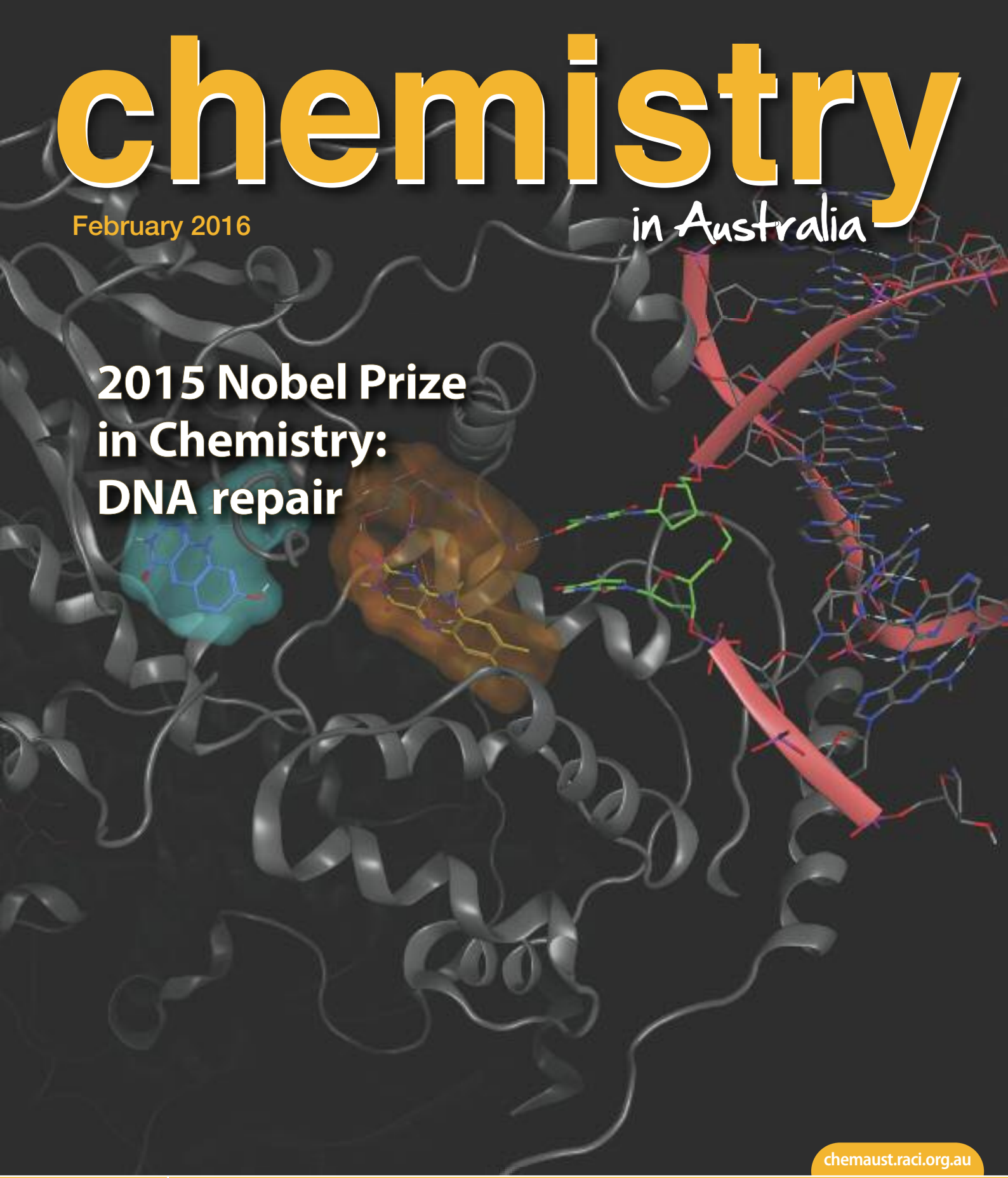
chemistry in Australia

February 2016



2015 Nobel Prize in Chemistry: DNA repair

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Royal Australian Chemical Institute

- Gamma activation analysis for gold
- Science and gender equity
- Streamlining chemical reactions
- 2015 RACI National Award winners

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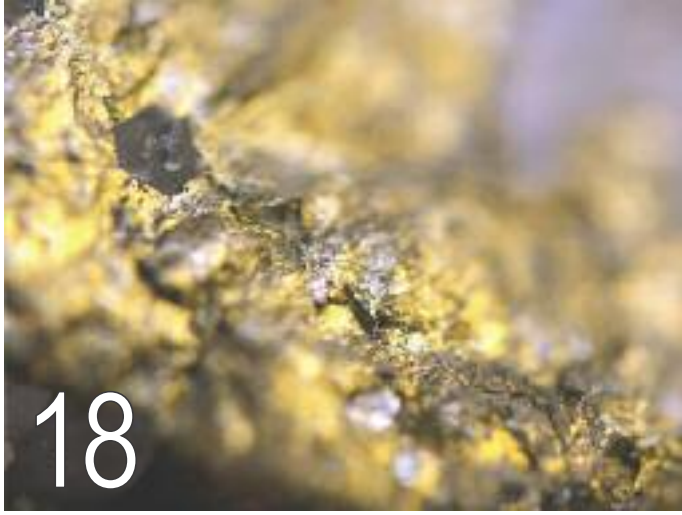

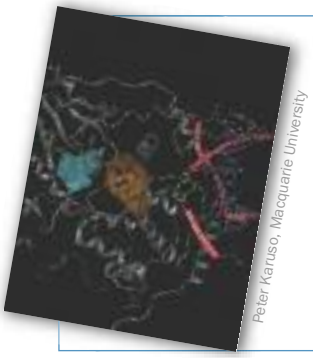
Peter Karuso, Macquarie University

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From the President

It has been most encouraging to see science (and innovation) at the forefront of Australian domestic politics in recent months. It is also reassuring to see broader bipartisan agreement from the major political parties on the importance of science and research to the nation's future. Governments may choose to prioritise the areas of scientific endeavour that warrant greater support but the acknowledgement by our political leaders (federal and state) that science and innovation is vital for the nation's future has not always been forthcoming. The funding mechanisms (e.g. grant schemes) and business incentives (e.g. taxation) put in place by governments are important catalysts of ideally spontaneous processes leading to innovation and economic advances. However, this pathway is very complicated.

Late last year I attended the inaugural Science Meets Business forum, run by Science and Technology Australia (STA). A stellar array of speakers and panellists was present, including outgoing and incoming Australian Chief Scientists Ian Chubb and Alan Finkel, CEOs of our major Commonwealth-funded research granting agencies ARC and NH&MRC (Aidan Byrne and Anne Kelso) and CSIRO CEO Larry Marshall, to name just a few. Past experiences and future opportunities were shared by all in what was a stimulating and engaging event. One of the key take-home messages was that Australia has an excellent track record in scientific *invention* (discovery through university-led basic research) but a less than impressive history of *innovation* through industry adoption with genuine value adding. The two words 'invention' and 'innovation' are in no way synonymous and a lot of work has to go into translating one into the other. Innovation policy is now on the agenda so the Australian scientific research community (with chemistry front and centre) has to take up the challenge but it needs the right people mediating the partnerships between academia, government and business.

Another major event run by STA is the upcoming annual Science Meets Parliament (SmP) meeting. In recent years RACI, though its membership of STA, has sent two RACI members to participate in the meeting and will be doing the same for SmP 2016. The focus of SmP is specifically on the relationship between policy-makers and the science community and how science can better inform decision-making. It also includes sessions on the role of the media and how scientists can better communicate their ideas. Everyone I've met who has attended SmP in the past has praised the event and having participated myself in 2014 I certainly concur. It's quite eye-opening to see so many parliamentarians showing a genuine interest in a topic that gets so little publicity in the mainstream media.

Around the world, we have seen a change in the political dialogue on major global scientific issues such as climate change and its knock-on effects such as more frequent extreme weather events and subsequent crop failures. The leaders of the world's largest economies (and populations) at the December COP21 Climate Conference in Paris all seemed to be singing from the same hymn sheet. There was unanimous acceptance that the scientific evidence cannot be ignored any longer despite the inconvenient conclusions that emerge from the data. Excuses cannot be made and courageous decisions will have to be taken to rein in our production of CO_2 in an effort to mitigate global temperature rises. The political will to 'do the right thing' based on sound science appears to be there and driven by an increasingly informed public who are more engaged in the topic than ever. The leaders of the world are attuned to the fact that the commitments they make now will affect the lives of future generations – well after their term of office. Long-term solutions to the global 'grand challenges' such as climate change, food and water security and sustainable (renewable) energy will be founded on scientific invention and innovation. Political courage and action to follow through on these advances are just as important.

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Researchers have the chemistry to make a star

Chemists have created a star-shaped molecule previously thought to be too unstable to be made.

The team created the five-pronged molecule [5]radialene, in work that could lead to more efficient ways to make medicinal agents, said lead researcher, Professor Michael Sherburn FRACI CChem from the Australian National University (ANU).

'This proof that we can make a compound that so many people thought couldn't be made opens up a world of new possibilities,' said Sherburn.

The chemical industry worldwide is worth nearly $1 trillion, making everything from cosmetics to cancer drugs. The vast majority of these important substances contain rings like radialenes.

'Hyper-reactive molecules like radialenes form more stable substances very quickly. Their reactions are some of the most powerful chemical transformations known,' Sherburn said.

Sherburn said that computations carried out on the Raijin supercomputer by collaborator Professor Michael Paddon-Row FRACI CChem from the University of New South Wales gave the team the confidence to try to create the elusive molecule.

'The compound is 10 000 times less stable than the others in the star-shaped radialene molecule family, which are themselves notoriously unstable. A previous research group describes spontaneous combustion of [6]radialene in air,' Sherburn said.

Sherburn and three generations of PhD students took nearly two years to develop a method to create [5]radialene.

Success came by preparing the molecule as a crystalline metal complex, which is stable because the metal shields the molecule from reaction. It also let the students use an X-ray technique to confirm their structure was correct. With the metal taken away, [5]radialene lives for only minutes even in very dilute solution at low temperature.

'Because the structure [5]radialene had never been seen in nature, we had to come up with a really creative method, something new and special,' Sherburn said.

'It was quite a day when the PhD students brought the X-ray crystal structure to me.'

Sherburn said the blue-sky nature of the research means it is impossible to predict the uses of the new techniques.

'We will always try to push back the boundaries of what is known, and what is thought to be possible,' he said. 'We have related projects underway that, if they succeed, will re-write the text books.'

The research is published in the *Journal of the American Chemical Society* (doi: 10.1021/jacs.5b07445).

AUSTRALIAN NATIONAL UNIVERSITY

Software update for Multiwave PRO

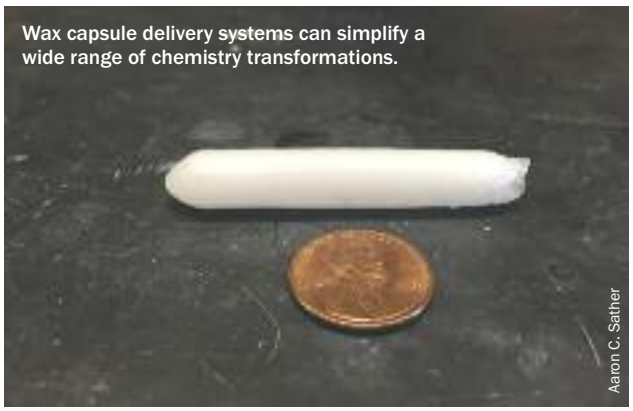
Anton Paar's flagship microwave reaction platform – Multiwave PRO – has received its first major software update, helping laboratories increase efficiency without additional cost. Multiwave PRO has become an IoT (Internet of Things) device and users can receive automated notification of completed runs and error reporting via email, as well as remotely control the instrument using VNC.

Reducing time to get results in the laboratory is a major concern of laboratory managers. Instruments are getting faster, but the biggest time drain is still the time between analytical steps. Laboratory technicians frequently find themselves waiting for a process to finish or walking back and forth between their desk and an instrument to determine if the process is completed. The software update for Multiwave PRO gives the user the ability to eliminate this wasted time.

This free software update, available on the Anton Paar homepage (www.anton-paar.com), builds on the already robust software package used by Multiwave PRO. Current features such as audio notification and visual notification on the 9" capacitive touchscreen, in addition to a variety of data export capabilities and a comprehensive video manual, make Multiwave PRO the easiest to use laboratory microwave platform on the market.

For further information, please contact MEP Instruments, ph. (02) 8899 5200, email info@mep.net.au or visit www.mep.net.au.

Wax capsules to save materials and streamline chemical reactions



Wax capsule delivery systems can simplify a wide range of chemistry transformations.

Chemists working in a variety of industries and fields typically go through a laborious process to measure and mix reagents for each reaction they perform. And many of the common reagents they use sit for months or years on shelves in laboratories, where they can react with oxygen and water in the atmosphere, rendering them useless.

In a paper published in *Nature* (doi: 10.1038/nature14654), researchers at MIT describe a technique that could help avoid this costly waste, and greatly reduce the number of steps a chemist must perform to prepare common compounds for use in a wide range of chemical transformations.

Aaron C. Sather, the lead author of the paper, is a postdoc in the lab of Stephen Buchwald, the Camille Dreyfus Professor in Chemistry. He and his colleagues have harnessed the power of a small, simple technology that could transform the benchtop practice of organic chemistry: the capsule.

Some labs use a glove box, an inert container that permits researchers to manipulate reagents in a controlled environment, isolated from the oxygen, carbon dioxide and water in ambient air. But many laboratories in industry and academia don't have glove boxes because they are expensive to maintain, and take up precious space, Sather says. As a result, many chemists avoid performing certain useful, but complicated, reactions because they require a glove box.

Many reagents and catalysts aren't used, simply because of this inconvenience. What's more, for a bench chemist working in materials science or pharmaceuticals, performing the complex sequence of steps to prepare certain compounds may be unfamiliar and onerous.

'If you can grab the reagents off the shelf and get the reaction to work without that expertise or a glove box, it's much more accessible', Sather says.

Paraffin delivery vehicles

Building on previous work by Douglass Taber at the University of Delaware, the researchers tried to disperse mixtures of reagents in molten paraffin wax, which has been demonstrated to protect oxygen- and water-sensitive compounds for long periods of time. But as the material cooled, certain dense reagents, such as caesium fluoride, would settle to the bottom. The scientists then decided to try making small capsules out of paraffin, enabling precise estimates of the contents for grab-and-go use.

'We thought, if we could enclose multiple reagents [and] catalysts in some way and actually know how much we put in,' Sather says, 'we could dramatically simplify chemical synthesis with these single-use capsules.'

Paraffin's physical properties make it ideal as a delivery vehicle for all kinds of chemical compounds. 'We wanted something that was inert, a long-chain hydrocarbon,' Sather says, 'that would have no competing side reactions with both catalyst and reagents. It's largely unreactive. Paraffin is insanely cheap, and nice and easy to work with. Paraffin doesn't pick up any water – it's just like grease.'

Upon heating, the paraffin capsule melts/dissolves in the reaction solvent, releasing its contents. After the reaction is finished, the paraffin can then be removed through precipitation, filtration and chromatography.

Sather and co-authors Hong Geun Lee and James Colombe made the capsules by hand, using a glass stirring rod to make the hollow shells. Then they filled them with dry reagents, and used a hot metal spatula to melt the wax and seal it off. The resulting capsules look like slightly bigger versions of the gelcaps sold over the counter at any pharmacy.

The team applied the paraffin capsule technology to a variety of reactions, focusing on combinations that are of broad applicability and interest across different fields, from making sensors to making pharmaceuticals. As an example, the researchers combined an oxygen-sensitive catalyst with caesium fluoride in capsules. They performed the same reactions using these capsules, and then in a glove box, and achieved similar results for both approaches.

A radically simplified process

Ironically, in order to prepare this glove box-free system, the group had to use a glove box to actually make the capsules. But the whole production process could easily be mechanised, Sather says, creating a low-cost, widely accessible alternative to glove boxes. Companies could sell hollow capsules for chemists to load themselves, or sell them pre-measured and pre-loaded.

Once they were made, the capsules dramatically simplified the benchtop chemistry. 'Instead of weighing out multiple reagents and catalysts, you're adding a capsule and weighing out one or two compounds,' Sather points out. 'It's really quick, especially for people who want to make a lot of molecules.'

The capsules also proved to be durable. The researchers took capsules filled with caesium fluoride – which is very water-sensitive – and immersed them in water overnight. The next day they took them out, dried them off with a paper towel and used them in a reaction.

'The result was the same,' Sather says. 'It told us that they're completely sealed. In terms of protecting water-sensitive compounds inside these capsules, the potential is huge.'

Sather says wider use of this technique could greatly extend the shelf life of common commodity chemicals. To demonstrate this, he and his colleagues prepared capsules containing multiple base-activated catalysts, along with strong bases, all mixed together in the solid state.

'They were still good after eight months on the benchtop, mixed together inside the capsule,' Sather says. 'There was no decomposition. And they weren't stored in any special way – just put in a plastic bin.'

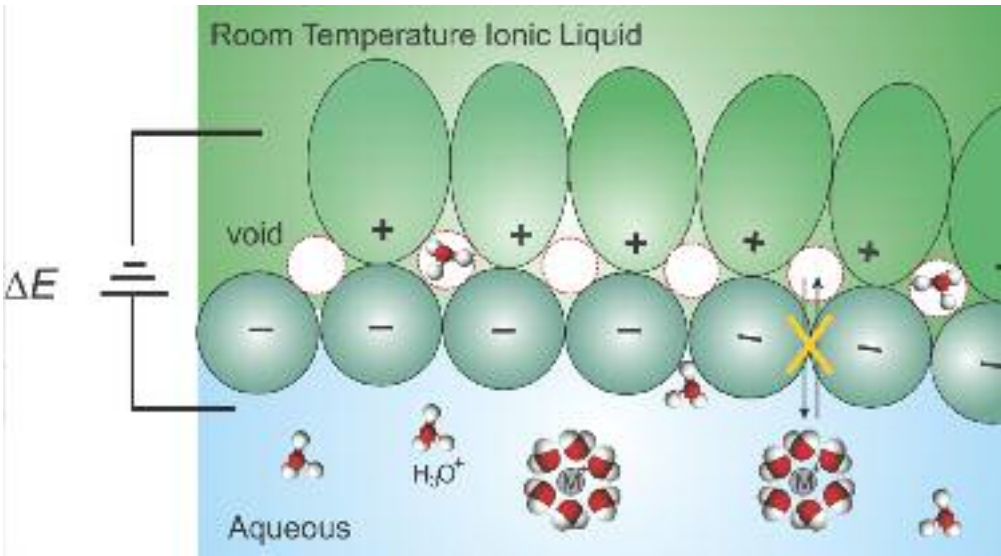
The researchers had similar success in an experiment conducted with a reagent that would degrade in hours if exposed to air; after more than a year of storage on the shelf in capsule form, there was no degradation.

Sather is most excited by the potential for this technology to make the work of chemists more efficient, and to widen access to demanding but useful reactions by overcoming the inconvenience and tedium associated with glove boxes.

JONATHAN MINGLE, MASACHUSETTS INSTITUTE OF TECHNOLOGY

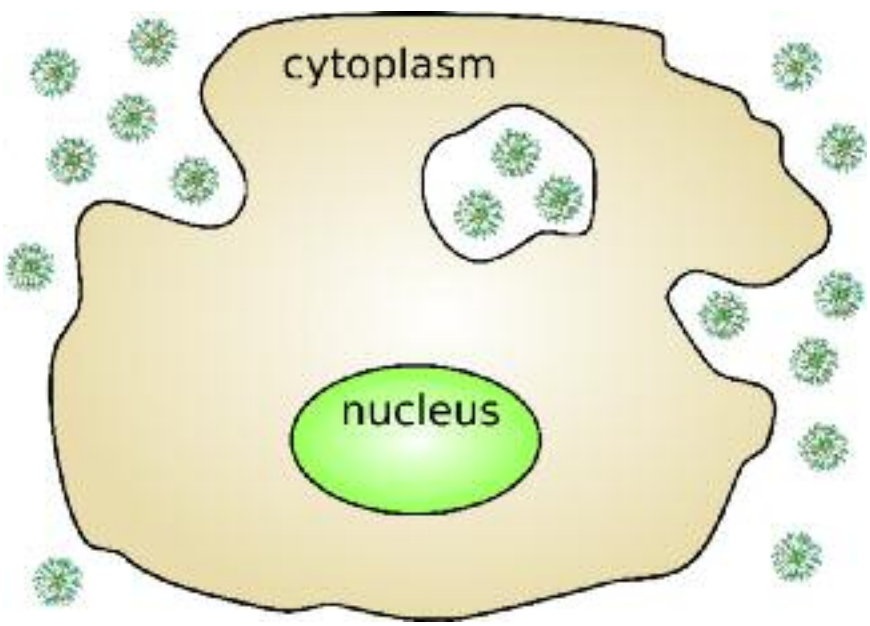
A new ion-transfer mechanism at liquid interfaces

Despite the interest in proton transfer and proton transfer-catalysed reactions at polarised water/oil interfaces, these reactions have hardly been studied at water/ionic-liquid interfaces. In previous years, researchers at Curtin University have explored ion transfer at interfaces between aqueous electrolytes and immiscible room-temperature ionic liquids for analytical purposes. In recent work using the ionic liquid trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate ($[P_{14,6,6,6}][FAP]$), an interesting background ion-transfer process was observed with acidic aqueous electrolytes but not with alkali metal salts. Using a variety of electrochemical methods, the ion-transfer process was shown to depend on concentration and to produce a new capacitive film at the interface (Alvarez de Eulate E., Silvester D.S., Arrigan D.W.M. *Angew. Chem. Int. Ed.* 2015, **54**, 14 903–6). This interfacial ion-transfer process can be explained by ion transfer into natural cavities within the ionic liquid matrix. Because of the finite size of these voids (radii 0.17–0.19 nm), small ions, specifically H_3O^+ and D_3O^+, can fit but larger ions such as hydrated alkali metal cations cannot. This phenomenon represents a new mechanism for size-dependent ion transfer at liquid–liquid interfaces.

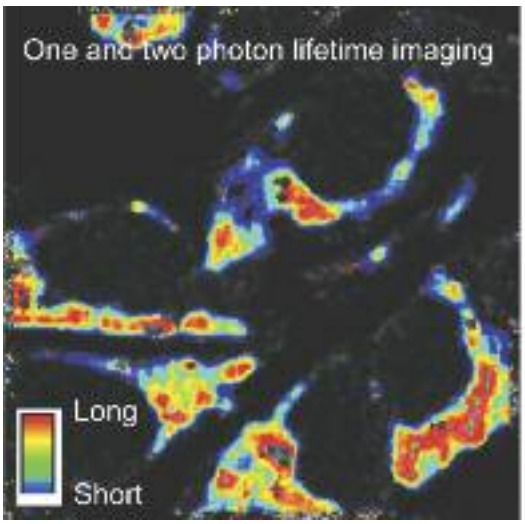


Personalised cancer targeting with dual functionalised nanoparticles

Understanding how therapeutic and diagnostic nanoparticles recognise diseased cells is essential for the development of effective and selective theranostics. Professor Bing Yan and his team from Shandon University have developed a library of gold nanoparticles that have been surface modified by a diverse selection of small organic targeting molecules and, optionally, by the tumour-targeting molecule folate. The uptake of these functionalised nanoparticles was found to differ widely across a panel of cancer cell lines. In collaboration with Professor Yan's team, Dr Tu Le and Professor Dave Winkler at CSIRO Manufacturing have developed quantitatively accurate and predictive models of the uptake of the nanoparticle library and teased apart the relationships between the surface chemistry of the nanoparticles and their cancer cell selectivity and extent of uptake (Le T.C., Yan B., Winkler D.A. *Adv. Funct. Mater.* 2015, **25**, 6927–35). They used a very robust machine-learning method developed in their group to predict uptake. A greater understanding of the molecular basis for targeting nanomaterials towards specific cells types will allow development of more effective drug-delivery systems, cancer treatments, therapeutic gene delivery, and diagnostic technologies.



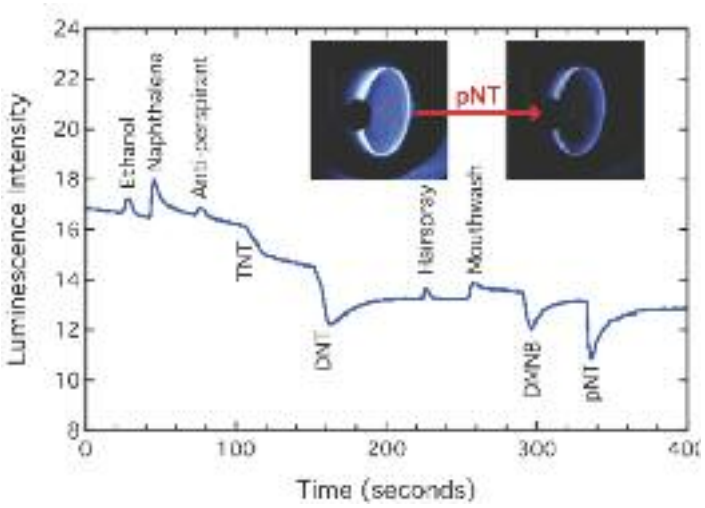
Optical solution to material science problem



Silicon quantum dots are of broad interest for their potential applications in optoelectronic devices, solar cells and fluorescent bio-imaging agents, primarily due to the low toxicity of silicon. A long-standing issue with silicon nanocrystals is that solution synthesis only produces blue-coloured nanoparticles. This is problematic in fluorescence bio-imaging for two reasons: biological background signals tend to influence the imaging process; and near-UV light is required for excitation, which can damage biological structures. Using an interdisciplinary, collaborative approach, Scientia Professor J. Justin Gooding, Scientia Professor Katharina Gaus and coworkers at the University of New South Wales approached this issue with an optical method. In a recent paper published in *Advanced Materials*, they used fluorescence lifetime imaging microscopy to solve the problem (Cheng X., Hinde E., Owen D.M., Lowe S.B., Reece P.J., Gaus K., Gooding J.J. *Adv. Mater.* 2015, **27**, 6144–50). By exploiting the long fluorescence lifetime of silicon quantum dots, they successfully de-convoluted signals of the nanoparticles from the biological background for both one- and two-photon channels. By further exploring the surface chemistry of silicon nanocrystals, they demonstrated for the first time that Förster resonance energy transfer can occur from silicon quantum dots to dye molecules immobilised on the particle surface, making the dye molecules glow.

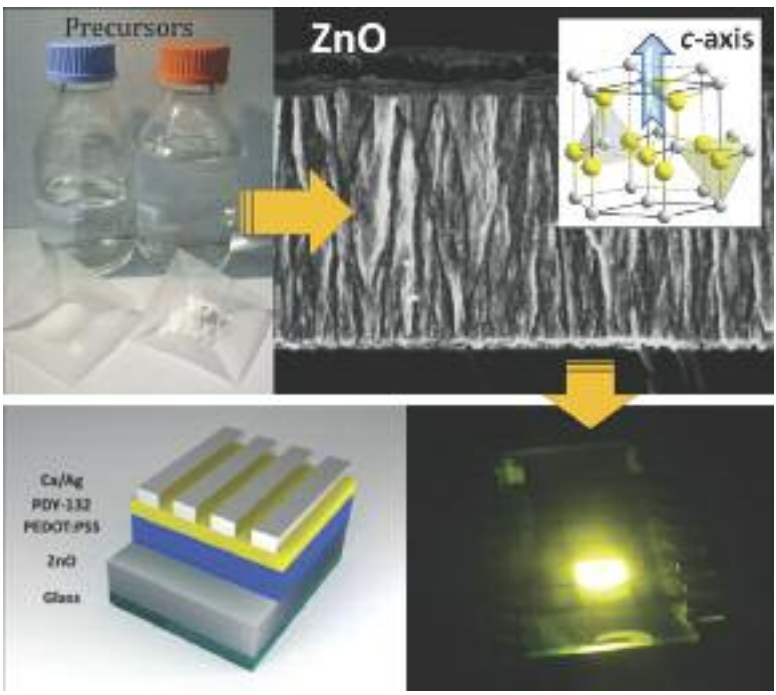
Detecting explosives with dendrimers

Explosive devices continue to be one of the most pervasive and destructive terrorist weapons. Unambiguous, selective and non-contact detection of nitro-containing explosives and taggants in the field is an important goal but is difficult to achieve with standard analytical techniques. The Centre for Organic Photonics & Electronics (COPE) at the University of Queensland has made a breakthrough in luminescence-based detection of explosive vapours, showing that luminescent dendrimers that incorporate a triphenylamine core can selectively detect nitro-containing explosives and taggants (Geng Y., Ali M.A., Clulow A.J., Fan S., Burn P.L., Gentle I.R., Meredith P., Shaw P.E. *Nat. Commun.* 2015, **6**, 8240). Using a combination of neutron reflectometry, quartz crystal microbalance and photophysical measurements, the COPE team determined that, while the vapours of both explosives and interferents can readily diffuse into and out of the dendrimer films, only the nitro-containing compounds interact electronically with the dendrimers and reduce the luminescence intensity. These results are a major advance in the development of sensing materials for non-contact detection of nitro-based explosive vapours, and deliver significant insights into the physical processes that govern sensing efficacy.

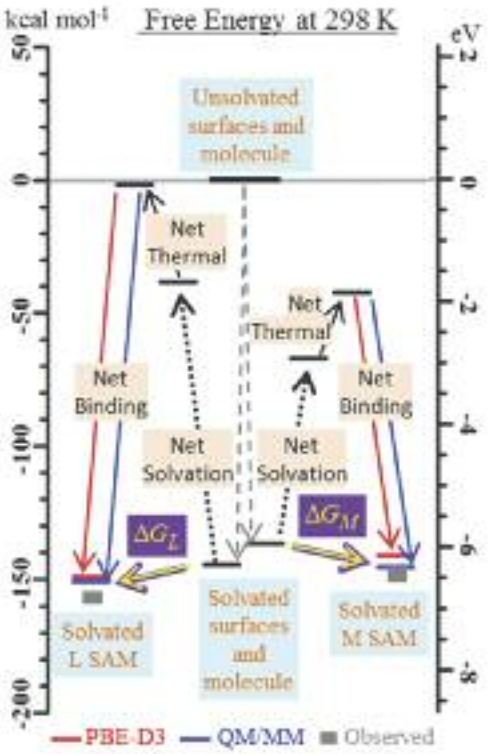


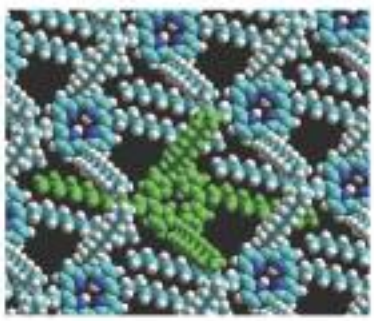
Flashed zinc oxide gives record electrode performance

As flexible electronics emerge in consumer markets, there is a progressive need for high-quality transparent conductors fabricated by inexpensive and industrially viable techniques. Zinc oxide (ZnO) is one of the most promising materials for this purpose due to its low cost, low toxicity, high transparency and high conductivity following doping. However, the high temperatures and vacuum conditions used to process ZnO electrodes currently limit widespread adoption. Researchers at Monash University and the CSIRO led by Associate Professor Jacek Jasieniak have overcome these problems by developing a novel synthetic method for producing ZnO coatings from water at low temperatures under 150°C (Della Gaspera E., Kennedy D.F., van Embden J., Chesman A.S.R., Gengenbach T.R., Weber K., Jasieniak J.J. *Adv. Funct. Mater.* 2015, doi: 10.1002/adfm.201503421). By harnessing tailored reaction chemistry and a photo-reduction step that consists of illumination of the electrodes with several millisecond pulses of white light, the team was able to fabricate ZnO with the lowest sheet resistance (40 Ω/□) ever reported for a transparent, intrinsically doped film. Compatible with common plastics used in flexible electronics, such as polyethylene terephthalate, and possessing nearly ideal sheet resistance for many consumer electronic applications, such ZnO electrodes may be a suitable replacement for the expensive and scarce indium tin oxide electrodes that are ubiquitously used in today's touch panels and displays.

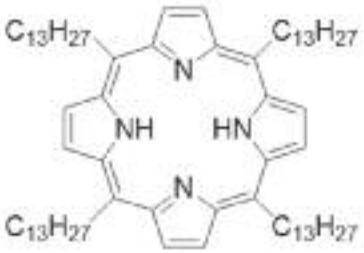


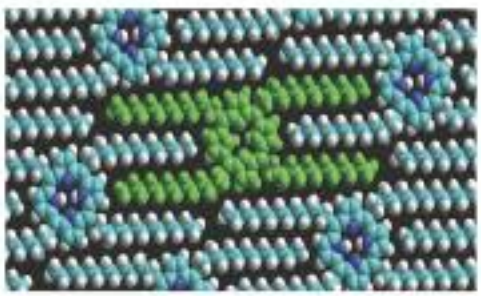
New tools for understanding how organic surfaces get dirty





M polymorph





M polymorph

Organic molecules, including proteins and polymers, stick to other molecules and to surfaces through weak but very numerous, widely distributed, van der Waals interactions. Recently, researchers at the University of Technology Sydney, the University of Sydney, the University of Melbourne, Shanghai University and Radboud University, led by Professors Jeffrey Reimers, Maxwell Crossley and Noel Hush, have developed new synthetic, scanning-tunnelling microscopy (STM), and density-functional theory methods to measure and predict free energies of formation of alkylporphyrin monolayers on graphite (Reimers J.R., Panduwinata D., Visser J., Chin Y., Tang C., Goerigk L., Ford M.J., Sintic M., Sum T.-J., Coenen M.J.J., Hendriksen B.L.M., Elemans J.A.A.W., Hush N.S., Crossley M.J. *Proc. Natl Acad. Sci. USA* 2015, **112**, E6101–10). Large intermolecular attraction energies were shown to drive dirtying of the surface from solution, but are nearly completely opposed by large desolvation forces and entropy effects. Subtle changes in the sums of these widely varying contributions control monolayer polymorphism. While measuring accurate free energies for the interactions of large organic systems is a severe modern challenge, this work shows how useful approximate values can be determined from a wide range of existing STM data. It also presents the first application to large-scale self-assembly of accurate free-energy simulation methods traditionally used by quantum chemists to understand small-molecule chemistry. These techniques will be applicable in a wide range of chemical and biochemical scenarios.

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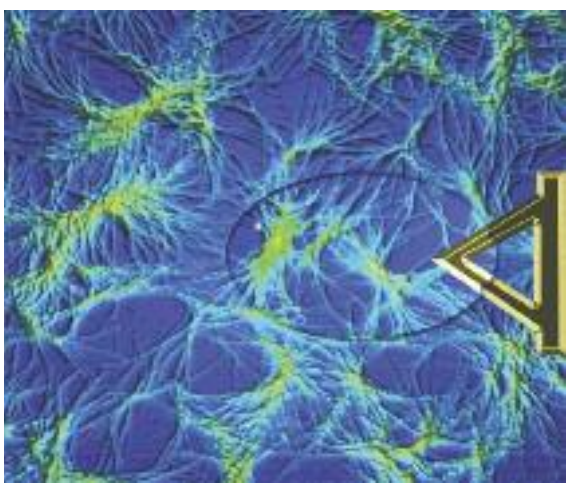
chemistry in Australia

Watching gels grow

Supramolecular gels are formed by molecules that assemble to form a solid network robust enough to immobilise a volume of solvent. An exciting feature of supramolecular gels is that they respond to environmental parameters such as pH, heat, light and chemical reactions. This opens up a range of potential applications such as drug-delivery systems, tissue engineering and sensors, to name a few. The dynamic nature of these systems also presents significant challenges for characterisation. Morphological examination using typical microscopic techniques such as freeze-drying followed by electron microscopy presents obvious pathways for artifacts to be introduced. Researchers at Curtin University, in collaboration with the University of Western Australia, have developed an experimental protocol to monitor gel fibre formation on the nanoscale, dynamically and in situ (Barker E.C., Goh C.Y., Jones F., Mocerino M., Skelton B.W., Becker T., Ogden M.I. *Chem. Sci.* 2015, **6**, 6133–8). Using an atomic force microscope tip immersed in a gelating droplet on a temperature-controlled stage, it proved possible to image supramolecular gel fibre networks in the process of forming, and disassembling, as a function of temperature. This technique provides a new approach to study the dynamics of supramolecular gel assembly and disassembly, particularly fibre–fibre interactions, at high resolution.



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.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to David.

chemistry in Australia

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The chemistry of DNA repair

2015 Nobel Prize in Chemistry I

BY **PETER KARUSO**

The 2015 Nobel Prize in Chemistry rewarded three researchers for the mechanistic understanding of DNA repair processes.

On 10 December 2015, the Nobel Prize in Chemistry was given to Tomas Lindahl (Clare Hall Laboratories, UK), Paul Modrich (Duke University School of Medicine, US) and Aziz Sancar (University of North Carolina, US) 'for mechanistic studies of DNA repair'. They made fundamental and ground-breaking discoveries on the enzymatic mechanisms of DNA repair. Lindahl discovered base excision repair. Modrich detailed the mechanism of mismatch repair and Sancar uncovered the mechanism of nucleotide excision repair and how 'photoreactivation' works.

Molecular biology's central dogma

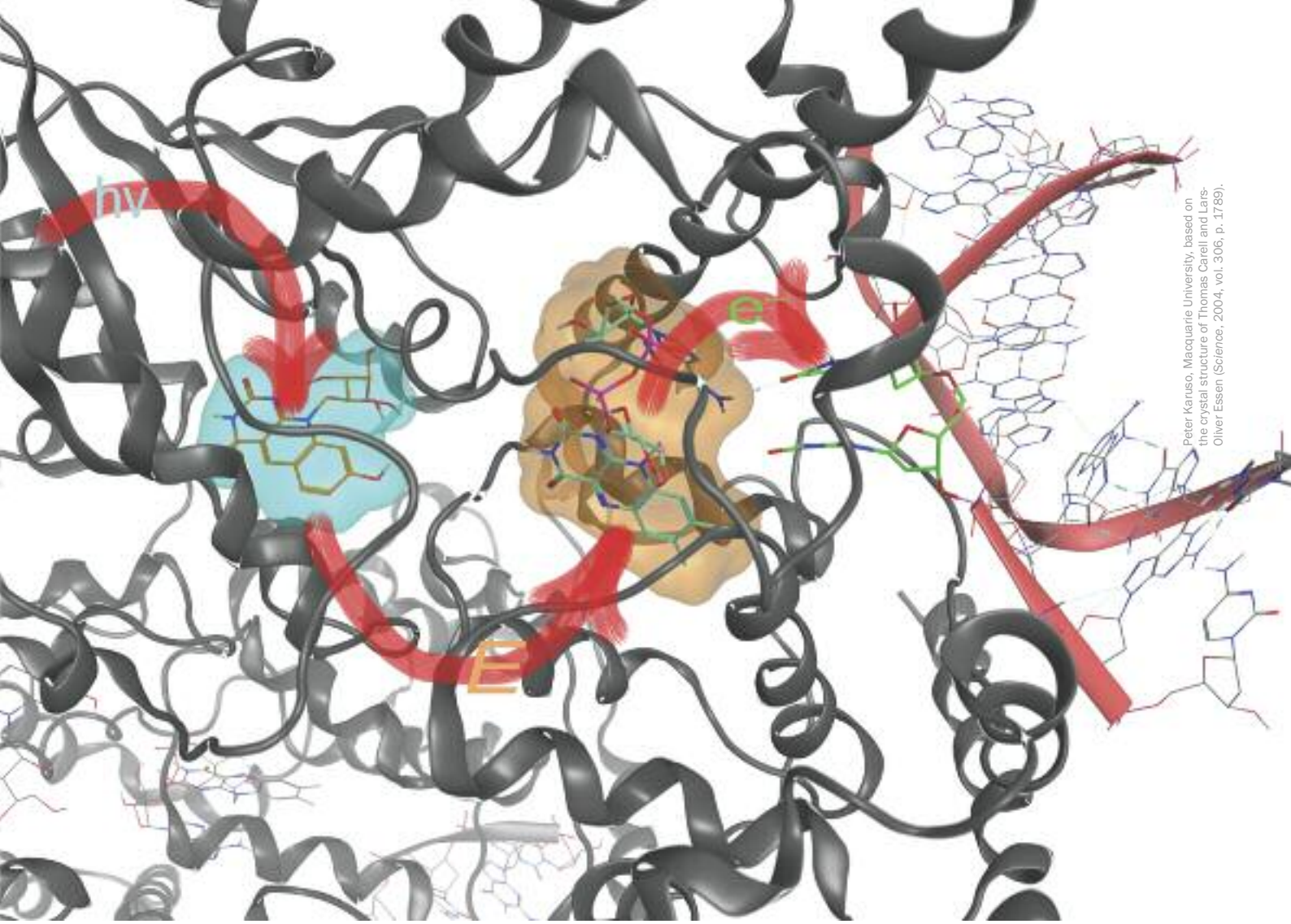
The central dogma of molecular biology was enunciated by **Francis Crick** in 1970. It states that all genetic information in a living cell is stored in its genome (DNA). The DNA is stored in the nucleus of the cell and made available by transcription to RNA (mRNA) and is subsequently translated to proteins by the ribosome.

Friedrich Miescher, in 1869, was the first to isolate DNA from the nuclei of cells. He called the compound 'nuclein'. It was not until 1944 that **Oswald Avery** suggested that this material carried the genetic code. While working at the Rockefeller Institute for Medical Research, US, he discovered that DNA from a virulent strain of a bacterium could permanently transform a non-virulent strain into a virulent strain. So started the race for the structure of the blueprint of life. **Linus Pauling** published the first structure of DNA in February 1953, but it was wrong, suggesting a triple helix.

Francis Crick and **James Watson**, using the information on the ratio of base pairs in DNA discovered by **Erwin Chagraff** (Columbia University) and the famous unpublished X-ray diffraction pattern ('picture 51') taken by **Rosalind Franklin** in May 1952 of a crystal of DNA, had a head start on Pauling. The pattern strongly suggested a double helix. By early 1953, Watson and Crick had correctly deduced the structure and published it in *Nature* on 23 April 1953, for which they received the 1962 Nobel Prize in Physiology along with **Maurice Wilkins**. Rosalind Franklin had died four years earlier of cancer at the age of 37. Ironically, the cancer was probably caused by DNA damage from exposure to X-rays throughout her career.

Herman Muller (University of Texas Austin), in 1927, had discovered that X-rays can lead to mutations in fruit flies and these mutations could be passed on to their offspring. Of course, DNA was not discovered to be the genetic material until 1944, at which time Muller's work was more fully appreciated and awarded a Nobel Prize in 1946. In 1933, **K.W. Hausser** and **H. von Oehmcke** discovered that far UV (254 nm) radiation can also cause genetic damage and turn banana skins brown. What was amazing was that the browning could be reversed by blue light.

It was known since 1878 that UV light, especially around 250 nm, killed bacteria, but in 1949 **Albert Kelner** (Cold Spring Harbor) made a truly remarkable discovery. He found that *E. coli* 'killed' with UV light could be reanimated with blue light (<450 nm) in direct parallel to Hausser and Oehmcke's work with bananas. **Renato Dulbecco** (Nobel Prize, 1975), during his time in Salvador Luria's lab in Bloomington, found the same thing with T2 bacteriophage (1950). This strongly suggested the target of UV damage was DNA. Dulbecco (1955) found that photoreactivation of T2 phages with daylight is effective only after the phage enter an *E. coli* cell. If one kills them with 254 nm light



Peter Karuso, Macquarie University, based on the crystal structure of Thomas Carell and Lars-Oliver Essen (*Science*, 2004, vol. 306, p. 1789).

outside of a cell, they stay dead. No one knew at the time how visible light could resuscitate bacteria and viruses killed with UV light but this was all about to change.

Sol Goodgal and **C. Stan Rupert**, while at John Hopkins in Baltimore (1958) in the lab of **Roger Herriot**, discovered that protein extracts from *E. coli* were able to repair UV-damaged DNA and reanimate dead viruses only if the mixture was exposed to daylight. This inducible repair activity found in the mashed-up *E. coli* was clearly due to a type of enzyme because it could be killed by heating, but it took until 1977 to find what the enzyme was.

Aziz Sancar

Born 8 September 1946 to a lower-middle-class family in Savur, Turkey, **Aziz Sancar** was the seventh of eight children. Even though his parents were illiterate, they valued education and gave their children the best education they could. Aziz excelled at science at high school and entered Istanbul University to study medicine but was more interested in chemistry. In the second year of his six-year degree, he studied biochemistry for the first time and decided then to be a research biochemist. However, after his medical degree, his biochemistry professor advised him to practice medicine, for at least a couple of years (1969–71) – which he dutifully did.

After two years as a GP in rural Turkey near Savur, Sancar applied for and was granted a NATO fellowship to visit Johns Hopkins University, where he worked with **Roger Herriot** (1971–2) and found out about 'photoreactivation' and the work of Sol Goodgal and C. Stan Rupert. Rupert was now a professor at the University of Texas, Dallas and still working on the putative enzyme that 'repaired' UV-damaged DNA that **Harold Werbin** had dubbed 'photolyase' in 1970.

After the NATO fellowship, Sancar returned to his medical practice in Turkey (1972–3) but was now fascinated by the field of DNA repair. He wrote to Rupert asking him to accept him as a PhD student. Sancar was accepted as a Masters student (1975) and then a PhD student (1977) at the University of Texas, Dallas.

During his postgraduate years in Rupert's lab (1974–7), Sancar made up for his lack of skill and expertise with plain hard work. Without much background in chemistry or biology, Sancar had great difficulty in the lab at the beginning. To compensate, he designed technically simple experiments. However, when even

Aziz Sancar in Stan Rupert's lab during his PhD, 1974.

Dr Sancar and Dr Rupert during the University of Texas, Dallas Alumni Gala in 2009 when Dr Sancar was named a University of Texas, Dallas Distinguished Alumnus.

these simple experiments repeatedly failed, his well-meaning benchmate suggested he had no talent for research and should return to medicine. Stan Rupert was, luckily, the perfect boss – patient and understanding, he understood his student's strengths and weaknesses. He was always encouraging, so Sancar persisted.

Sancar much later recounted that Rupert 'as both a scientist and a gentleman, he has been the most influential person in my career'.

Some 11 months later, Sancar got his 'simple' experiment to work and had produced a strain of *E. coli* deficient in the photolyase gene. At about the time Sancar started his PhD, the field of recombinant DNA and molecular cloning was born and the first gene cloned east of the Rocky Mountains (according to Sancar anyway) was photolyase in 1976 (Sancar A., C.S. Rupert, 'Cloning of the *phr* gene and amplification of photolyase in *Escherichia coli*' *Gene* 1978, vol. 4, p. 295). After a four-month return to Turkey to complete his compulsory military service, Second Lieutenant Sancar returned to Dallas to find out what the chromophore in photolyase was that allowed it to use blue light to repair UV-damaged DNA. However, Stan Rupert said he had done enough and needed to write up his PhD, which he did. Hoping to continue studying DNA repair, he wrote to all the labs in the US studying this, trying to secure a postdoctoral appointment. Unfortunately all rejected his application. Meanwhile his fiancée, fellow PhD student, Gwendolyn Boles, had landed a postdoctoral fellowship at the State University of New York, so Sancar started looking for jobs in the north-east. **Dean Rupp** at Yale was interested in cloning DNA repair enzymes, so he took a job there as a lowly laboratory technician in 1977.

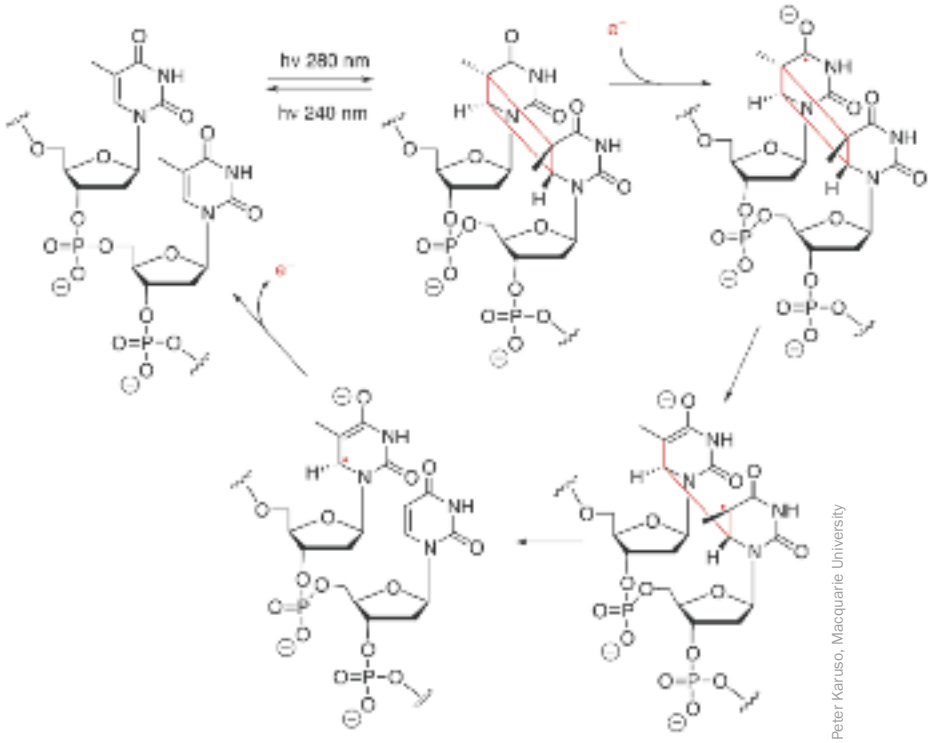
Yale University has a long history in DNA repair (Rupp W.D. *Yale J. Biol. Med.* 2013, vol. 86, p. 499) dating back to 1957 when Senator Prescott Bush (Republican, CT), father and grandfather of the well-known US Presidents, approached researchers at Yale to investigate the health hazards of nuclear testing. This led to a concentration of researchers including **Paul Howard-Flanders**, **Richard Setlow** (until 1961), **Jane Setlow** and **Philip Hanawalt** (PhD, 1959) who were studying the effects of radiation on DNA from 1959 to1961. At about the same time (1960), two Dutchmen (**Rob Beukers** and **Wouter Berends**, Technical University of Delft) published a paper identifying that UV light (280 nm) dimerised thymidine to make cyclobutane rings and that this could be reversed with 240 nm UV light in the same repair process discovered by Stan Rupp and Sol Goodgal in 1958. By 1961, Hanawalt had moved to Stanford and Dick Setlow to the Oak Ridge National Laboratory. After reading the papers of the Dutchmen, Setlow set out to prove them wrong. In 1964, Setlow, Hanawalt and Howard-Flanders separately published papers that showed that bacteria repair thymine dimers with enzymes that remove the dimer and replace it with undamaged bases and that this does not require light at all. Hanawalt and his first PhD student **David Pettijohn** went on to show that short patches of DNA are replaced around the damaged thymidines. They named this 'repair replication', now known as 'nucleotide excision repair' (NER) or the 'dark reaction'.

In 1974, Hanawalt organised the first DNA repair conference in Squaw Valley, California, drawing some 200

participants, including Aziz Sancar, **Tomas Lindahl** and **Paul Modrich**.

When Sancar arrived at Yale in 1977 as a lab technician, W. Dean Rupp was involved in the major challenge of identifying the enzymes responsible for this dark reaction. The year before, **Erling Seeberg** (Forsvarets forskningsinstitutt, Norway) and **Peter Strike** (University or Liverpool, UK) first purified enzymes involved in DNA repair. While Seeberg and Strike had no direct connection to Yale, both their PhD advisors (**Ivar Johansen** and **Peter Emmerson**) were postdocs for Paul Howard-Flanders in the early 1960s. With the addition of **Frank Hutchinson** and **Charles Radding**, Yale was a hotbed of research on DNA repair.

Feeding off this exciting environment, Sancar got more involved in research and Rupp proved a valuable mentor. From 1979 to 1980, Sancar cloned several *E. coli* genes (*uvrA*, *uvrB* and *uvrC*) involved in DNA repair. To isolate the proteins, Sancar invented the maxicell technique. This relied on a DNA-repair-deficient strain of *E. coli* that Sancar had developed (Sancar, Hack, Rupp *J. Bacteriol.* 1979, vol 137, p. 692) and remains his most cited paper. After the cells are transformed with a plasmid of interest, the cells are irradiated with UV light, which selectively damages large pieces of DNA (the chromosome), leaving the small plasmids to continue to replicate and express protein. In conjunction with radioactive amino acids, it was relatively easy to use gel electrophoresis and autoradiography to identify the proteins encoded by the plasmid. This led to the rapid isolation and identification of the enzymes involved in the dark reaction. To Sancar's surprise, the combination of *uvrA*, *uvrB* and *uvrC* did not excise just the damaged bases but cleaved the eighth phosphodiester bond 5′ to the thymidine dimer and the fourth or fifth phosphodiester 3′ of the lesion (Sancar, Rupp (1983) *Cell* 1983, vol. 33, p. 249). The repair is completed by uvrD (a helicase, which removes the excised strand), PolI (DNA polymerase that fills in the missing DNA) and finally a ligase that stitches the two phosphodiester bonds back together.



Peter Karuso, Macquarie University

Thymidine dimers are formed under the action of UV light by a [2+2]-photocycloaddition. Photolyase repairs this damage by excitation of methylenetetrahydrofolate (MTHF) with blue light followed by resonance energy transfer to flavin adenine dinucleotide ($FADH^-$), which transfers an electron to the thymidine dimer, catalysing its repair and final transfer of an electron back to $FADH^•$ (see image p. 15).

Papers in *PNAS* and *Cell* clearly showed that Sancar was more than a laboratory technician from a third-world country. His in vitro reconstitution of the NER enzymes landed him a job as Associate Professor of Biochemistry at the University of North Carolina at Chapel Hill in 1982. Here he returned to his PhD project and in a series of papers from 1984 to 1989 described the mechanism of photolyase and discovered that it contained two chromophores – flavin adenine dinucleotide ($FADH^-$) and a pterin (methylenetetrahydrofolate).

While photoreactivation (photolyase) was the first form of DNA repair identified, it is not found in mammals, which rely on NER to correct UV damage. However, unlike bacteria that use just three enzymes to affect NER, humans require 15 enzymes. Reconstituting these enzymes in vitro and showing that they can repair damaged DNA was a *tour de force* (Selby, Sancar *Science* 1993, vol. 260, p. 53) that Sancar says is his most aesthetically pleasing paper. Photolyase does have a human counterpart though; it is not involved in DNA repair but, coming full circle, Sancar has discovered that this protein is a photoreceptor and responsible for maintaining our circadian rhythm.

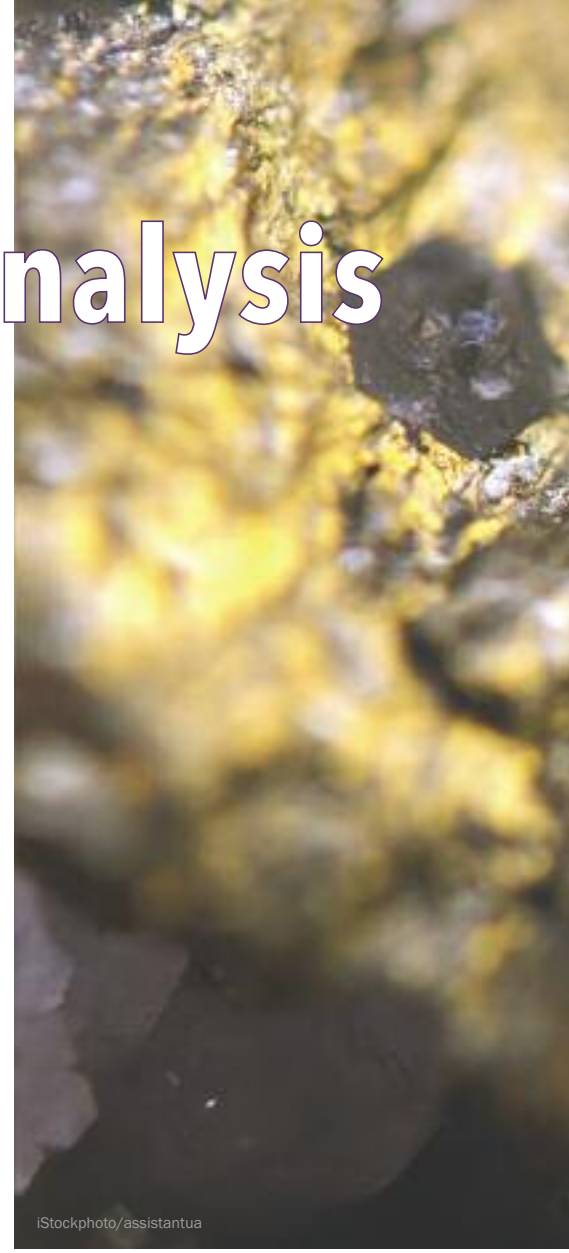
This year's Nobel Prize recognises Aziz Sancar for elucidation of the mechanism for 'nucleotide excision repair' and the photoreactivation of bacteria and viruses killed with UV-light. We know now that NER is just one type of DNA repair and that there are numerous types of lesions that affect DNA. In the next issue, we will look at the two other major DNA repair mechanisms: base excision repair (Tomas Lindahl) and mismatch repair (Paul Modrich).

Peter Karuso FRACI CChem is the Professor of Chemistry at Macquarie University, Sydney. Part II will appear in the next issue.

Gamma activation analysis
A new gold standard?

BY **DAVE SAMMUT**

A gold assay developed by CSIRO Minerals may avoid interferences that frustrate current methods.


iStockphoto/assistantua

First discovered in the Australian colony in 1823 by Government Surveyor James McBrien, gold has played a huge role in the development of Australia as a nation. It wasn't the first mineral mined or exported from Australia – by 1823, more than 3000 tonnes per year of coal was being mined and hand-loaded by convicts into ships at the port of Newcastle – but it played a major role in defining the country we live in today.

In 2014, Australia was the world's second largest producer of gold (after China), producing over 270 tonnes of the yellow metal. Mined in almost half the countries of the world, gold had a global production in 2014 of 2860 tonnes, according to the US Geological Survey.

The dominant gold assay method at present is fire assay. A known quantity of crushed ore (usually 30–50 grams) is mixed with flux in a refractory crucible. The flux is typically a mixture of sodium bicarbonate, potassium carbonate, sodium borate, lead oxide and either flour or iron metal as a reducing agent, depending on whether the ore is an oxide or a sulfide.

The mixture is heated to 1000–1200°C. Via a complex series of reactions that depend on the sample chemistry, the lead is reduced to a 'button' of metal alloyed to the precious metals in the sample, while the remainder separates as a slag.

The lead buttons are put into porous crucibles made of 'bone ash' (MgO), termed 'cupels', which are then re-heated to 1000°C in a muffle furnace under oxidising conditions. The lead melts and oxidises to PbO, which in turn melts and is drawn into the pores of the cupel by capillary action. The gold remains in the base of the cupel as a 'prill', which is then assayed for metal content.

Fire assay is a time-consuming, destructive technique. The accuracy is limited to around 5% for typical ore samples, on top of the error rate in the sample preparation (see box). Yet such is the demand from gold (and platinum group metals) exploration and mining that Australian laboratories collectively produce as much as 100 tonnes per month of lead-contaminated cupels as hazardous waste.

CSIRO has introduced a potentially game-changing assay technique – gamma activation analysis (GAA). Much less labour intensive, and with no hazardous waste, it should enable detection of all of the gold in a sample, regardless of the chemistry or matrix. DCS Technical spoke to Dr James Tickner about CSIRO Minerals' work on this new analytical method.

CSIRO's GAA testing uses a high-power electron linear accelerator (LINAC) X-ray source developed by Mevex Corp Ltd of Ottowa, Canada. It produces an electron beam of around 8.5 MeV directed onto a water-cooled copper target, which produces X-rays via the Bremsstrahlung process. Samples are placed in 300 mL containers positioned close to the target. The electron beam is rastered over a calculated path on the copper

to ensure uniform irradiation of the sample.

Tickner notes that there is no simple distinction in energy between X-ray and gamma radiation. Instead, the convention is that 'X-ray' refers to radiation generated electrically, while 'gamma' refers to energy from nuclear reactions. GAA is then so-named for historical reasons, with intense, high-energy gamma-ray sources being initially used.

Bombarding the sample with high-energy X-rays induces nuclear reactions in the elements of the sample, and the resulting isotope decay reactions generate characteristic gamma rays that can be compared to standard samples for quantified elemental analysis.

For gold analysis, the most important reaction is the excitation of the 409 keV, 7.73 second half-life isomeric state. This half-life allows the sample to be moved between the irradiation and measurement zones, protecting the liquid nitrogen-cooled germanium detectors from the intense radiation required to excite the isomer.

A 'monitor foil' is used to correct for variations in the X-ray flux from the source, or changes in detector efficiency. This is simultaneously irradiated and measured with the sample. If done correctly, both are subject to nearly identical changes in activation, allowing normalisation of any variation in the analytical factors.

Following irradiation of the sample, the decay gamma rays are measured

Sampling challenges

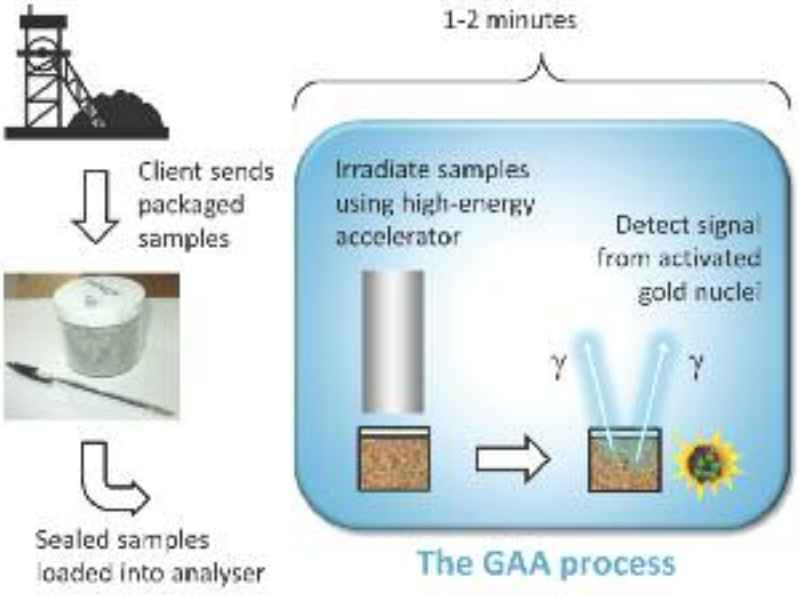
Gold is only very sparsely dispersed through the Earth's crust. The average gold grade for operating gold mines in 2012 was only 1.06 g/t (1.06 ppm) (bit.ly/1LQJKZQ). Even the average for the world's top ten mines was only around 15 g/t in that year (bit.ly/1GMz1AW). And these figures are the averages for the *ore* itself, before recovery efficiencies are taken into account for the beneficiation of the ore into concentrate, and the extraction of the gold from the concentrate to metal (typically via cyanidation).

Overall, this means that for every tonne of gold produced, these mines drilled, blasted, carried, crushed and processed more than one million tonnes of host rock, plus uncounted millions more of 'overburden', the valueless spoil that has to be removed before the mines even get to the ore.

From an analytical chemists' perspective, the challenges in this endeavour are huge. Finding one gram of gold dispersed through a tonne of material is very much 'needle in a haystack' territory.

The gold may be either widely dispersed or 'nuggetty' within the sample; the latter gives extremely heterogeneous samples. Due to its high relative density, gold often separates via simple movement under gravity. This property can be a major advantage for the beneficiation via shaking tables, spiral or rotary classifier, or simply by panning for amateur enthusiasts, but requires careful attention during sample preparation for assaying.

After the initial challenge of getting a representative sample from some tonnes of coarse source material, the operator needs to crush and homogenise the sample, then sub-sample via riffle splitting or classic 'cone and quarter' methods. A key problem with this is that good sampling requires skilled operators, and results are therefore subject to random and operator-based error.



and related back to the gold concentration via the sample mass. A Monte Carlo simulation is used to calculate a mass/density correction factor, which Tickner reports as giving surprisingly high accuracy in the correlations, in the region of 1%.

Tickner says that the technique is not entirely novel. Originally suggested as a possible gold analysis method in the 1960s by groups in the US, the method was first applied in an industrial setting in the 1970s in the former Soviet Union. Unfortunately, details available in the English language literature are limited.

GAA has commonalities with both X-ray fluorescence (XRF) and neutron activation analysis (NAA). Like XRF, GAA uses incident X-ray radiation. However, whereas XRF induces only energy shifts in the electrons to measure the resulting releases on the return to ground state, GAA induces much larger changes at the nuclear level. Essentially, the higher energy X-rays of GAA blast neutrons out of the nucleus, or cause shifts between nuclear energy levels, producing unstable nuclei that subsequently decay.

NAA similarly induces nuclear reactions in the target elements by adding (nuclear reactor generated) neutrons to the nuclei. However, the technique is relatively unselective, as many common rock-forming elements are capable of absorbing neutrons and becoming radioactive. This creates a large background of gamma radiation across the energy spectrum and therefore reduces sensitivity. Typically, samples must be left for a long time (usually more than seven days) to allow this background to decay before sensitive measurements for trace elements such as gold can be performed.

By using electrically generated X-rays, GAA is able to 'tune' the incident energy to target the desired elements. This works particularly well for gold, which activates at lower energy than

'Invisible gold'

There is a niche but persistent concept in gold circles termed 'invisible gold'. Put simply, this is gold that, for various reasons, is supposedly present in samples but simply doesn't show up in conventional fire assay techniques, or by acid digestion and spectroscopic analysis.

In theory, it is certainly at least conceivable. If gold were locked in refractory particles, particularly if that gold were encapsulated at the nano-scale so that none was exposed at any particle surfaces, perhaps it might not be available for any of the chemically based analyses. If it can't react or dissolve, then it can't be measured by any of the existing techniques.

GAA may answer this question once and for all. Free from matrix effects and chemical reactions, GAA comes down to the pure physics of the sample. If it is present, then the atoms should be activated and the resulting isotopes should decay.

In the interview with DCS Technical, Dr James Tickner of the CSIRO noted that the technique had been trialled on several purported invisible gold samples. For those samples, he concluded that the gold 'was indeed invisible'. He went on to state that 'If the gold does not show up in a brute force nuclear reaction, then [if it were actually present] this would require a Nobel Prize-winning change to our understanding of physics.'

A typical gold mine would drill ten kilometres or more diamond drill cores such as these each year.

many other elements. And by avoiding activating many background elements, the sensitivity of the technique can be improved.

Tickner explains that GAA is applied at a high-grade mine in Uzbekistan based on the old Soviet work, apparently achieving a 0.5 ppm detection limit. Using the newer high-energy X-ray sources developed for the medical sterilisation and industrial radiation markets, and improved detector systems, Tickner and the team are aiming for limits in the low tens of ppb.

Despite the high energies of the source X-rays, the resulting isotopes have very short half-lives. This yields rapid measurements, in the order of around 1–2 minutes, rather than the 30–60 minute measurements typical to NAA. This also means that the technique is non-destructive, which could be of particular benefit to the mining industry. During exploration, each metre of core can cost thousands of dollars to obtain, and with only limited quantities available, the samples can have multiple uses.

GAA uses much larger samples than fire assay, typically around 500 grams. This has the potential to reduce the effects of sampling error (by averaging out variation to some extent). Interestingly, the quantity is not defined by mass itself, but by the fixed volume of the sample container.

The technique has the advantage over XRF that the higher-energy incident and decay radiation largely removes matrix interferences: particle size, packing density and sample distribution.

Free from the requirement for a nuclear reactor to generate the high-energy source, Tickner envisages that GAA could become a portable technique. However, 'portable' is in this case a relatively loose term. With the required shielding and equipment, a single unit could be the size of a shipping container. Even so, this offers potential advantages for field use in minerals exploration.

To date, the CSIRO team has concentrated its efforts on gold, having tested a wide range of samples in summer campaigns at Mevex Corp's facility in Canada. This has included ores, concentrates, tailings and carbon samples (from CN^- processing), with the typical range of sulfides, oxides and silicates.

The work has concentrated on investigating and refining the technique, with a particular emphasis on the subtleties of the density correction. Tickner now has his eyes set on establishing a commercial analysis facility in Adelaide, probably in 2016–17. Likely costs associated with this method, which may be the main potential disadvantage, have not yet been disclosed. I'll be keeping a close eye on this for my consultancy's gold samples.

Dave Sammut FRACI CChem is principal of DCS Technical, a boutique scientific consultancy, providing services to the Australian and international minerals, waste recycling and general scientific industries.

GAA across the periodic table

Approximately half of the periodic table will respond to gamma activation. However, although weighted towards higher atomic numbers, the response is not linear. Adjacent elements can have quite different activations, and it is therefore fortuitous that the technique is so well suited to an element as commercially important as gold.

Fortunately for the mining industry, other key commercially relevant elements are also well suited to GAA. Copper offers a strong activation that is both easy to observe and measurable across the useful commercial range of concentration.

Silver and lead are straightforward, and while zinc is somewhat more difficult, it is still measurable with GAA.

Platinum group metals are measurable, but less sensitive than gold due to higher energies of activation and resulting greater difficulty of separating background radiation from co-activated elements, particularly given the typically low concentrations of platinum group metals in samples. As such, for now GAA will probably be more suited to platinum group metal concentrates and metal accounting, rather than ore samples.

Rare earths, uranium and thorium are accessible by GAA. Higher energy X-ray sources will be required before iron will become practical for precision work.

For gold analysis, key interferences are elements such as Ba, Br, U and Th, which fission at low energy, pushing up the background and reducing sensitivity. However, interference typically occurs at closer to the per cent level, which is not common for those elements in commercial mineral samples.

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Changing the gender landscape of science academia

Modelled on a UK charter, the Science in Australia Gender Equity pilot envisages positive change for both women in science and Australian research in general.

BY **MADELEINE SCHULTZ**

The issue of under-representation of women at senior levels in science research has been studied for many years both in Australia and internationally. Women usually leave the science research workforce for either structural or cultural reasons.

The structure of an academic system is such that it rewards those who are able to work full time (frequently with workloads requiring well over 40 hours a week) for a continuous period, with extensive networking through conferences involving multiple days and long-distance travel.

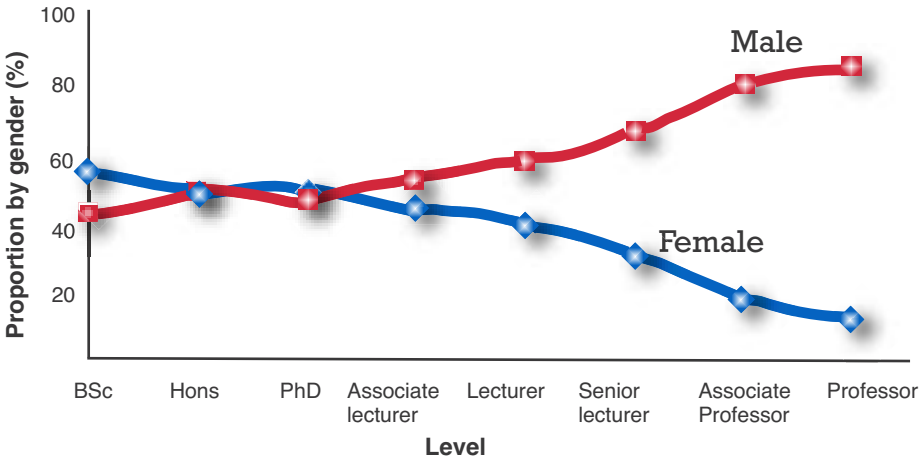
A critical period of a woman's academic career, the transition from postdoctoral appointments to a substantive position, is likely to coincide with the time when she may decide to have children. However, academic demands don't satisfactorily accommodate maternity leave, part-time work, flexible hours or limited ability to travel. Traditional family roles allow men more than women to undertake such work patterns.

Cultural reasons for the loss of women from science research are more subtle and complex. Unconscious bias has been identified as a fundamental cause of the loss of women from science research positions. This is the bias that leads to identical resumés or online courses being judged more positively when they are thought to

originate from men. It results in negative judgements of women for confident and assertive behaviour, the same behaviour for which men would be admired or rewarded.

Subtle yet pervasive consequences of unconscious bias include not inviting women to speak at conferences or to serve on committees or in other responsible roles. It can mean that women are not provided with important information that is given through informal channels.

A further cultural aspect is the recognised tendency to appoint in one's own image, which means that existing predominantly male hierarchies have an inherent inertia. The knock-on effects of these small but cumulative gendered practices on promotion, collaboration and academic success result in the situation illustrated in the so-called scissors graph, shown here for all natural and physical sciences in Australia.



For natural and physical sciences, the proportion of women drops significantly over the progression from undergraduate through the academic levels. This data was collected by the Australian Council for Educational Research and represents all tertiary institutions in Australia in 2011, with numbers ranging from tens of thousands for bachelor degree students through to hundreds for professors.

Women in the science research workforce: the scissor effect

The finding, that the proportion of women drops significantly over the progression from undergraduate study through the academic levels was one outcome of a recent, comprehensive study led by Sharon Bell and Lyn Yates and funded by an ARC Linkage Grant (2011–14). The study investigated gendered career paths and critical career transitions in chemistry and biology in Australia, using a combination of surveys, focus groups and analysis of existing data sets (full report at bit.ly/1MjI5NV). The RACI was an industry partner on the grant and CEO Roger Stapleford contributed to the project.

The point at which the scissors diverge, that is the career stage at which the proportion of men increases, has moved backwards in recent years: in 2007, women held more level A (the lowest level substantive academic role) positions than men, but this has now been reversed. Although analogous data specific to chemistry has not been gathered separately, the situation in our discipline very likely parallels that shown.

The point at which the scissors diverge, that is the career stage at which the proportion of men increases significantly, has moved backwards in recent years ...

The loss of women from the science research workforce is a complex problem that defies simple remedies. As Bell and Yates and others have identified, the solution requires cultural change on the part of institutions as well as changes to employment practices. Bell and Yates characterise the academic workforce as a marathon, in which multiple factors combine over many years to lead to success. Specific strategies that have been shown to improve the proportion of women in academic positions include requiring a balance of women and men to sit on selection and promotion committees, requiring formal and transparent processes for all decisions that affect seniority and funding, and providing mandatory training in the manifestations and consequences of unconscious bias.

As part of their ARC project, Bell and Yates have developed a website that includes a toolkit (bit.ly/1kuIqCt) aimed at senior leaders, team leaders and individuals (see images). This toolkit provides information to understand the cultural shift required from scientists and senior management to reduce the loss of women from science research positions.

The Athena SWAN charter

In the UK, the Athena SWAN charter was launched in 2005 to advance the career progression of women in science at UK universities. The charter is run by the Equality Challenge Unit, a charity funded by a group of representative and funding bodies in higher education in the UK. The ten principles of the Athena SWAN charter (bit.ly/1MjJnsc) can be summarised as a commitment to the following major goals:

- advancing gender equality in

academia, in particular, addressing the loss of women across the career pipeline and the absence of women from senior academic, professional and support roles
- tackling the gender pay gap (Note that in Australia this is also a federal requirement under the Workplace Gender Equality (Minimum Standards) Instrument 2014 of the Workplace Gender Equality Act 2012.)
- removing the obstacles faced by women, in particular, at major points of career development and progression, including the transition from PhD into a sustainable academic career
- addressing the negative consequences of using short-term contracts for the retention and progression of staff in academia
- making and mainstreaming sustainable structural and cultural changes to advance gender equality, recognising that initiatives and actions that support individuals alone will not sufficiently advance equality.

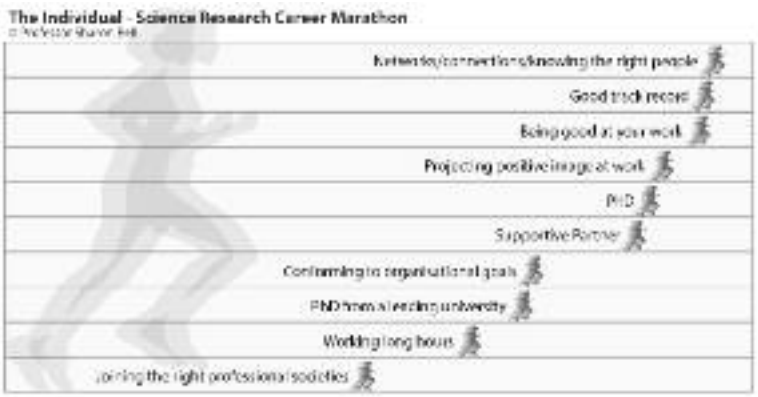
When institutions sign up to Athena SWAN, they commit to the ten principles. Once an institution has joined, both the whole institution and its departments can apply for Athena SWAN awards. These are awarded on the basis of performance at bronze, silver and gold levels. The criteria examine:

- academic staff career transition points (recruitment, promotion, those selected for research quality assessment exercises)
- career development
- flexible working and career breaks (including maternity and paternity leave)
- organisation and culture (including proportion of women in senior management, workload model).

There are currently 134 Athena SWAN institutional members and 483 award holders in the UK, and the program was recently launched in Ireland.

A preliminary review of the impact of Athena SWAN was conducted after five years of operation and found significant improvement in the percentage of women at all academic levels in several institutions; comparative data could not be obtained due to changes in reporting details (bit.ly/1Wxr35s). A more detailed study into the impact of Athena SWAN membership and awards was undertaken in 2013 (bit.ly/1MBdUgS). It was found that membership does impact positively on the culture of institutions, particularly if senior management is committed to change. A full statistical analysis of the impact of Athena SWAN after ten years of operation is underway and will be published in 2016.

The UK National Institute for Health Research (equivalent to the NHMRC) has instituted a requirement for an Athena SWAN Silver award for several of its funding schemes, amounting to approximately 25% of total funding awarded by the NIHR. This requirement will first be applied in the upcoming funding rounds starting in 2016.



Science in Australia Gender Equity

In November 2014, the Australian Academy of Sciences hosted a Science in Australia Gender Equity (SAGE) Forum with around 140 stakeholders to discuss the best approaches to improve gender equity in STEM (science, technology, engineering and mathematics). Up until that point, no national strategy to improve gender equity in STEM existed. It was agreed by the participants that concerted action across the

sector is required, and the approach chosen was to trial the Athena SWAN charter in Australia. This was launched in September 2015. Prior to this national approach, some individual institutions already had established gender equity programs including the Walter and Eliza Hall Institute of Medical Research (bit.ly/1kcbhvY). The discipline of engineering had also already released a comprehensive strategy to improve gender equity across their industry (bit.ly/1MJE8UE). However, chemistry was not involved in any such strategy and the RACI has no gender equity statement or policy similar to that of the Australian Academy of Technological Sciences and Engineering (bit.ly/1MBe8oe).

The pilot of Athena SWAN in Australia is being overseen by the Australian Academy of Sciences. The 32 institutions involved (bit.ly/1NR2NUv) are required to collect data on their current gender equity status, practices and policies, to identify areas of potential improvement and to implement action plans to improve gender equity for their staff.

The process begins with the appointment of a self-assessment team, which meets and puts together the data required for application for membership. Each institution is expected to develop their own action plan for improvement as part of their application. The team has the on-going task of monitoring implementation of the action plan, including how it will interact with other relevant committees and structures within the institution.

The actions suggested by Athena SWAN to improve gender equity in STEM encompass all aspects of academic life.

Recruitment processes: Women (and men where underrepresented) should be explicitly encouraged to apply. Recruitment panels should have a gender balance (not a token woman) and should be trained, including on the existence of unconscious bias.

Promotions: Identification of candidates and communication of the process and criteria should explicitly target women. The criteria for promotion should include the full range of work-related activities (including administrative, pastoral and outreach work) and should be sensitive to the impact of career breaks. Training or mentoring should be offered around promotion and the process should be transparent and fair.

Flexible working: Arrangements should support staff who may need to change their working patterns. A formal, institutional-level approach should cover absences of staff who take extended absence rather than relying on their colleagues. This should include arrangements to enable staff to keep in touch during leave, and to support staff before and upon their return to work. Managers should be supported in managing flexible working arrangements and the options available should be communicated to all staff. Staff transitioning from part-time to full-time work should be supported with mentoring or coaching support and a phased increase in workload or working pattern. The timing of meetings and social gatherings should consider those with caring responsibilities and part-time staff.

Child care: Child care with extended opening times and sufficient places should be provided at institutions.

Culture: Consistent HR policies about equality, dignity at work, bullying, harassment, grievance and disciplinary processes should be enacted. Any identified differences between policy and practice should be addressed. Staff with management responsibilities should be up to date in their HR knowledge.

Senior roles: Heads of schools, faculties or departments should be decided by a transparent process. Any specific gender underrepresentation should be addressed. Targeted support or leadership training should be provided for potential future senior managers to improve any gender imbalance on committees; role rotation, deputising and shadowing can be used as well as increasing the size of the committee if necessary.

Workload model: This should include teaching, pastoral, administrative and outreach responsibilities. It should be fair and transparent, and periodically reviewed by a gender-balanced committee.

Events: Gender equality should be built into organisation of events. This includes speakers and chairs in seminars, workshops and other relevant activities.

Outreach activities: While it is important to have underrepresented groups involved in outreach, often people from these groups end up doing a lot of outreach, which can affect other parts of their job, particularly research. Outreach should be formally recognised and included in workload modelling.

Action plans for Athena SWAN should be SMART (specific, measurable, achievable, relevant and time-bound) and prioritised, and responsibility for completing actions should be distributed across a range of staff.

Diverse groups in research have been shown to lead improved outcomes compared with homogeneous groups. The Australian model of Athena SWAN should benefit Australian research as well as individual women in their research careers.

On 7 December 2015 the federal government announced that it will support the expansion of the SAGE pilot to cover more Australian science and research institutions. This funding is part of a total $13 million to be spent over five years on several initiatives to encourage more women to choose and stay in STEM research, careers, startups and entrepreneurial firms.

Madeleine Schultz MRACI CChem was a senior lecturer in chemistry at Queensland University of Technology until recently and is currently working at the European Molecular Biology Laboratory in Heidelberg, Germany, synthesising fluorescent dyes for live cell microscopy. She maintains a mailing list for women in chemistry in Australia; if you would like to be included please email her at madeleine.schultz@qut.edu.au.

2015 RACI National Award winners

Applied Research Award

Professor Anthony Weiss FRACI CChem is the world leader in human tropoelastin research and synthetic human elastin. His laboratory is making human elastic materials that accelerate the healing and repair of arteries, skin and other 3D human tissue components. Anthony holds the McCaughey Chair in Biochemistry, leads the Charles Perkins Centre Node in Tissue Engineering and Regenerative Medicine, and is Professor of Biochemistry and Molecular Biotechnology in Molecular Bioscience at the University of Sydney. He also has appointments at the Bosch Institute and Royal Prince Alfred Hospital and is Distinguished Visiting Professor Brain Korea 21, and Visiting Professor in Biomedical Engineering at Tufts University, US.

Anthony is a Fellow of five societies, including Fellow of the Royal Society of Chemistry (UK), Fellow of the Australian Academy of Technological Sciences and Engineering (Australia) and Fellow of the American Institute for Medical and Biological Engineering (US). He is on seven editorial boards. He works at the interface of science, technology and industry. He has 30 awarded patents, is a serial entrepreneur, biotechnology company founder, and promoter of national and international technology development, and has been given a substantial number of national and international awards and prizes.

Citation: Contributions to Chemistry and the Profession

Dr Clarence J. Ng ('Clarrie') FRACI CChem, FAIFST graduated from the University of New South Wales and joined Arnott's Biscuits Ltd in 1972 as a research chemist developing new analytical methods using instrumentation (AA, HPLC, GLC). Over the next 31 years he held positions of Research Supervisor Analytical Services (including Microbiology), Company Analyst (procedures and quality systems) and Specifications & Regulatory Affairs. His duties extended outside the laboratory into product development, process development and food labelling. He also represented Arnott's Ltd in the Cooperative Research Centres for Wheat Breeding specific for Biscuits and Bake Vision of Biscuits. In conjunction with Macquarie University, the Bake Vision project involved development of a laboratory computer vision system to measure biscuit bake colour and taking it to the factory floor.

Clarrie became an RACI student member in 1969 and joined the Analytical Chemistry Group (NSW) in 1982. His roles within this Group have been Secretary, Chairman and Treasurer. As Chairman he fostered the Group's aim to use the profit from seminars to support undergraduate students through prizes at NSW universities and travel bursaries to the annual R&D Topics Conference. He also represented the Group on the NSW Branch Committee (Chair, Fellowship Committee) and the Analytical Division Standing Committee. He has been on the organising committee of numerous state and national conferences and seminars. He retired from the Analytical and Environmental Chemistry Committee in 2014 to enjoy more time with his grandchildren.

Other professional duties have been with Australian Institute of Food Science and Technology (Scientific Affairs Committee), NATA (Chemical Testing Assessor and Chair, Food & Drug Technical Group) and Standards Australia.

After retiring from Arnott's, Clarrie established a consultancy providing food labelling of biscuits and snack foods. He has also continued his involvement with Scouts Australia since 1987, currently as Group Leader of 1st Brush Park Scout Group.

Dr Richard Thwaites FRACI CChem was born and educated in the UK, graduating from the University of Oxford in 1967 with the degrees of MA and DPhil in Chemistry. After working in London, he was sent to Australia in 1970 on a temporary secondment, but decided to stay. He worked for Albright & Wilson (Australia) Limited in Melbourne and Sydney in a variety of roles, including development, production, marketing and general management and was also Business Manager of the CRC for Bioproducts and Commercialisation Director of the CRC for Industrial Plant Biopolymers. He retired from paid employment in 2008.

Richard became a Member of the RACI in 1971 and a Fellow in 1994. He chaired the Qualifications and Accreditation Committee from 2003 to 2012, and was Victorian Branch President from 2012 to 2014. He is currently Victorian Branch Treasurer and Member of the *Chemistry in Australia* Management Committee.

Richard, who gained a Graduate Diploma in Theology from the Melbourne College of Divinity in 2012, is also a Member of the Australian Institute of Company Directors, a Member of the Royal Society of Chemistry, a former President of the Council of

Whitley College and Secretary of the Ashburton Baptist Church. He is currently Deputy Chair of Ashburton Baptist Community Services Inc., is the convener of the Society of Chemical Industry (Australia Group) and is a member of the Committee of the Oxford University Society in Victoria.

Richard is married to Sandra: they have three adult children and one grandchild.

Professor Joe Shapter FRACI CChem obtained his PhD from the University of Toronto in 1990 working with Professor J.C. Polanyi on the detection of small molecules and the determination of their energies. From 1990 to 1996, he worked at the University of Western Ontario (London, Ontario) building a scanning tunnelling microscope and lecturing first-year chemistry.

In 1996, he moved to Flinders and is now Professor of Nanotechnology and Dean of the School of Chemical and Physical Sciences. Prof. Shapter led the establishment of and is now course coordinator for the Flinders Bachelor of Science Degree in Nanotechnology (2000-2003, 2007-present). This was the first degree of its kind in the world. He was the founding Director of the Defence Science and Technology Organisation (DSTO) funded Centre of Expertise in Energetic Materials (CEEM) and is currently the Director of the South Australian node of the Australian Microscopy and Microanalysis Facility (AMMRF).

Joe has served the RACI in various capacities. He has served in several executive roles in the South Australian Branch, was a board member for two and half years and has been a long-standing member of the Membership Assessment Committee (MAC). He was recently Congress Chair for the RACI National Congress held in Adelaide in December 2014.

Cornforth Medal

Dr Lara Malins MRACI was born in 1987 in South Carolina, US. In 2009, she completed her undergraduate studies in chemistry as a Trustee Scholar at Boston University, where she worked in the laboratory of Associate Professor Scott Schaus on the synthesis of purine-based natural products. She was awarded an International Postgraduate Research Scholarship in 2010 to undertake her PhD at the University of Sydney in the group of Professor Richard Payne. Her doctoral research focused on the development of novel peptide ligation methodologies for the synthesis of biologically relevant and post-translationally modified peptide and protein targets. After completing her PhD in 2014, she remained at the University of Sydney for a short postdoctoral stay in the Payne laboratory. In June 2015, she relocated to The Scripps Research Institute in La Jolla, California, where she is currently a postdoctoral research associate in the laboratory of Professor Phil Baran.

Fensham Medal: Outstanding Contribution to Chemical Education

Professor Brian Yates FRACI CChem was appointed as the Dean of the Faculty of Science, Engineering and Technology at the University of Tasmania in July 2015. Professor Yates is a researcher with an international reputation for computational chemistry and a highly commended teacher.

Brian has carried out research in computational chemistry with particular applications to organometallic, inorganic and organic chemistry. He has received considerable grant funding and has published over 150 papers.

Brian has also built up a strong reputation for teaching excellence. He has been awarded competitively funded teaching development grants at the national (CAUT/CUTSD, ALTC) and state levels, and he has been rewarded with local and national teaching excellence awards (the 2006 Carrick Australian Award for University Teaching Excellence in Physical Sciences, the 2007 Medal of the Chemical Education Division of the RACI, and the 2010 Vice-Chancellor's Individual Citation for Outstanding Contribution to Student Learning from the University of Tasmania). In 2010–2011, he was appointed as an Australian Learning and Teaching Council (ALTC) Discipline Scholar in Science. During this time he worked in partnership with Professor Susan Jones to facilitate the development of a set of nationally agreed learning and teaching academic standards in science higher education. These Threshold Learning Outcomes for Science were endorsed by the Australian Council of Deans of Science in 2011 and a number of implementation projects are currently underway.

Brian was an Executive Director (Engineering, Mathematical and Information Sciences) at the Australian Research Council from 2013 to 2015. In this role, he helped to develop new initiatives within the ARC to support research excellence in Australia, as well as overseeing grant awarding processes and the development of research management software.

H.G. Smith Memorial Award

Professor Calum Drummond FRACI CChem has research interests in the area of advanced materials, including application to energy storage and biomedical products. He has been an author of over 200 publications. Calum is a graduate of the University of Melbourne (BScEd, BSc(Hons), PhD and DSc).

Calum has a strong interest and passion for the commercialisation of research outcomes. 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. Before this, he was Chief of CSIRO Materials Science and Engineering (CMSE). Prior to becoming a Chief, Calum was seconded from CSIRO to be the inaugural Vice President Research at CAP-XX. CAP-XX develops supercapacitors for consumer electronic products. In 2006, CAP-XX listed on the London Stock Exchange.

The outstanding calibre of his research has been recognised through the award of the Victoria Prize for Science and Innovation in the Physical Sciences Category (2015), CSIRO Fellow designation (2013; CSIRO's highest award for exceptional scientists), World Economic Forum Global Technology Pioneer (2005; awarded to CAP-XX), Frost and Sullivan (USA) Excellence in Communication and Information Technologies Award (2006; awarded to CAP-XX), an Australian Research Council (ARC) Federation Fellowship (2003–10), an ARC Queen Elizabeth II Fellowship (1990–93), the inaugural R.J.W. Le Févre Memorial Prize from the Australian Academy of Science (1989), the RACI Rennie Memorial Medal (1989), the RACI Applied Research Award (2002), the RACI Industrial Chemistry Division R.K. Murphy Medal (2004), the RACI Green Chemistry Challenge Award (2005), the RACI Physical Chemistry Division Medal (2006), CSIRO Medal for Outstanding Research Achievement (2004), CSIRO Medal for Business Excellence (2011), Distinguished Lecturer Award from The Colloid and Surface Chemistry Division of the Japanese Chemical Society (2011), Distinguished Paper Award of The Soap and Detergent Association (USA) and The American Oil Chemists Society (2001), both the David Syme Research Prize (2002) and the Grimwade Prize in Industrial Chemistry (1995) from the University of Melbourne, and a Rothmans Foundation Fellowship (1990; declined).

Calum is a Fellow and former Director of the Australian Academy of Technological Sciences and Engineering (2006; FTSE), a Fellow of the Australian Institute of Company Directors (2004; FAICD), past RACI Honorary General Treasurer and Council member, and a Fellow of the Royal Society of Chemistry (2012; FRSC; UK-based).

He is an adjunct Professorial Fellow in Chemistry at the University of Melbourne and an Adjunct Professor in Chemical Engineering at the University of Queensland. He has held an Adjunct Professorship in Chemistry at the University of Sydney.

Le Fèvre Memorial Prize – Australian Academy of Science

Professor Chengzhong (Michael Yu) received his PhD in 2002 from Fudan University, China. He joined the University of Queensland in 2010 as a group leader at the Australian Institute for Bioengineering and Nanotechnology. He has established a research group at the University of Queensland with a focus on functional materials and their applications in health, energy and environmental protection. Professor Yu has made significant contributions to the fundamentals of self-assembly of nano-structured materials and has invented many functional materials with diverse applications in drug delivery and water treatment. He has published over 170 journal papers, which have been cited over 7900 times resulting in an *H*-index of 46. He has attracted over $7 million in competitive grant funding in Australia and 12 grants in China.

Leighton Medal

Armed with a Diploma of Applied Chemistry and a PhD degree, **Professor Ian Rae** FRACI CChem went forth into the wide world of chemistry in 1964. At first his career followed a traditional path – overseas postdoctoral experience followed by 27 years at Monash University broken by periods of sabbatical leave in Britain, America and Argentina. As he moved into university administration and eventually to a sort-of-retirement, his laboratory bench was replaced by an armchair from which he remains involved in chemistry as an adviser, writer and historian.

Ian is perhaps best known to chemists for his monthly Letter in *Chemistry in Australia*, and has recently become co-editor of the journal *Historical Records of Australian Science*. Ian is a Fellow and past president of the Institute, and a Fellow of the Australian Academy of Technological Sciences and Engineering. While continuing to hold a position as Honorary Professorial Fellow at the University of Melbourne, he has had major involvements with Australian government agencies and the United Nations Environment Programme.

Masson Memorial Prize

Johnathon Robertson (Student Member) was born in NSW in 1994, before moving to Tasmania in 1997, where he completed primary school, high school and college. In 2013, he enrolled in a BSc at the University of Tasmania where he has majored in Chemistry, Biochemistry and Plant Science. In 2016, he will undertake his Honours year in the field of Organic Chemistry with Dr Alex Bissember at the University of Tasmania.

RACI Chemistry Educator of the Year Award

Dr Natalie Williamson MRACI CChem completed her BSc(Hons) and PhD in organic chemistry at the University of Adelaide. The opportunity to do some teaching in the undergraduate chemistry laboratory during her postgraduate studies ignited her interest in learning and teaching. Natalie is currently a senior lecturer and the Level I Director, Chemistry, in the Department of Chemistry at the University of Adelaide, and is responsible for over 1000 first-year students who commence their chemistry studies each year at the university.

She was appointed to the university in 2009, and teaches in eight undergraduate courses at first-, second- and third-year level. Natalie enjoys helping students find their own way to understanding using a mixture of interactive classroom activities, humour and immediate feedback to engage students in the learning process. Natalie chaired the committee that oversaw the recent revision of two of the Department of Chemistry's first-year courses, resulting in their complete restructure and the use of Process Oriented Guided Inquiry Learning (POGIL). This work was awarded funding and professional development support through the ALTC and SaMnet, with Natalie invited to speak at two education conferences about the development and impact of the new courses.

Since her appointment, Natalie has received a number of teaching awards, including the Executive Dean of Sciences Award for Excellence in Teaching in 2009 (first five years of teaching award) and 2014 (team award) and an ALTC Citation for Outstanding Contributions to Student Learning (2010). Natalie was named Early Career STEM Educator of the Year at the 2013 SA Science Excellence Awards and received the University of Adelaide's Stephen Cole the Elder Award for Excellence in Teaching in 2014.

Rennie Memorial Medal

Dr Colin Jackson MRACI graduated from the University of Otago, New Zealan, with a BSc(Hons). He then studied for a PhD in chemistry at the ANU, after which he worked at CSIRO as a research team leader. In 2009, he was awarded a Marie Curie Fellowship to work at the Institute of Biological Structure in Grenoble, France. He returned to ANU in 2012 to establish a chemical biology research group. He has published over 50 research papers and several patents and has been awarded a number of prizes and fellowships, including an ARC Future Fellowship and the 2015 ACT Scientist of the Year RACI Post Graduate Student Travel Bursary.

RACI Post Graduate Student Travel Bursary

The following students have won a Travel Bursary: Arthur Zavras (University of Melbourne), Shu Lam (University of Melbourne), Megan Cook (University of Queensland), Daniel Pasin (University of Technology Sydney), Jessica Pandohee (RMIT) and Joana Da Rocha (University of New South Wales).

ASVO award for best oenology paper

Dr Geoff Scollary FRACI CChem (Honorary Principal Fellow, School of Chemistry, University of Melbourne, and Adjunct Professor, Charles Sturt University) and Dr Andrew Clark (National Wine and Grape Industry Centre, CSU), together with Paris Grant-Preece (CSU) and Natalie Cleghorn (Yalumba), have been awarded the 2015 Oenology Paper of the Year by the Australian Society of Viticulture and Oenology (ASVO), the society that owns and publishes the *Australian Journal of Grape and Wine Research*.

The ASVO jury selected the paper titled 'Copper(II) addition to white wines containing hydrogen sulfide: residual copper concentration and activity' for making a significant contribution to the debate on the use of copper in winemaking as studies into its effective removal are important for today's wine industry. This, the jury commented, is particularly relevant with the rapid transition to alternative closures to cork.

After several years of wine research in the University of Melbourne, Geoff was appointed as foundation Director of the National Wine and Grape Industry Centre in 1997, returning to the School in an honorary position on retirement from the NWGIC.

The award was a magnum-size engraved decanter – all the authors are waiting for their next meeting for its 'baptism'.

Centenary Book – volunteer helpers required

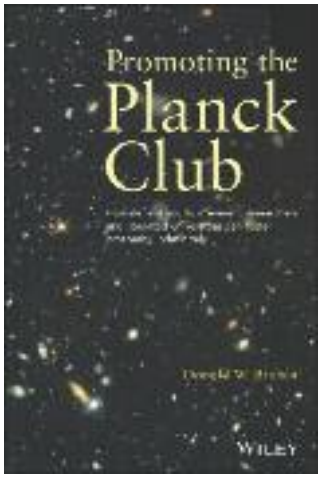
In 2017, the RACI will be 100 years old and to celebrate this mega RACI milestone, the Centenary Committee is working to write a coffee-table-style book covering the Centennial RACI history. Obviously this is an enormous project and we are looking for interested parties to research and write relevant pieces on important events and people over the years.

We also wish to make contact with anyone in possession of past RACI-related documentation, letters, records and, in particular, photos that can be incorporated into the project.

If you are interested, please contact Roger Stapleford (roger.stapleford@raci.org.au).

As your RACI member magazine, *Chemistry in Australia* is the perfect place to voice your ideas and opinions, and to discuss chemistry issues and recently published articles.

Send your contributions (approx. 400 words) to the Editor at editor@raci.org.au.



Promoting the Planck Club

Braben D.W., John Wiley, 2014, paperback, ISBN 9781118546420, 222 pp., $88.95

Promoting the Planck Club is a passionate development exploring the proposition that defiant youth, irreverent researchers and liberated universities can foster prosperity indefinitely. Author Donald Braben presents interesting vignettes on scientists from Max Planck onwards, who exemplify these characteristics, thus qualifying for membership of his Planck Club, and who have made enormous contributions to scientific progress. Most of the book is devoted to the biographies of this select group. Inevitably, these interesting tales feature instances of adversity, resolute and often unrecognised genius, and a certain amount of serendipity. They are enjoyable reading.

Braben concludes the way to foster future prosperity is to withdraw a lot of the shackles constraining scientific research and let more people follow their passions and ideas. The pay-off will be significant societal advantage from discoveries arising from this strategy, just as there has been great economic and social advancement from discoveries made by members of the Planck Club. Does the argument hold up? Well, only partly in my view.

Braben concludes the way to foster future prosperity is to withdraw a lot of the shackles constraining scientific research and let more people follow their passions and ideas.

Dr Davis McCaughey AC, one of Victoria's notable governors, said 'students need time to waste and places to waste it in, if they are to become reflective men and women'. You could equally say this of scientists; if you want people to reflect, and to think deeply, then you are unlikely to succeed if you feed them a diet of research grant applications to apply for, reinforced by smacking them about the ears for enhanced productivity and basing their promotion on the length of their publications ('Never mind the quality: just feel the width!'). And imposing what must seem like an interminable regime of justifying their very existence. And yet, many (most?) young Australian researchers are faced not only with fierce competition in the job market, but extreme competition in career advancement, often based on some score achieved on what is a quintessentially un-scorable scale. Not a lot of attention to Pasteur's Chance favours the prepared mind'. A very Hobbesian world view, indeed, unleavened by McClelland's Theory X – Theory Y! Fortunately, the Australian Government has flagged an end to the 'publish or perish' culture hitherto applied to university research funding (*The Age*, 16 November 2015, p. 8), although adopting a cautionary approach, one ought probably 'always keep a hold of nurse for fear of finding something worse'.

How do you judge quality? Well, for a start you'd need an agreed definition. Everybody knows quality when they see it, but then everybody looks through different eyes. If you want to explore this further, then try Robert M. Pirsig's *Zen and the art of motorcycle maintenance*. One thing is for sure, it is not something you are likely to be able to quantify with a number (and isn't that exactly what we try to do?). I suppose if you equate quality with output, then where research grants are concerned, about the best you can do is apply a version of the Markovnikov rule, which I learnt as, 'To him who hath shall be given'. It more or less works with racehorses, so why not scientists? Alas, not much help to the maiden (of either gender!)

We seem to lurch about in Australia, unfettered by anything remotely resembling a national science policy. What should be our national balance between pure research (in a sense our membership dues for 'world knowledge incorporated') and applied research (directed at attaining some national economic advantage)? How do we balance serendipity, by its very nature probabilistic, against strategic research, by its very nature goal-oriented? And perish the thought of what you can do when purity strays! Lewis and Randall, in the introduction to their seminal thermodynamics text, wrote of 'cathedrals of science', constructed by 'a few architects and many workers'. How do we pick the architects of the future? (And particularly when most of us are closer to the bricklaying end of things than to the drawing board.)

My short answer (my long answer too) is, I don't know! Having read Braben's book, which I enjoyed, I really have more questions than answers. I'm pretty sure the present system is seriously broken, but Braben's book doesn't lead me to pontificate on any solution. It's worth reading. See what you think.

R. John Casey FRACI CChem

Secret science: a century of poison warfare and human experiments

Schmidt U., OUP, 2015, hard cover, ISBN 9780199299799, 672 pp., £25

Let me tell you from the start: *Secret science* is sobering and, in many ways, profoundly worrying and depressing reading. It is a 'far-from-light' work and probably not for the faint of heart, despite its obvious erudition and scholarly mien. It is not a chemistry book. Rather, it is about the history and ethics of deployment of chemical research in pursuit of military goals. Author Ulf Schmidt is Professor of Modern History at the University of Kent, with research interests in the history of modern medical ethics, warfare and policy in 20th century Europe and the US.

Near Ypres at about 5 p.m. on 22 April 1915, German engineers released 600 tons of chlorine, sending a rolling cloud of choking green gas, about 7 kilometres wide and 1.5 metres high, towards the Allied trenches. This action, at Fritz Haber's instigation (who, nevertheless, was awarded the 1919 Nobel Prize for Chemistry, to the shock of the *civilised* world … well, to the winners of World War I, anyhow), killed an estimated (albeit possibly over-estimated) 5000 soldiers and seriously injured about 10 000 more, marking the start of a new form of human bastardry – chemical warfare.

We all know there are 'spooks' behind curtains observing us (for instance our internet usage, our telecommunications, our shopping habits, our medical history, our driving practices, the places we go, and the people we see) and that our governments (notionally our 'betters') cynically manipulate public discourse and indulge in varied nasty, restrictive and unpleasant actions, on our behalf, frequently without any genuine approval, endorsement or, indeed, real informed cognizance and scrutiny by the general population (cloaked as 'operational matters'). In general, you could say we pay our taxes, take our choice and fairly largely ignore these less pleasant aspects of our existence, unless and until they directly impinge on us. This book takes us behind the barbed wire fences and walls of secrecy and traces the detailed and documented history of development and testing of chemical and biological weapons, principally by Britain (Porton Down), the US and Canada. And, it describes very unpleasant stuff.

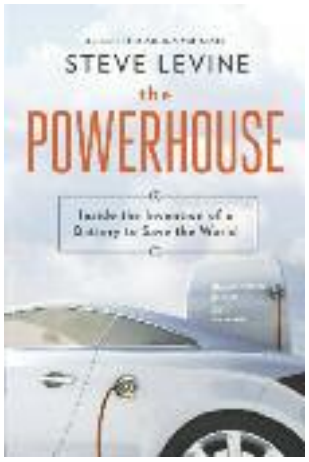
It is a story of what can, and did, happen when clever people are allowed to 'play', unsupervised by any moral or ethical restraints, with some of the most noxious substances in creation. It is a story of how, over the last hundred years, scientists, military people and senior civil servants have contrived to obtain enormous resources by indulging in flexible justification strategies about national security in order to fund experimental research into chemical and biological warfare, conducted in top secret, locked establishments.

Overall, what is perhaps most disturbing is the cavalier attitude taken to human beings, and animals, in trial exposure to chemical and biological agents. Many of the medical experimenters do not appear to have encountered any conflict between their Hippocratic Oath and inflicting unconscionable, sometimes life-long, suffering on uninformed human subjects. When things went badly wrong, veils of secrecy, obfuscation, deceit and dishonesty were the order of the day.

And the methodology of poisoning just kept on getting better and better as we (well, our agents, anyway) advanced from chlorine and phosgene, through mustard gas (currently in use in Syria) to VX agents, truth drugs (like LSD), incapacitating agents (like CS gas), and biological toxins (think anthrax). You'd have to be stark staring bonkers to knowingly expose yourself to these agents! Unless, of course, you weren't actually told. So, when you are next fulminating about the demands of the 'bloody ethics committee', or wondering why the trial you think you might participate in has just sent you a 15-page consent form when all they want is a few millitres of your blood, then just remember it is all about making *you* think and making sure *your consent* is informed. And it is way ahead of the (demonstrated) alternative.

I found this book deeply depressing and distressing. It has enhanced my general cynicism and scepticism, and caused me to reflect on what is right and what is wrong (it all depends on where you are standing). I also realise anew just how lucky I am to live in Australia where the probability of deployment of these terrible weapons seems presently small. If you seek a well-researched account of a side of secret warfare, the development of chemical and biological weapons and their testing on human subjects, then I doubt you'll find a better book. It is a compelling account. You also need a certain 'stomach'/courage to cope with some of the instances of man's inhumanity to man, inflicted by people who were basically just like you and me, and who believed they were working for the public good. All war is evil, but to this chemist at least, chemical warfare seems particularly so.

R. John Casey FRACI CChem



The powerhouse: inside the invention of a battery to save the world

LeVine S., Viking Penguin, 2015, hard cover, ISBN 9780670025848, 308 pp., $32.99

Battery technology will change the world, and the race is well and truly on to be the nation to make the next big breakthrough. Set against a backdrop of growing environmental need, financial reward of untold proportions, and all-important political power, is the story of a team of researchers at Argonne National Laboratory in Chicago, their collaborator, Silicon Valley start-up company Envia Systems, and their nickel manganese cobalt ('NMC') battery technology.

In *The powerhouse: inside the invention of a battery to save the world*, Steve Levine looks at the personalities, the deals, and the strategies that have underpinned battery research and commercial licensing in Argonne and Envia over the past ten years or so. He also looks at how these factors have influenced their failures and successes in the race to provide automotive and tech giants including General Motors, LG, Apple and Samsung, but also the US Government, with the breakthrough they all so desperately want: a battery not only cheaper to manufacture but safer, and more powerful and durable than existing technology.

Having been granted access to Argonne for two years to follow this story, Levine focuses on the people rather than the science, interspersing the present-day narrative with short biographies of key players such as John Goodenough, Mike Thackeray, Khalil Amine, Jeff Chamberlain, Atul Kapadia and Sujeet Kumar and how they came to play the roles they did. Through having 'lived' in the battery world for this substantial period of time, you get a strong sense of Levine's connection to the personalities in this story – their demeanour, tone and energy – and a connection to the atmosphere at meetings and conferences that only comes through firsthand experience. For these reasons, this book would suit people with an interest in the business of innovation and the role of intellectual property in negotiating funding and industry partner deals. It would also be of interest to those who would like to gain a general perspective of the way the battery industry is shaping up from the inside, and in particular, across the public/private divide.

Notwithstanding these positives, I found Levine's almost purposeful avoidance of battery science in this book a great disappointment. Although focusing on the players who did the science rather than on the science they did certainly improves accessibility for a non-science literate audience, a few simple diagrams, some equations, and some more detailed scientific discussion would have added a great deal of substance and interest to the story. This book is also very US-centric, and is thus imbued with a healthy dose of US nationalism (and anti-China sentiment), which in the end I found a bit tiresome. I am also not sure this book meets its own brief as a 'thrilling' account of the next technological age. While Levine has done an admirable job of condensing a vast array of people, places and information to arrive at the story in this book, the challenge was always going to be making the 'climaxes' – successful licencing deals, takeover bids, or awards of funding, which are inherently most interesting to those directly affected – exciting to outsiders.

Overall, *The powerhouse: inside the invention of a battery to save the world* is a decent story of the 'drama of technological competition', but readers will need to look elsewhere for insights into the technology itself.

Jessica Chadbourne MRACI CChem

iStockphoto/Jirkab

Technology in labs: where will IT take us?

The manufacturers of key laboratory equipment have forever looked for new means to improve and differentiate their equipment. A key means for achieving this has been, for example, labour-saving technologies such as higher throughput lab equipment and automated sample loading and unloading.

In clinical and industrial test labs where high volumes of standard testing are the primary function, there already exists very high degrees of automation and short cycle time testing. The higher revenues in this sector have allowed equipment manufacturers to invest heavily into product development to create these customer benefits. R&D labs have benefited from these technology upgrades by a 'trickle-down' effect.

The introduction of labour-saving automation and high-throughput technologies in labs is nowhere near complete but I would suggest that we are not at some point where there will be a sudden surge in new automation or increased throughput equipment. The transition in labs away from manual labour towards higher-throughput and automated equipment has been and will remain a steady process.

An interesting transition that is going on right now is the repurposing of newly available and now very cheap IT technologies – smartphone apps, wireless data connection to equipment, cloud data storage and analysis, crowdsourcing and others – for application in the labs. In July 2014, for example, I reviewed a number of new smartphone and web-based apps that aim to radically improve lab productivity related to data capture and analysis.

My view is that there will be a rush of newly available IT products for lab use in the next decade. Critical to this trend is the relatively low cost of developing these products; all that is required is the re-engineering and re-purposing of existing IT technologies, providing an attractive return on investment in new product development.

The result of this uptake in IT technologies in the labs will probably be fairly neutral to employment but it may be accompanied by an increasing fraction of lab workers looking at computer screens. Also I would note that some of these screen-facing employees may not be local to the lab, or even to Australia.

After all, the point of many IT technologies is to remove employment where possible, to increase productivity on labour, and to disconnect the place of labour from a physical location of high capital equipment investment (e.g. a lab). Whether or not we agree that this results in good outcomes is hardly the point – this is a trend that seems virtually unstoppable.

On the larger issue of the outlook for employment in the labs of Australia, ponder this press release (bit.ly/1HtbhBN): 'A lack of skills in Science, Technology, Engineering and Mathematics (STEM) in the current and emerging workforce is holding back Australia's economy. A recent survey by AIG [bit.ly/1Qr3A12], which spoke to 300 businesses across the country, found nearly half were having difficulty recruiting technicians and trade workers with STEM skills.'

I believe that 'STEM' is a case of a false grouping. There's IT and there is the sciences (including mathematics in Australian universities) and the non-IT engineering studies and these should not be grouped together in the context of policy development.

The real issue is that businesses are having trouble hiring IT workers at reasonable cost because these graduates are in such demand. If you subtract IT types from STEM and re-polled all those businesses, they would likely answer 'we hardly need any of them (science graduates and old-school engineers) and when we do there is no issue finding them'.

One result of pushing STEM education is that we have graduates in the sciences who study for years and ultimately are forced to seek employment outside of their fields of expertise.

We are already training way too many scientists and it makes no sense to 'double down' on this problem. Also, under-employment in the sciences puts downwards pressure on salaries, which will likely lower the quality of candidates entering undergraduate science.

We are in the digital age and the relative demand for scientists will likely continue to decline over the next few decades. On the other hand, we won't be able to train enough IT graduates.

I am sure that tertiary educators know that a large percentage of both undergraduates and postgraduates in the sciences will not get jobs in their chosen field and will end up elsewhere. They may be able to justify this by assuming that the rigour of training in the sciences will successfully enable these graduates to retrain and succeed in many other career paths.

However, I am not sure that graduates facing large HECS debts would view the situation with the same indolence.

Surprisingly there is no readily available information on how many graduates get jobs in their field of training. The primary source of information for people entering tertiary training, the Graduates Careers website (www.graduatecareers.com.au), is sadly lacking in readily available access to this critical information. This urgently needs to be addressed.

I would suggest that the biggest impact on employment in the labs of Australia will not be the introduction of new technology. The overtraining of employees for this sector is a more immediate issue.

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Ingenious vs obvious: is your invention patentable?

Dr Andrew Gregory, Registered Patent Attorney, FB Rice

In many industries inventions provide solutions to known problems. Although an invention may be useful, an inventor has to prove that their invention justifies the granting of a patent.

Patent law dictates that to qualify for patent protection, all inventions must be novel and possess an inventive step. Establishing novelty is generally a factual exercise – is the invention new as compared with known information (prior art)? However, establishing that an inventive step exists and an invention is not obvious, is somewhat subjective in nature and often difficult to prove once the invention is disclosed due to hindsight.

Nevertheless, 'simple' inventions can be protected as long as at least a 'scintilla of invention' is present. Even if an invention hinges on a 'minor' modification, factors that can tip the scales in an inventor's favour are cases where:

- there has been a long-term need for a particular invention; and/or
- competitors have failed to find a solution; and/or
- commercial success.

Usually the first time an applicant has to justify their inventive step is during examination of a patent application. An examiner compares the features of the invention as recited in a claim with the prior art. To satisfy the inventive step criterion, an applicant must convince the examiner that their invention is not obvious in view of the prior art.

The general test for an inventive step is whether a hypothetical skilled person in the same technical field could make the invention without any ingenuity. If the examiner concludes that this hypothetical person could have made the invention based on information contained in the prior art (using common general knowledge in the relevant technical field), then the invention lacks an inventive step. It is then necessary to submit arguments or refine the scope of the invention to convince the examiner otherwise.

A strong indicator for an inventive step is where an invention unexpectedly works despite the established prior art suggesting otherwise.

A strong indicator for an inventive step is where an invention unexpectedly works despite the established prior art suggesting otherwise. Going against convention indicates there has been a 'light bulb moment' where an inventor has been inspired.

Importantly, patents can be granted for new uses for known articles, especially where previously unknown advantages are indicated. For example, combinations of known pharmaceutical compounds may meet the inventive step threshold if an inventor identifies an unknown benefit, e.g. synergistic properties, when treating a medical condition.

While there are many hoops to jump through in order to protect your intellectual property, identifying the merits and benefits of an invention is an important first step. In practice, this requires a detailed knowledge of the prior art before a patent specification is prepared. This knowledge will guide how best to describe the invention, and, more significantly, how to distinguish over the prior art. In this way, it is more likely that an inventive step will be correctly identified and the features conferring the inventive step fully described.

In all technical fields, the importance of a thorough understanding of the prior art gained through searching the literature, particularly patent literature, cannot be underestimated.

For more information, email agregory@fbrice.com.au.

Improving laboratory learning

Laboratories are the signature pedagogy in chemistry education (see April 2005 issue, pp 11–12; September 2013 issue, p. 35). Good laboratory learning engages students in the practices of science at many levels, including but not limited to the development of technical skills, demonstration of theoretical concepts, development of generic skills such as occupational health and safety practices, team work, verbal and written communication skills, and many others. However, many laboratory programs do not realise their potential. Some reasons for this are fear of chemical hazards, poor pedagogy, out of date practices, uninteresting activities, lack of class time, and lack of expertise on the part of the teacher–instructors. A typical example would be a year 12 teacher developing a laboratory activity, but the year 9 classroom teachers either not using the activity or omitting parts of it because they lack confidence with the concepts.

Teachers investigating the (left) breaking strain of polystyrene in an experiment on composite materials and (right) the corrosion of metals at an ASELL for Schools workshop at Mooroolbark College, Melbourne, November 2015.

The ASELL (Advancing Science and Engineering through Laboratory Learning) project and its earlier incarnations (see March 2001 issue, pp. 37–8) have shared the best laboratory activities from many Australian universities sine 1999. There are guidelines for comprehensive documentation, so that technical staff can set up the experiment at a new institution and novice instructors can run experiments with confidence. ASELL methodology also enables the evaluation of the effectiveness of the laboratory activities, and this data can be used either for systematic improvement of a not-quite-right activity or for benchmarking. Along the way, ASELL also provided professional development and created a network of educators interested in laboratory learning.

The Office of the Chief Scientist has noted that the STEM disciplines are in danger of decline and recommended that ASELL for Schools should be part of the solution. Since 2012, ASELL for Schools has worked with school teachers to improve student engagement in science by enhancing laboratory experiences, and building capacity amongst teachers through opportunities to refine teachers' pedagogical content knowledge through the processes of reviewing experiments, implementing these procedures in their science classes and reflecting on their classroom practice. ASELL for Schools has expanded the project to five states and territories through a grant of about $2 million from the Australian Maths and Science Partnerships Program, with additional support from the Australian Council of the Deans of Science, Australian Government Office for Learning and Teaching's ReMSTEP program, and other sources.

Typically, a school teacher collaborates with the ASELL team of university scientists, engineers and educators to enhance an existing laboratory activity, which is not currently achieving desired learning outcomes, or to design a new activity. Experiments are radically re-thought and aligned with intended learning outcomes and what is interesting and relevant to students. Such experimental activities are showcased at a workshop, which has a combination of hands-on practical, professional development and networking sessions. School students and teachers critique the laboratory activities, with feedback leading to a further round of enhancements. Finally, the laboratory activity is implemented and evaluated in the teacher's school. Another important aspect is that the workshop participants disseminate the ASELL ideas as they report back to their colleagues in their own schools.

During 2015, ASELL for Schools workshops have been run in Adelaide, Armidale, Darwin, Melbourne, Parramatta, Port Macquarie, Sydney and Tamworth, with shorter professional development sessions in Adelaide, Launceston, Melbourne, Perth, Sydney and elsewhere. Many more collaborations and workshops are planned for 2016 and 2017. For further information about ASELL for Schools, please contact Manjula Sharma or Vicky Tzioumis vicky.tzioumis@sydney.edu.au.

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Wine metabolomics – what's in a name?

Metabolomics continues to be a rapidly emerging field of analytical science with particular relevance to food authentication. The recent review of metabolomics and wine (Alañón et al., *TRAC* 2015, vol. 74 pp. 1–20) describes metabolomics as the application of 'powerful, robust analytical techniques' such as NMR, LC-MS, GC-MS and FTICR that provide 'high-dimensional data that require advanced chemometric tools in order to handle these datasets appropriately and to assess the chemical composition holistically'. All a bit of a mouthful really, but it does get the concept across.

In searching for a simpler descriptor, some authors have been using *wineomics* and even *oenomics*. Recently, in a study on wine polyphenolic compounds, *polyphenomics* has been coined. These terms do not differentiate between targeted or untargeted metabolomics. That is, while the targeted approach may seek information including absolute concentration for specific metabolites, the untargeted approach is more useful for sample discrimination as it allows a rapid assessment in a semi-quantitative manner of the compounds that can identify unique patterns in the distribution of selected classes of compounds. This had led to the development of *shotgun polyphenomics* in one recent study (Alvarez-Casas et al. 2014).

The In Vino Analytica Scientia (IVAS) conference in July last year (see my December 2015 column, p. 35) had a major focus on metabolomics in relation to grapes and wine. The keynote lecture in the metabolomics section was presented by Vladimir Shulaev of the University of North Texas, US, on the application of sub-2 µm particle CO_2-based chromatography with mass spectrometric detection for a targeted approach to *lipidomics* (another name!) in grapes. This strategy provides a rapid approach to identifying different grape genotypes.

Constructing a pipeline for wine characterisation by GC × GC with mass spectrometric detection was the title of the keynote lecture in the chemical analysis section presented by Silvia Rocha from the University of Aveiro, Portugal. A quick keyword search indicates that *pipeline* is now widely used in metabolomics. In 2005, Kell et al. (*Nat. Rev. Microbiol.*, vol. 3 pp. 557–65) described a pipeline as commencing with the sample, followed by footprinting (now more commonly fingerprinting) using a technique such as GC × GC to give a table of peaks upon which chemometrics treatment will lead to metabolite identification. I find the need for a new term such as pipeline to describe what is clearly standard analytical science (sample through to result) of little value. I have long argued that a proper understanding of analytical science commences with the sample and ends with the result; that is, it is more than just instrumental measurement. Irrespective of this point, the results shown by Silvia in her lecture clearly underscored the advantages of the strategy adopted for wine characterisation (see *Microchem. J.* 2014, vol. 116, pp. 107–17).

The keynote lecture by Aaron Fait from Ben-Gurion University of the Negev, Israel, outlined experiments to investigate the effects of abiotic stress (light and temperature) on the metabolite profiles and gene expression in red grape berries. Experiments were performed using a cell suspension exposed to elevated temperature and light, separately and in combination. Metabolite profiling was achieved with LC-MS and GC-MS with quantitative PCR for selected genes. Full details of this intriguing story can be found in *Frontiers in Plant Science* (doi: 10.3389/fpls.2015.00728). The approach is a step forward in providing information to winemakers and oenologists on what changes in grape-growing and winemaking practice may be required to handle grapes grown under extreme abiotic stress conditions.

Chloé Roullier-Gall from the Université de Bourgogne, France, and the Helmholtz Zentrum Munchen, Germany, presented an intriguing metabolomics study on oxygenation processes occurring in the 'prise de mousse' stage of champagne production. These days, the bottles are commonly closed using crown seals although progressive loss of CO_2 and ingress of O_2 through the closure does occur. Post-prise de mousse, the wine in bottle remained on the yeast lees for 4 and 6 years in the experiments described in Chloé's presentation. Samples were analysed by FTICR-MS and UPLC-QTOF-MS followed by extensive chemometrics. The work was structured around the impact of grape cultivar (Chardonnay, Pinot Noir, Pinot Meunier), vintage (2006 and 2008) and degree of oxygenation. The results showed that vintage and cultivar characteristics were drivers of the metabolomic fingerprints and that *discriminant chemical signatures* were obtained for wines with different levels of oxygen ingress. Hopefully, this work will be published in full soon, as it is an amazing study.

Continuing with the Champagne theme, Philippe Jeandet, University of Reims, France, described the analysis of a 170-year-old champagne recovered from the Baltic Sea, a process that was called 'deep sea ageing'. In addition to simple sensory analysis, the metabolomic approach used a raft of methods including FTIR-MS, UPLC-QTO-FMS, 1D and 2D NMR, stir-bar GC-MS and, for good measure, element identification by ICP-AES and ICP-MS. It was argued that this extensive metabolomic and *metallomic* study provided insight into winemaking practices used 170 years ago as there were markers identified for barrel ageing and Maillard reaction products. This work we were told revealed the 'extraordinary *archaeometabolome* and elemental diversity in the form of chemical signatures' relevant to champagne science. You can read all about it in *PNAS* (2015, vol. 112, pp. 5893–8) and you may well find a few more new terms to add to your metabolomics vocabulary.

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Of thee I sing (part 2): bosses

A few months ago (August 2015, p. 40), I wrote about some of the students I have had the privilege to mentor and how much they contributed to my success as a scientist. However, it would be remiss of me to not speak about the other side of the coin: bosses.

It may be a cliché to complain about horrible bosses, but in my experience, there are either a whole slew of excellent bosses out there, or I have managed to be employed by a statistically improbable number of good ones. So I'd like to take the opportunity to sing the praises of some of them (anonymously, of course).

I should preface this by saying that I have consistently changed my research focus (if not my entire career) once every three years, on average. What this means is that every boss I've had has had to roll the dice on hiring me. This alone might weed out the brave bosses from the discreet and may explain why I've had so many great ones.

... in my experience, there are either a whole slew of excellent bosses out there, or I have managed to be employed by a statistically improbable number of good ones.

One boss, in particular, exemplifies this reluctance to bring in an unknown element. Let's call this boss 'Rob'. Rob said to me two weeks after hiring me that he didn't usually like to hire university-trained students. They, in his experience, had too many book smarts and were completely useless in the lab. He confessed that HR had liked me a lot more than he had, but also conceded that I was far from useless in the lab. In fact, two months after I joined, Rob pretty much handed me the reins of the lab and made time to do more important managerial things. I really appreciated his hands-off approach and it motivated me to do my best to live up to his faith in me. Rob ended up driving me to work and back every day of the week (a 30-minute commute), offering to make my temporary contract permanent and arm-twisting management into giving me five weeks of leave so I could go to the US and get married in style!

Another boss who (I think, anyway) didn't regret rolling the dice on me was 'Seb' (for the purposes of this column). Seb and I didn't always see eye to eye on the direction my research should take, but after a couple of spirited conversations, he decided to let me do my thing. I chose to do a different project from the one he proposed and I chose to give my student another project from the one he proposed. I did random experiments and told Seb after the fact about both the successes and failures. Seb only seemed to focus on the former. Even after all the head-butting, Seb and I still remain on great terms and he continues to write excellent references for me. In fact, Seb was the one who recommended me to my next boss, 'Hal'.

Hal (who, to no one's surprise doesn't go by that name outside this column) hired me after meeting me twice and talking to Seb once. Further, he hired me to do a project for which I had absolutely no experience. And even further, he allowed me to try new things to make the project work. The project did work. However, his ability to let me try things is not what impressed me the most about Hal. I was a new father when employed by Hal and as a father, there are things far more important than work. And Hal understood this. He understood the last-minute leave requests, the dashing out of meetings and the otherwise erratic behaviour only a newly minted father would engage in and for this, my family and I are very grateful.

Last but not least I want to talk about 'Jim'. Jim was my first boss and in many ways he is the one who I wanted to emulate going down the science route. Jim was the head of the school when I was working for him, and had constant demands on his time. But he always found time for his group. I did three projects with Jim because he was the most understanding, relaxed and genial professor I have encountered. I keep thinking that if ever I become a professor, I'm going to be a professor like him.

All my bosses have taught me a whole bunch of things to do right to get the best out of people (and let's be honest, a few things to do wrong too). I am a much better employee now thanks to their guidance and I'm determined that if I'm ever a boss, I'll be an awkward chimera of Rob, Seb, Hal and Jim.

The author is currently just the boss of his son. And that is only when his wife isn't home.

Remembering the third-year lab

The experiments in organic chemistry undertaken by third-year students during my time at Monash challenged with a sequence that included some unusual mechanisms, one of them for a molecular rearrangement. The sequence started with benzaldehyde, Ph–CH=O, which was reacted with sodium cyanide to give benzoin, Ph–C–CH(OH)–Ph. In the reaction, two molecules of benzaldehyde were joined by a new carbon–carbon bond and there was some redistribution of the hydrogen atoms. I remember pondering over the pronunciation of benzoin: it was always 'oh-in', whereas acyloin – the generic name for an α-hydroxy ketone – was some sometimes 'oh-in' but just as often 'oyn'.

Stage two in the sequence was the oxidation of benzoin to benzil, Ph–CO–CO–Ph, through reaction with nitric acid. Nitric acid is mainly notable for its strongly acidic nature and its use as a nitrating agent, but this reaction served as a reminder that nitrogen in oxidation state +5 is a powerful oxidant. That's why nitrates or nitro compounds are present in most explosive mixtures.

But, back to the lab, where stage three involved the reaction of benzil with strong alkali in aqueous alcohol, leading to the anion of benzilic acid, $Ph_2C(OH)–COOH$. The free acid was obtained by working up the reaction mixture. The structure of this product was in doubt for some years after it was first reported in the 19th century because it was not suspected that a molecular rearrangement had taken place. Later, the mechanism was the subject of debate and experimentation by chemists for many years before it was finally nailed down as involving migration of a phenyl group in an anionic intermediate. This was all good fun, but what I didn't know (and what we never told the students) is that the outcome of the reaction is solvent dependent. Sodium ethoxide in ethanol cleaves the benzil molecule to give benzaldehyde and ethyl benzoate. 'Benzilic acid appears only in traces' according to Lachman, who researched the reaction in 1923. It's also the source of a rare error in Fieser and Fieser's *Organic chemistry* (third edition, 1956). If you think about it, the rearrangement is accompanied by addition of a molecule of H_2O ($C_{14}H_{10}O_2 \rightarrow C_{14}H_{12}O_3$) and so could not have proceeded in the absence of water. Even a little water in the mixture is enough to ensure the formation of benzilic acid, according to Arthur Michael (1853–1942) who published his work in 1919. Yes, that's Michael of the Michael addition, another of the iconic reactions of organic chemistry.

I was alerted to all this by reading a fascinating book by Yale organic chemist Jerome A. Berson, entitled *Chemical discovery and the logicians' program: a problematic pairing* (2003). The first report of the reaction between benzil and alkali was in 1836 by Auguste Laurent (1807–1853), who identified the products as benzoic acid and (probably, since the oil was hard to characterise) benzaldehyde. Justus Liebig (1803–1873) also investigated this reaction. Liebig repeated Laurent's experiments, although maybe not under exactly the same conditions, and in 1838 reported the isolation of the new substance. Next year the Russian chemist Nikolai Zinin (1812–1880) confirmed Liebig's work and named the new substance benzilic acid.

Liebig was scathing in his criticism of Laurent's work and of Laurent himself, just part of his running battle with the French chemists over the structures of organic substances. When I looked at the originals, I found that experimental details in the French and German articles were scanty and it seems to me likely that Liebig had not realised that he and Laurent had not, strictly speaking, performed the same experiment.

As I was reminiscing over the hours spent in third year lab, I recalled another benzaldehyde experiment that occasionally caused a problem. We had the students condensing benzaldehyde with acetone in the presence of dilute alkali to form benzalacetone, $Ph–CH=CH–CO–CH_3$. The sticky liquid product was purified by distillation under low pressure, and mastering this technique was the main point of the exercise. Students, being more or less beginners of the fine arts of organic chemistry, often got some benzalacetone on their skin. It seemed to have no effect on most people who contacted it, but for some it produced an itchy red rash that was short-lived but worrying. I recall being phoned by an anxious parent whose son developed such a rash in the evening after his lab class. Drawing on my own experience and those of others, I advised that it would disappear within 24 hours and that the sort of antihistamines that were available in most households could bring some interim relief. I heard no more about it over the weekend and the student reported that the rash had, indeed, rapidly subsided.

Touching base with French chemistry again, I remember writing in my April 2014 letter that I would check up on the Eiffel Tower to see whether Chevreul had been reinstated. Indeed he has, as the photograph shows.

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.

events

PhysChem 2016
2–5 February 2016, University of Canterbury, Christchurch, NZ
www.physchem2016.com

Safety in Laboratories – RMIT Short Course
8–10 February 2016, RMIT University, Melbourne, Vic.
www.shortcourses.rmit.edu.au

7th Heron Island Conference on Reactive Intermediates and Unusual Molecules
9–15 July 2016, Heron Island, Qld
www.Heron7.org

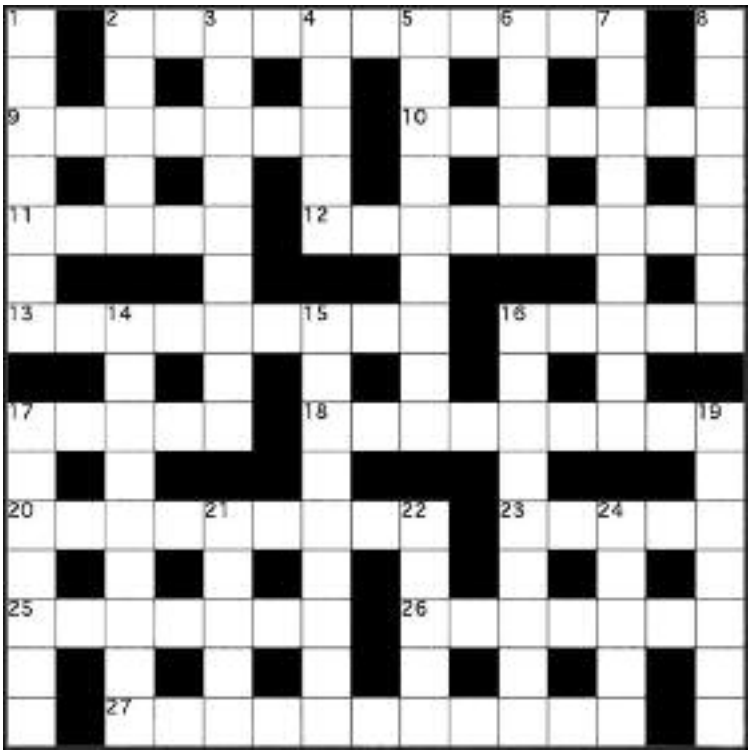
European Symposium of Biochemical Engineering Sciences (ESBES)
11–14 September 2016, Dublin, Ireland
www.esbes2016.org

sudoku solution

From December 2015/January 2016

Am	Md	Cf	Cm	Fm	Es	Bk	Pm	No
Pm	Bk	Es	No	Am	Md	Cf	Fm	Cm
Cm	No	Fm	Cf	Bk	Pm	Es	Am	Md
Md	Cm	Pm	Fm	No	Cf	Am	Bk	Es
No	Fm	Am	Es	Cm	Bk	Pm	Md	Cf
Cf	Es	Bk	Pm	Md	Am	No	Cm	Fm
Bk	Am	No	Md	Es	Cm	Fm	Cf	Pm
Es	Pm	Md	Bk	Cf	Fm	Cm	No	Am
Fm	Cf	Cm	Am	Pm	No	Md	Es	Bk

cryptic chemistry



Across

2 Loose pin. Fly around the compounds. (11)
9 Opposed to using silver stain complex. (7)
10 Broken nails after actinide holds a carbon atom with two amine groups attached. (7)
11 Prune her subject: argon. (5)
12 $R_2NO\bullet$ from NI_2 dextro-rotation?! (9)
13 This one is moist. Turn around. (9)
16 Cover inapt fix. (5)
17 Reading about loss of sodium chine. (5)
18 Compounds new born clays. (9)
20 Unreacted compound is not looked after. (9)
23 Changed shape of solid, perhaps. (5)
25 It's an enzyme X so idea falters. (7)
26 Flowers certain for fun time. (7)
27 $C_{10}H_8$ from H_2 panel. Neat! (11)

Down

1 Ranks carbon misses. (7)
2 Locate phosphorus mesh. (5)
3 Wrong angle. Drop 74 and move around if you want to be effective over a large distance. (4-5)
4 A lot of times garnet forms in rises. (5)
5 A big molecule which stretches atom or else loses oxygen radical. (9)
6 A reference to a carbon–nitrogen double bond found in *Weilheim in Oberbayern*. (5)
7 A good person with talent provides some resistance to change. (9)
8 Sodium odour being generated. (7)
14 Decline donation of electrons. (9)
15 Wrong in right. (9)
16 Shop changed pH in first evidence of PH_3. (9)
17 Support singers Spooner says are unpleasantly loud and harsh. (7)
19 165876839? Look at it. (7)
21 Temperature slope down and out. (5)
22 Change to model taken in. (5)
24 Cloud computing platform blue. (5)

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

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Private Fleet offers you savings of up to 20% off your next car purchase. Free access to the service (normally $178), 12 months road side assistance and more is included.

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Student spirit: young chemist groups in the RACI

From the east coast to the west, young chemists are surfing, socialising and networking as part of RACI activities.

The winning table at the pub quiz night held by the RACI Young Chemists Group of SA.

The fantastically chic inner-city venue, deliberately away from the partisan environment of a university, helped the informal feel and set the tone of activity for the Victorian Young Chemists Group.

South Australia

It was a pub quiz night, held at the UniSA City West Bar on Adelaide's North Terrace last October, that welcomed 50 young chemists to the newly formed RACI Young Chemists Group of SA. Students, young professionals, enthusiasts and even SA branch committee members attended the inaugural event, which tested general knowledge over six rounds of trivia, an assortment of bonus table questions and three exciting mini games. The event offered a perfect environment for young chemists from around the state to meet new friends, have a few drinks and enjoy the fun-filled program in a relaxed atmosphere.

In a very lively event, teams debated the history of Escher's Staircase; confused the meaning of 'googology'; pondered which outdoor sport Nobelist Robert Grubbs most enjoys; and, at the end of the night, showed their artistic talent in a game called Plastic Swayze, where teams sculpted a plasticine figure of the famous 90s actor to the soundtrack of *Ghost*. Prizes were given throughout the night, including a healthy selection of chocolates, bottles of wine, gift vouchers and signed sports merchandise. Congratulations to the winning team, a group of PhD students and postdoctoral researchers from the chemistry department at Flinders University. Special mention also goes to the team of research students from the University of Adelaide who won the Plastic Swayze competition.

Thank you to all participants in the Young Chemists Group of SA pub quiz night. The group is driven to foster a close network of students, early-career professionals and researchers, and to connect these people with the RACI. We encourage all young chemists to be involved. Future events in SA, including pub quizzes and social networking occasions, will be announced during the year.

Matthew Norris MRACI (matthew.norris@flinders.edu.au) and **Sophia Ackling** (student member), chairs of the RACI Young Chemists Group of SA

Victoria

The inaugural event for the Victorian Young Chemists Group was held in September last year in Melbourne, and the feedback from our trivia night was very positive. We had 75 students register, with the low price of $10 (including food!) adding to the attraction. The professional quiz company QuizMeisters did a superb job and injected more life into the evening than any of us could have mustered. Rather than pit universities against each other (perhaps a future event), chemistry-themed teams comprised members from across the institutions, including some participants from industry, to promote networking. The fantastically chic inner-city venue, deliberately away from the partisan environment of a university, helped the informal feel and very much set the tone for what we envisage the Young Chemists Group becoming.

The Branch hopes to step back a bit and allow Young Chemists to run their own events while offering our support and access to our networks and contacts, which will allow their initiatives to flourish. The group has a social media presence on both Facebook (www.facebook.com/RACIVicYC) and LinkedIn to engage members and non-members in the activities. Keep an eye out there for forthcoming events.

Keeping younger members actively involved is essential to a healthy future of any professional society and should be seen as a responsibility of more established members. We were lucky to have input from enthusiastic students from universities and research institutes. We could not have held the event without sponsorship from the chemistry departments at the University of Melbourne and Monash University, Monash Institute of Pharmaceutical Sciences, and Walter and Eliza Hall Institute, in addition to the very generous provision of prizes from ChemSkill. Thank you all!

Dave Turner MRACI CChem, **Julia Stuthe** MRACI CChem (Victorian Branch Vice President, julia.stuthe@csiro.au) and **Brittany Howard** MRACI

Students visiting booths at the careers night in WA.

Student surfing at Scarborough Beach, WA.

Western Australia

There's been plenty happening in the West too. 'Worst interview experiences' was a well-attended Tertiary Student Group event in July during which a local member of the Kelly Scientific Team outlined basic interview 'do's and don'ts' and a panel and the audience shared their worst interview experiences. The experiences were many and varied: one of the panel members once interviewed a candidate who, after being introduced and sitting down, proceeded to put up his feet on the desk and immediately ask 'Well how much are you going to pay me?'. It was during the WA mining boom, I suppose …

Also popular was this year's annual careers night in October. Booths were set up by a number of chemistry employers and could be visited by undergraduate and postgraduate students in a one-on-one setting and informal atmosphere. A number of well-attended career-specific lectures were given during the evening. The participants must have enjoyed themselves – the RACI received several membership applications after the event!

In Perth, there is always time for some great marine social activities. To help clear the mind and mix in the great WA outdoors, in May a student social surfing event was organised at a local beach (advertised as the world's best!). It was supervised professionally by a surf school who managed to get most of us to stand up on a board (except the WA President, but he's working on it). A brief ocean science presentation and a nice meal rounded off a great day.

A careers evening and surfing day will be held again in 2016, and we will host sausage sizzles at the various university campuses. Check the WA Branch newsletters for details or look out for a poster on university campus.

Alf Larcher FRACI CChem, WA Branch President (wa-president@raci.org.au)

Esters and their smells

Courtesy James Kennedy (jameskennedymonash.wordpress.com)

	methyl 1 carbon	**ethyl** 2 carbons	**propyl** 3 carbons	**2-methyl propyl-**	**butyl** 4 carbons	**pentyl** 5 carbons	**hexyl** 6 carbons	benzyl benzene ring	**heptyl** 7 carbons	**octyl** 8 carbons	**nonyl** 9 carbons
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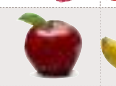
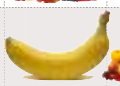
ethanoate 2 carbons								JASMINE 			
propanoate 3 carbons											?
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pentanoate 5 carbons					ETHEREAL					?	?
hexanoate 6 carbons											
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heptanoate 7 carbons						?					?
salicylate from salicylic acid			MINT	WINTERGREEN	STRONG			DIFFERENT PEOPLE PERCEIVE DIFFERENT AROMAS!	?		?
octanoate 8 carbons											
phenylacetate benzene ring + 2 carbons	STRONG							JASMINE	none!		?
nonanoate 9 carbons										?	
cinnamate benzene ring + propenol											?
decanoate 10 carbons			OIL				?	?	?	?	?
undecanoate 11 carbons			?	?	?	?	?	?	?	?	?
laurate 12 carbons			?				?			?	?