometallic chemistry and/or non-linear optical materials research.

Humphrey is a recipient of the RACI's Organometallic Award (1998), Inorganic Division Award (Burrows Award) (2008) and H.G. Smith Memorial Medal (2010). During 22 consecutive years of service to the RACI, he held a number of positions in both the ACT Branch and the Inorganic Division, and served as President of the former and Chair of the latter. He has been particularly active in conference organisation, chairing or co-chairing 16 conferences and symposia, including RACI Inorganic Division meetings and OZOM conferences.



Margaret Sheil Leadership Award

Mary Garson FRACI CChem is a professor



of chemistry at the University of Queensland. She graduated from the University of Cambridge, UK, with PhD and MA degrees, after which she undertook postdoctoral studies in Italy. This was followed by a college research fellowship at

New Hall, Cambridge, and then a two-year period as a medicinal chemist at Smith, Kline and French Research, UK (later Glaxo Smith Kline). She started her independent research career with a Queen Elizabeth II Research Fellowship held at James Cook University of North Queensland (1983–6). Prior to joining the University of Queensland as the first female academic staff member in chemistry in 1990, and later as the first female professor of chemistry in Queensland, she held an academic staff position at the University of Wollongong.

Garson has made significant contributions to the fields of terrestrial and marine natural products, biosynthesis and chemical ecology for over 40 years. She has completed more than 400 scuba dives for sample collection; the flatworm *Maritigrella marygarsonae* ('little female sea tiger') is named in her honour.

Garson has made many service and leadership contributions to women in chemistry both within Australia and overseas. In 2011, she created and convened a global breakfast event 'Women sharing a chemical moment in time' for the International Year of Chemistry. This global event will be repeated in 2019 during the centenary celebrations for IUPAC. In recognition of her significant role supporting female scientists, Mary was included in the Queensland Government's online tribute gallery *Everyday women, extraordinary lives* in 2011. She was awarded the most senior award of RACI, the Leighton

Memorial Medal given in recognition of outstanding service to the Institute, in 2011. In 2013, she was honoured as one of 12 international recipients of the Distinguished Women in Chemistry or Chemical Engineering award of IUPAC.

Garson has served the RACI in various capacities, including as Queensland Branch President, and as Chair of the International Relations Committee, and thereby a member of the National Committee for Chemistry. She chaired the board of Australian Science Innovations, with responsibility for Australia's teams in international science Olympiads between 2002 and 2005. She has been involved with the International Union of Pure and Applied Chemistry (IUPAC) since 1994, including as President of Division III (organic and biomolecular) for the 2014–15 biennium. She currently chairs the international Management Committee, overseeing planning of the centenary year of IUPAC in 2019, and has been elected a member of the Bureau of IUPAC for 2018–21.

Masson Memorial Award

Liam Burt (student member) grew up in the seaside town of Penguin in north-west Tasmania. He completed his BSc (chemistry and physics) at the



University of Tasmania in 2017. Along with several undergraduate research projects at his native university, he has engaged in two summer research programs with Professor Anthony Hill at the Australian National University between 2016 and 2018. He will undertake Honours in Chemistry at the University of Tasmania with Dr Alex Bissember beginning in 2018 and his project will focus on the development of new visible light copper-photocatalysed reactions.

RACI Educator of the Year

Erica Smith MRACI

CChem holds a BSc(Hons) from the University of Sydney, a Master of Science with Distinction from the University of Greenwich (UK), and a Doctorate in Theoretical and Computational Chemistry from the University of Houston (USA). She was an Associate Professor of Chemistry at Lonestar College (USA) before returning to Australia to take up a postdoctoral research fellowship at the CSIRO, where she worked on computational animal genetics for livestock breeding. She is currently a senior lecturer in chemistry at the University of New England.

Smith's scientific research utilises computer simulations to gain atomic level understanding of biological and industrial systems with a focus on processes that occur at interfaces. She

has published research on chemical education and is a member of the RACI Chemical Education Division committee. She also has several years' experience working in STEM-based industries in Europe and Australia.

Smith is a passionate and dedicated educator. She has extensive experience with school outreach programs, including leadership of two programs designed to inspire students and create equity within STEM disciplines. She has received a University of New England Excellence in Teaching Award, an Australian Awards for University Teaching Citation for Outstanding Contribution to Student Learning and is a senior fellow of the Higher Education Academy (UK).



Rennie Memorial Medal



Liz New FRACI CChem undertook her undergraduate and Masters studies at the University of Sydney before completing her PhD studies in 2010 at the University of Durham (UK). She was then a Royal Commission for the Exhibition of 1851 Research Fellow at the

University of California, Berkeley. In 2012, she returned to the University of Sydney, holding an ARC DECRA from 2012 to 2014, and a Westpac Research Fellowship from 2016.

New's research focuses on the development of small molecule chemical sensors for the study of oxidative stress and metal ions in biology. Her research awards include the Premier's Prize for NSW Early Career Researcher of the Year (2016) and the ChemComm Emerging Investigator Lectureship (2017). New was the 2014–15 RACI NSW Nyholm Lecturer and the 2017 RACI Tasmania Youth Lecturer, and she currently serves on the executive of the Australian Academy of Science's Early-Mid Career Researcher Forum. She is also passionate about teaching, and has received awards, including the RACI Chemistry Educator of the Year (2016).

Rita Cornforth Lectureship



Lidia Matesic MRACI CChem completed a BMedChem (Hons) degree and graduated with a PhD in chemistry in 2011 from the University of Wollongong, where her research focused on the targeted delivery of novel anticancer agents. In 2011, she commenced a postdoctoral fellowship at the Australian Nuclear Science and Technology Organisation (ANSTO).

She now works at ANSTO as a radiochemist where her primary research interest has been in the field of radiopharmaceutical development using the radioisotope, fluorine-18. In particular, her research involves the synthesis of radiopharmaceuticals by using microfluidic flow chemistry.

In 2012, she was awarded an Early Career Fellowship from the Australian Academy of Science to work at Centre Cycon in Caen, France, on the development of new radiopharmaceuticals to diagnose stroke. Her other scientific achievements include a Fresh Science NSW Award (2016), the RACI NSW Nyholm Lectureship (2016–17) and a HOPE Fellowship from the Japan Society for the Promotion of Science (2017). Matesic is actively involved in the RACI NSW Branch, where she has been the Treasurer since 2016.

Weickhardt Award

Calum Drummond FRACI CChem is a graduate of the University of Melbourne (BScEd, BSc(Hons), PhD and DSc). He has been an Australian Research Council (ARC) Queen Elizabeth II Fellow and an ARC Federation Fellow.



Drummond is currently RMIT Deputy Vice-Chancellor Research and Innovation and Vice-President. He joined RMIT University, as Deputy Vice-Chancellor Research and Innovation, in 2014 from CSIRO where he was Group Executive for Manufacturing, Materials and Minerals. Immediately prior to this CSIRO Group Executive appointment, he was Chief of CSIRO Materials Science and Engineering (CMSE). Before becoming a Chief, Drummond was seconded from CSIRO to be the inaugural Vice President Research at CAP-XX, an Intel portfolio company. CAP-XX develops supercapacitors for consumer electronic products. In 2006, CAP-XX listed on the London AIM.

Drummond is an author of over 200 publications. His research interests are in the area of advanced materials, including application to energy storage and biomedical products. He has a strong interest and passion for the commercialisation of research outcomes.

Drummond was nominated the Weickhardt Award for his roles as a researcher and project leader in many translation projects of chemical research to benefit industry and the Australian economy; an organisational science and innovation leader creating research and innovation ecosystems that support value creation for companies operating in Australia; and a member of governance and advisory boards for governments and industry.

From testosterone to dogs, and physics for babies: five fascinating books in 2017

In my mild-mannered persona as an academic in science education, I teach and research ways that science can be better taught in Australia and globally.

But every year I also explore the world of science books. I scope what's new and interesting for my not-for-profit science book blog, and the Big Ideas Book Club I help run in Melbourne.

In 2017, five books in particular grabbed my attention, covering the fields of psychology, biology, history and physics.

How men and women behave

Testosterone rex: unmaking the myths of our gendered minds, by Cordelia Fine, Allen and Unwin



This book won the Royal Society Book Prize in 2017. The author is University of Melbourne's Cordelia Fine, an academic working in historical and philosophical studies with a background in experimental psychology.

With discussion of feminism in the media on a regular basis, this book provides an important critique of previous research that has linked many underlying societal assumptions about testosterone to explain behaviour of both men and women. For example, 'men engage more in risk-taking behaviour'.

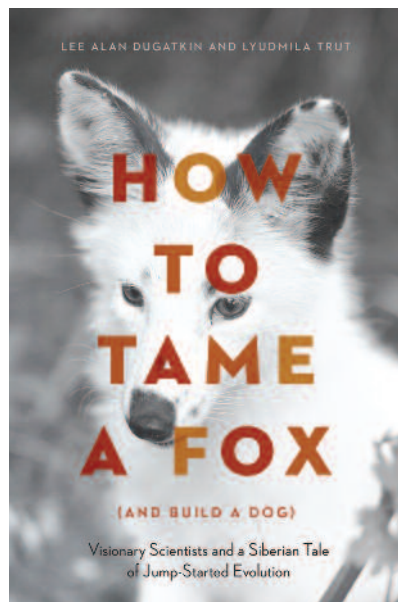
Many of us assume that science is done without prejudice, but Fine

highlights how social factors influence what research and concepts are considered important. This can compound an over-simplified notion of how testosterone affects us both biologically and socially.

Fine covers a wide range of topics in this short book, and often I found myself wanting to know more. But I think she successfully achieves her aim of getting us to reconsider some assumptions in our everyday lives. She helps the reader realise that when it comes to testosterone, things are a little bit more complicated than we may have assumed.

Where dogs came from

How to tame a fox (and build a dog): visionary scientists and a Siberian tale of jump-started evolution, by Lee Alan Dugatkin and Lyudmila Trut, University of Chicago Press



This book is at the top of my holiday reading list. It's part of a wave of science books directed at understanding the inner minds of dogs, their behaviour and their evolution.

Growing up with chihuahuas in the house, it can be difficult to reconcile how my family dog had somehow evolved from the wolf. While foxes are not wolves, the question of how wild animals can be

domesticated was investigated by a team of researchers in Siberia, commencing in 1959, led by Dmitri Belyaev and Lyudmila Trut. The latter is currently head of the research group at the Institute of Cytology and Genetics of the Siberian Department of the Russian Academy of Sciences, and one of the authors of this book.

The premise was quite simple: to recreate the process of domestication from wolves to dogs – a process that is estimated to span 15 000 years – by selecting and breeding foxes on the basis of their tameness.

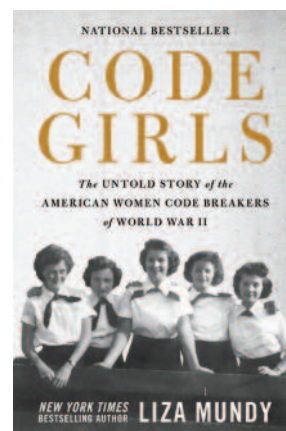
Trut and co-author Dugatkin (a biologist and science writer) write about the history, politics and outcomes of this experiment, including genetic, behavioural and physical changes seen in wild foxes as they became tame foxes with floppy ears, curly tails and an interest in human companionship.

This looks perfect for anyone interested in the history of dog-kind, and in how scientists answer questions about our relationship with our closest companions.

Women deciphering military codes

Code girls: the untold story of the American women code breakers of World War II, by Liza Mundy, Hachette Book Group

Code girls is one of several recent books that tell stories about women's involvement in history and science – others include *Hidden figures* (2016), *The radium girls* (2016), *Rise of the rocket girls* (2016), and *The girls of Atomic City* (2013). The previously untold stories of these remarkable women are being recorded as they get older, and as previously classified documents are shared with the public.



This particular book tells the story of some 10 000 women who were recruited by US military intelligence during World War II to decipher Japanese and German military codes. A great opportunity for highly educated women, they were taken from around the country and moved to live in dormitories in Washington and Arlington. Here, they had to deal with sexism, bureaucracy, relationships and new-found freedom.

To prepare the book, author Liza Mundy – a journalist who has written for the *Washington Post* – interviewed 20 of these code girls, who over 70 years ago had taken a vow of secrecy about their work.

Due to the age of the women, Mundy worked diligently to locate them:

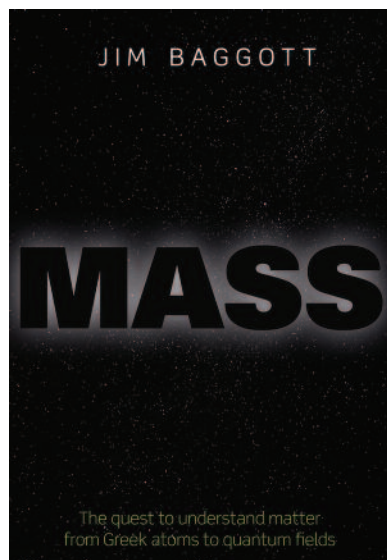
I literally cold-called most of the women, and they were delighted to hear from someone who wanted to know about this.

I was struck by the number of adult sons who were really proud of what their mothers had done and had wanted them to tell the story forever.

This book captures the highs and lows of these brave women, and celebrates their rich and varied impact on generations of women working in science and technology.

A journey through mass

Mass: the quest to understand matter from Greek atoms to quantum fields, by Jim Baggott, Oxford University Press



Mass is one of those terms that many of us first encounter in primary school, but what is it, really?

Popular UK science writer (and former scientist) Jim Baggott takes us on a journey through mass. He presents early philosophical considerations, how mass influences the elements of the periodic table, and then to modern considerations of mass that have come from recent work from quantum physics, field theory and the standard model.

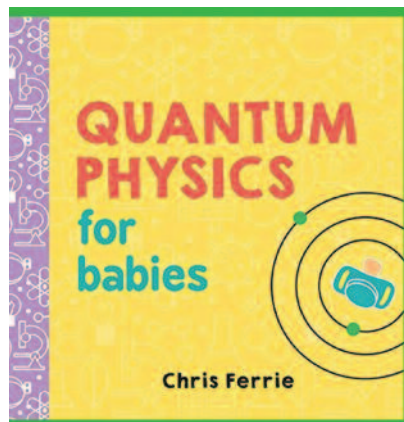
Typically, we consider that mass is a property that all things ‘possess’, but Baggott asks us to reconsider this idea, and to think that mass is an outcome of what things ‘do’.

If this has left you scratching your head, don’t worry; Baggott is a skilled writer, as Kevin Orrman-Rossiter writes in his review:

I found his concluding chapter ‘Mass without mass’ to be a great example of his writing in Mass. In this he brings us to the question of matter – via a familiar and everyday substance – frozen water, an ice-cube. He asks ‘What is this cube made of? What is responsible for its mass?’ Using this simple example, he recaps and brings to a prosaic conclusion what is an enthralling, philosophically deep and scientifically rich, story.

Good for chewing, and learning

Quantum physics for babies, by Chris Ferrie, Source Books Inc.



This is part of the Baby University series of board books written for babies.

Author Chris Ferrie is an academic from the University of Technology Sydney, who conducts research into quantum physics.

The question immediately comes to mind: ‘Can you teach quantum physics to babies?’. My immediate answer would be ‘no’, but that isn’t Ferrie’s intention. He wants the book to be a starting point of exploration of a wider scientific world for children, but also for parents to dip their toes into an area they might feel uncomfortable with. He says:

many parents I talk to find mathematics and science scary. Whether it is intentional or not, they steer [their children] away from these topics.

I purchased the Baby University series of books for my little person, who likes to chew them. But with him, I have enjoyed the colourful and varied diagrams that represent the complex quantum concepts with minimal text.

The book is a way for parents and children together to explore science concepts and connect to the ideas and representations that they use. Science has its own language of words and images, and the earlier we explore these, the less mysterious and unknowable science will seem to be.

These are just a selection of the many science books that come out every year to enlighten, enthrall and entertain us. I struggled to suggest only five books.

When you choose a book to get you through the holiday break, make sure you have a look at what science has on offer, whether it’s about birds, space, the human body, psychology or robots. Science offers us a new perspective on the world – one that is intriguing, affirming and full of life; it’s not just about equations and numbers.

George Aranda is a lecturer in science education at Deakin University. First published at The Conversation (www.theconversation.com).

Research, development, demonstration and commercialisation

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The thrust of most, but importantly not all, basic research is to develop a commercial process or product. In most instances, the path from basic research to commercialisation progresses through the intermediate stages of development, which aims to prove up the research on a small scale (often called bench scale), and demonstration in which larger process plant is used to produce product on sufficient scale for market evaluation.

For some commercial products, this process can take many decades while other basic research progresses to commercialisation within a decade. This time scale appears to depend on market demand and acceptance for the final product. For instance, lasers were discovered in the 1950s but it was not until the 1980s that their commercial use took off; for many years, lasers were considered a solution looking for a problem. By contrast the discovery of high-brightness blue-light-emitting diodes revolutionised lighting within a decade from their discovery in 1995. Today, the use of LEDs is widespread.

Lasers and LEDs are based on the same basic research into doping semiconductors with alien materials. This fact reinforces the view that some basic research should be supported for its own sake, not just research that might have an immediate commercial outcome.

Passing from research to development results in many bright ideas falling by the wayside as fundamental issues become more closely defined. Sometimes success requires progress in an unrelated area.

The transition from bench scale to demonstration requires significant levels of funding, which means many more personnel become involved and research workers have to be able to communicate with people with non-scientific backgrounds. However, in my experience, scientists and engineers in managerial roles tend to be more sceptical than non-scientists towards new ideas; often people with a science or engineering background focus on finding problems (i.e. reasons not to fund development) rather than the blue-sky opportunities that may ensue from success of a development.

One of the hurdles faced by projects transitioning from research into development is that quite a lot of research is funded on a 'me too' principle, and success at the research level forces funders to ask: 'Why are we doing this research at all?' My first industrial research project (developing new catalysts for elastomer production) fell on this question. Often this has overtones of *Yes, Minister*, with research aimed to give the organisation (or government) blessing on what it would like to see achieved, not to actually achieve something of merit that would result in difficult funding questions. I fear there is a lot of this around.

The demonstration stage involves interaction with the market (i.e. people willing to pay for the product), and feedback – which can be quite unexpectedly critical of the product – is an important part of the process. This stage of the process often attracts critics (usually not directly involved). In

One of the main problems with Australian government intervention in the development process is that there is a strong tendency to believe foreign technology promoters rather than local experts, whose views are often ignored completely ...

'The plastics project that went to waste' (May 2016, p. 34), I gave an illustration of a project that failed at this stage. However, if the project passes successfully through demonstration, then the next stage is commercialisation. This stage involves serious amounts of money and many more non-scientific personnel.

Back in the 1970s, ICI developed and commercialised dry powder fire-extinguishers. The inventor, Dr Derek Birchall, discovered the fundamentals when he put some potassium oxalate into a Bunsen flame (flame test) and noticed, as well as the usual lilac coloration, a large hole appearing in the flame, the consequence of CO and similar radicals quenching the flame. He developed the idea, with the final commercial product using a potassium bicarbonate/urea complex (Monnex™). He was invited to the official launch, which involved hundreds of people, very few of whom he knew, and who kept asking him what his role in the development had been.

It is notable that at the stage prior to commercialisation, science and engineering are only one, and not a dominant one, of the many inputs into the decision-making process. People's careers and egos often come to the fore and organisational political considerations are often dominant. Naysayers are often openly shunned.

As noted, the time from research discovery to commercialisation can be quite long and steps are often taken to shorten the process. One successful way is to increase the scale of the development program so as to produce a significant volume of product. Du Pont used this method successfully in the development of their production of hexamethylene diamine by hydrocyanation of butadiene. However, this approach is fraught with danger and there have been many failures in omitting trials at larger scale. The root cause is generally engineering in nature because, as scale increases, fluid flow often moves from laminar to turbulent, which can change thermal equilibria and fluid behaviour within the system. Often this can be overcome by re-engineering reactor design, but at additional cost, which upsets the project funders.

One of the main blocking points in private industry is justifying funding at demonstration level and then addressing

issues of technical risk, a major concern in the finance community, in a commitment to a commercial venture. These issues seem to be much lower for governments (using other people's money) and there are many examples of government-sponsored development moving rapidly because of political considerations rather than because of technical issues.


This is shown by the rapid Chinese development of a large coal-to-chemicals industry (see July 2015, p. 36). The technology was demonstrated by several US and European chemical and engineering companies, but it took the central planning of the PRC to spur commercialisation. However, not all attempts proved successful, with the PRC withdrawing from coal hydrogenation to produce fuels, a technology that was at a similar stage in the development process.

We may be seeing Australian governments trying to force the pace of development in an attempt to solve the east coast energy crisis by promoting and quickly introducing novel battery back-up and other unproven systems for both domestic and base-load power – technologies that are still not proven in terms of cost-benefit, durability, safety and reliability.

One of the main problems with Australian government intervention in the development process is that there is a strong tendency to believe foreign technology promoters rather than local experts, whose views are often ignored completely – what used to be called the cultural cringe. Back in the 1980s, I was working at BHP with several academic and CSIRO groups on a large gas to fuels project and we were surprised to learn that the Commonwealth was funding, to the tune of \$90 million, a US entrepreneurial group to do the same.



Duncan Seddon FRACI CChem is a consultant to coal, oil, gas and chemicals industries specialising in adding value to natural resources.



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Adding water to wine

The heading above is the title of a 2002 article by Jancis Robinson (bit.ly/2BVGD6X), referring to the addition of water to grape must to dilute the sugar concentration before fermentation, thereby giving a lower alcohol concentration in the finished wine. Perhaps trying to give some biblical justification to the addition of water, the term ‘turning water into wine’ has been coined by some (bit.ly/2pJI8Qj).

The need to find a way to reduce the sugar concentration is driven by various factors, including the demand in the marketplace for wines with lower alcohol concentration, the potential problem with ‘stuck’ fermentations (see below) and the maximum alcohol concentration that some countries impose on imported wine. Without going into the reasons for high grape sugar concentration here, the options to lower the final alcohol concentration are to either remove some alcohol after the fermentation by costly technology (see October 2012, p. 39) or reduce the sugar concentration by adding water prior to the fermentation. Of the two, water addition is by far the cheaper and quicker way to reach the desired goal.

Dilution of grape must with water has been carried out in Australia and other countries for a long time. It is just that until the end of 2016, the process was illegal. Food Standards Australia New Zealand (FSANZ) approved the addition of water to ‘facilitate wine fermentation’ (see FSANZ Application A1119). The wine industry argued that the need for water addition is a consequence of high sugar must causing slow or ‘stuck’ ferments. With non-functioning yeast, the resulting wine can be high in residual sugar and/or extensive production of acetic acid may occur (see bit.ly/2pAPu8k on this fermentation issue). The New Zealand wine industry could not see the need for adding water because there is little opportunity for grapes grown there to achieve the high sugar levels found in some regions of Australia. FSANZ, in a delightful inter-government solution, argued that the practice of water addition was to be optional and not mandatory and thus would not be required for New Zealand wineries. The amount of water that can be added, or perhaps the degree of sugar adjustment that can be achieved, is regulated. Practical issues regarding water addition are described in an AWRI technical note by Geoff Cowey (*Aust. NZ Grapegrow. Winemak.* 2017, vol. 639, pp. 88–9).

While some new-world wine countries now allow water addition, many countries do not. If the addition of water to grape must remains illegal, then there needs to be an accepted procedure for assessing if water has been added. Here, analytical chemistry rises to the fore, as it does in so many other wine characterisation/authentication issues (see the blog at bit.ly/2C9nqvp). The $^{18}\text{O}/^{16}\text{O}$ ($\delta^{18}\text{O}$ -value), measured by isotope ratio mass spectrometry, is the accepted standard method for detecting water addition.

It has been known for some time that after véraison (the transition from berry growth to berry ripening) the ^{18}O isotope



is enriched in grape water. This isotope enrichment process is in part a consequence of biotic factors that include sugar photosynthesis and the grape cultivar, and the abiotic factors of region, climate, rainfall and harvest timing. The frustrating issue when using the $\delta^{18}\text{O}$ -value for legal authentication is that the level of ^{18}O enrichment varies from year to year as well as between countries and regions within countries. Thus the creation of medium-to-large-scale data banks of standard wines is a prerequisite for the success of this method. In 1991, the EU commenced the creation of such a data bank for EU wines as well as one for non-EU countries that import wine into Europe (see Christoph et al. 2015, doi: 10.1051/bioconf/20150502020; Rossmann et al. *Z. Lebensm. Unters. Forsch. A* 1999, vol. 208, pp. 400–7). More recent work has attempted to use the $\delta^{18}\text{O}$ -value for wine ethanol in combination with the $\delta^{18}\text{O}$ -value for wine water (Perini, Camin, *J. Food Sci.* 2013, vol. 78, pp. 839–44), but this seems to be more academic than of direct practical use at this stage.

I first came across the application of stable isotopes for wine authentication at the first two *In Vino Analytica Scientia* conferences in 1997 and 2001. One presentation related to the issue of a wine available in the market place and labelled as a wine from EU country-1 that showed characters that questioned its claimed origin. Using the measured $\delta^{18}\text{O}$ -value, it was demonstrated that the wine actually came from grape juice concentrate, sourced from EU country-2, which had been broken down to an acceptable sugar concentration by water addition prior to fermentation. Intriguingly, the legal point was presented as a case of consumer fraud, even though there was nothing particularly wrong with the wine itself. This takes us into a debate of retail ethics, fraudulent behaviour and analytical chemistry, a topic perhaps for another day.



Geoffrey R. Scollary FRACI CChem (scollary@unimelb.edu.au) was the foundation professor of oenology at Charles Sturt University and foundation director of the National Wine and Grape Industry Centre. He continues his wine research at the University of Melbourne and Charles Sturt University.

Squeezing the life out of them

This little story started in the dentist's waiting room, where the most readable thing on the coffee table was a foodie magazine, and my eye was taken by an advertisement for 'cold pressed milk'. Hmm, there had to be some chemistry here, I thought.

The few details in the advertisement, a few more on the website that was mentioned there, and a fair bit that was alluded to but not clearly stated, led me to understand that subjecting milk to high pressure was a way of killing off microorganisms that could cause spoilage. In this, 'cold pressing' was about as effective as pasteurisation, in that there was not total elimination of microorganisms but their numbers were reduced so that the shelf (or refrigerator) life of the milk was increased. There were sly allusions to the taste of pasteurised milk and claims that unlike the heat-treatment processes, cold pressing did not change the chemistry in any detectable way.

The publicity for this new technique also stressed that the milk had not been homogenised, so a fresh bottle had a layer of cream at the top, just like good old milk. I wasn't sure whether pasteurisation and homogenisation were inevitably linked, but the advertising asked me to believe that this was the case. The advertisement said that cold pressing was good for fruit juices, too, by which I understood that the actual juicing operation was not conducted under high pressure, but the microorganism count of the product was reduced by subsequent pressure treatment and the shelf life was accordingly extended.

I turned to the literature – to wit, a 750-page multi-author book – to find out more about it. The technique is at least a century old but it was not until the 1990s that it became popular, notably by Japanese food producers. It is described as a 'commercially viable technology', a phrase that carries with it a hint of a technology looking for applications. In general, the product to be treated is contained in flexible packages, possibly vacuum-packed, so that hydrostatic pressure applied to the packaging can be transmitted evenly to the contents. The

... the product to be treated is contained in flexible packages, possibly vacuum-packed, so that hydrostatic pressure applied to the packaging can be transmitted evenly to the contents.

acronym HHP – high hydrostatic pressure – is adopted in technical literature but I can understand that 'cold pressing' sounds less high-tech and more user friendly.

The pressures for milk are mostly in the range of 400–600 megapascals. For most of us this is unfamiliar territory, but a typical car tyre pressure is 200 kilopascals, over 1000 times smaller. The process is normally conducted at about room temperature, so I take the reference to 'cold' as meaning 'not heated' – that is, not pasteurised by heat shock in the conventional way. The pressure is exerted for just a few minutes, during which there is warming of the milk, but only by a few degrees Celsius, because milk is not very compressible. By contrast, when air is compressed, say in a bicycle pump, it gets hot because the change in volume is much greater and the change in temperature is correspondingly greater. Detailed chemical examination of 'cold pressed' milk has revealed nothing much in the way of molecular change, but some changes in the casein micelles have been noted, especially when HHP is applied for longer periods. Proteins can be denatured, but they retain their nutritive value, and proponents claim that there is no difference in taste.

It's easy to understand why a bacterium, essentially a bag of cytoplasm enclosed in a cell wall, can be killed by pressure that 'pops' the container and spews out the contents. What about the other potential food contaminants, the viruses, I wondered. A virus has no cell wall, but consists of nucleic acid coated with protein and sometimes an extra layer of lipid. If the virus could survive high pressure, then pressure-treated food could still deliver a dose of gastro or even hepatitis. Early experiments suggested that viruses were extremely resistant to the effects of high pressure, but it turned out that the test organism, tobacco mosaic virus, is an unusual one, requiring over 900 megapascals to inactivate it. Later work showed that the viruses we might be exposed to in contaminated shellfish – hepatitis and the noroviruses that cause gastroenteritis – can be inactivated by about half of that pressure. Some viruses, after deactivation by pressure treatment, can still provoke an immune response and this observation has opened the way to new techniques for the preparation of viral vaccines, although to the best of my knowledge none has been produced in that way and applied to immunisation.



Ian D. Rae FRACI CChem (idrae@unimelb.edu.au) is a veteran columnist, having begun his Letters in 1984. When he is not compiling columns, he writes on the history of chemistry and provides advice on chemical hazards and pollution.

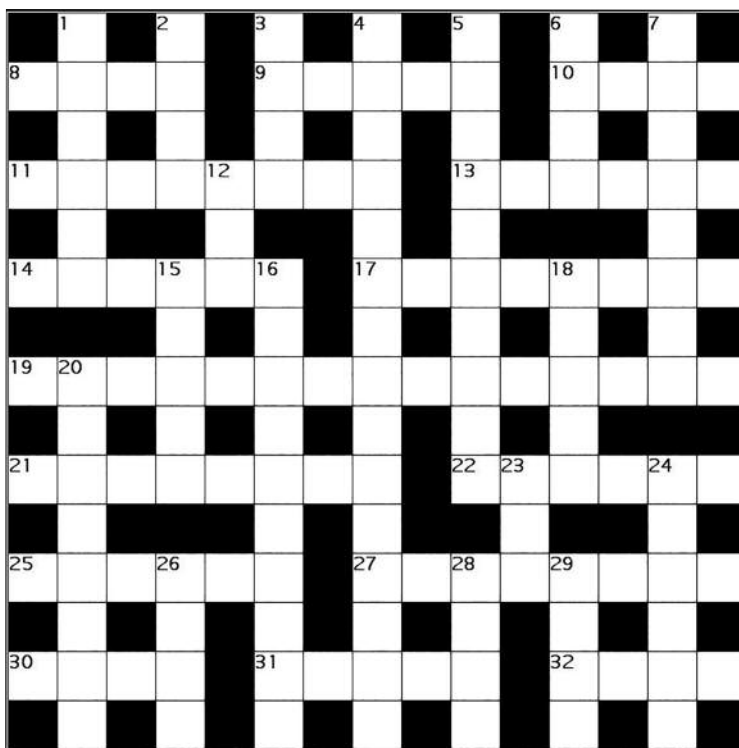
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altamet.com.au/conferences/alta-2018

AOCRP-5 – 5th Asian & Ocean Regional Congress on Radiation Protection
20–23 May 2018, Melbourne Vic.
aocrp-5.org

Macro 18 – World Polymer Congress
1–5 July 2018, Cairns, Qld
macro18.org

8th International Conference on Environmental Chemistry and Engineering
20–22 September 2018, Berlin, Germany
environmentalchemistry.conferenceseries.com



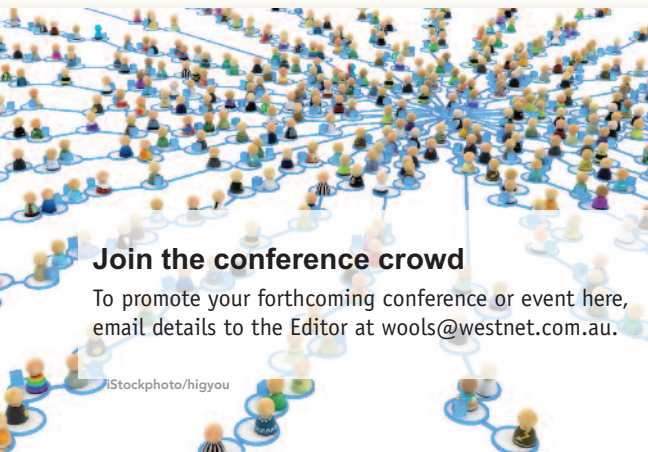
Across

- 8** Pitch record. (4)
9 Element after element after element remains. (5)
10 Rotate time vessel. (4)
11 Use on rum cocktail a lot. (8)
13 Injecting act to send an echo-request packet. (6)
14 Oxygen, sulfur and iodine in parent metal. (6)
17 Smart! Tin used for relay. (8)
19 Promising spirit introduced by William Rankine. (9,6)
21 Say solid is used with iodine in place of oxygen, for waste removal. (8)
22 It's Delfware, a tin glazed pottery container. It's consuming! (6)
25 Quartz is 14320. (6)
27 Time music genre is catching. (8)
30 Compound to add interest. (4)
31 Reel comes back in circles. (5)
32 Lug to 52. (4)

Down

- 1** Symposia for uranium manuscript. (6)
2 Used to tungsten before. (4)
3 Circle overhead dropping information from chlorine, perhaps. (4)
4 Perhaps melting point hastens air damage. (5,10)
5 Ionized sea storm yielded R_2N_2 . (10)
6 Surfing aid ends beach front support group. (4)
7 Overlooking 87 nanogram over broken 26 Down. (8)
12 Organocopper complex used in air-cushion vehicle construction. (3)
15 Model is perfect. (5)
16 Encountered a second bar and will stay like that for a while. (10)
18 Pleasant dessert. (5)
20 Centres endorsed assigned actinium salt first. (8)
23 A melting point that is current. (3)
24 Thorium, nickel and neon, thank you. (6)
26 Absorbed by first immune network theory outcome ... (4)
28 ... and therefore following aluminium. (4)
29 Getting up a thirst held course. (4)

Graham Mulroney FRACI CChem is Emeritus Professor of Industry Education at RMIT University. Solution available online at Other resources.



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The quiz has been in operation since 1982, growing from humble beginnings into an international event spread over 21 countries, seven languages, 1400 schools and more than 100 000 students.

The ANCQ is a unique chemical education activity.

It provides a major focus for secondary school students on the relevance of chemistry in an exciting and stimulating way. It is not a nationwide assessment of chemistry knowledge, but rather a promotion of chemistry that allows teachers and students to gauge their level of teaching and learning.

The quiz comprises 30 multiple-choice questions and takes one hour to complete. It is available both in hard copy and online.



**Registrations open:
Monday 5 March 2018**

Entry cost: \$6 per student

Website: www.ancq.com

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