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- Turning graphene into 'black gold'
- 'Science meets business': interview with SCI's Sharon Todd
- Hydrogen: fuel of the (far-distant) future?



Celebrate the festival of Chemistry

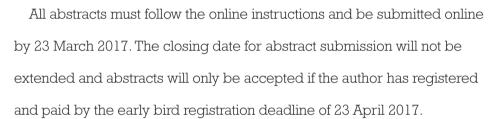
Call for abstracts





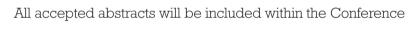


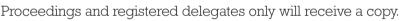




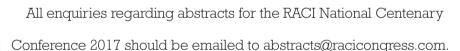














Dates and deadlines

Call for abstracts closes

Authors notified of results

April 2017

Presenter/early bird registration deadline

23 March 2017

April 2017



For more information about submitting an abstract, including FAQs, a template and list of themes, visit http://racicongress.com/RACIConference/call-for-abstracts.php.

chemistry

March 2017





cover story

Rise of the machines. The 2016 Nobel Prize in Chemistry. II

The Nobel Laureates in Chemistry for 2016 have designed and synthesised molecular systems that can be taken out of equilibrium and into higher-energy states in which their movements can be controlled. Molecular machines will likely lead to nanorobots, sensors, storage devices and perhaps even artificial life.

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24 Light, soap and magnets turn graphene into 'black gold'

Some clever chemistry is employing magnetism and a light-sensitive soap to turn simple graphene into a super-material with applications in water purification and electronic device.

26 'Science meets business' at the Centenary Congress

Dave Sammut speaks with Sharon Todd, SCI's Executive Director, about the organisation, its activities and its plans to participate in the 2017 Congress.

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Marking a centenary, in print

Congratulations, RACI, on the milestone of your centenary. Chemistry in Australia sits proudly beside you (as it has in one form or another since 1934) to record and share your history.

Part of that history, of course, is that the R in RACI arrived (courtesy of a supplementary royal charter) in 1953; similarly, the name Chemistry in Australia follows the Journal and Proceedings of the Australian Chemical Institute.

Our centenary content kicked off last month when we profiled the RACI National Awards, and some of last year's winners explained what the awards mean to them. Please consider marking this special year by nominating yourself or someone else (see page 24 of the February issue or see www.raci.org/awards).

It's fitting that, in the month of International Women's Day, our conference update in this issue introduces some of the outstanding female plenary speakers for July's Centenary Congress. Meet professors from California Institute of Technology, Imperial College London, the University of Wisconson-Madison and Tsinghua University (p. 30). Sharon Todd discusses her role as Executive Director of SCI (formerly Society of Chemical Industry) and the organisation's involvement in the Congress, in an interview with Dave Sammut

Elsewhere in this issue, Peter Karuso concludes his profile of the 2016 recipients of the Nobel Prize in Chemistry. Several chemistry laureates (if still living) would have been marking

their personal centenaries this year: John Kendrew (Nobel recipient 1962), Robert Burns Woodward (1965), John Cornforth (1975), Ilya Prigogine (1977), Herbert Hauptman (1985), William Knowles (2001) and John Fenn (2002).

In future issues, we will overview the conferences planned as part of the Festival of Chemistry within the Centenary Congress, and Ian Rae will take us back to the research days of 1917. Andrew Holmes, a Centenary Congress plenary speaker and President of the Australian Academy of Science, will write for us as he reaches 50 years as an RACI member.

This centenary year is bookended by significant anniversaries of other science bodies. CSIRO was formed 100 years ago last year, and the Royal Society of Chemistry marked its 175th year, including its 175 Faces of Chemistry exhibition (September issue, p. 28). Looking forward, the Australian Journal of Chemistry will reach its 70th year in 2018. Much later this year, Mary Garson will introduce the planned activities of IUPAC for its centenary in 2019.



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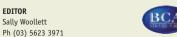
Sally Woollett (editor@raci.org.au)

Some centenarian chemists

Chemist	Centenary year	Known for work in
Foil A. Miller	2016	Infrared and Raman spectroscopy
Cai Qirui	2014	Catalytic chemistry
Dan Eley	2014	Eley-Rideal mechanism in surface chemistry
Adam Bielanski	2012	Inorganic chemistry textbooks
Malcolm Renfrew	2010	Teflon
Ray Crist	2000	Chemistry education and the Manhattan Project
Waldo Semon	1998	Polyvinyl chloride
Nellie May Taylor	1985	Chemistry education
Joel Henry Hildebrand	1981	Liquids and non-electrolyte solutions



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Chemistry publishers commit to integration with ORCID®

The Royal Society of Chemistry and the Publications Division of the American Chemical Society (ACS) have become signatories to the ORCID Open Letter, reasserting the commitment of both organisations to enhancing the scholarly publishing experience for researchers worldwide who are involved in chemistry and allied fields.

The commitment by these two global chemistry publishers to undertake new workflow integration with technology infrastructure provided by ORCID, a not-for-profit organisation that provides unique identifiers for researchers and scholars, will enable both societies to provide unambiguous designation of author names within chemistry and across the broader sciences. This partnership with ORCID will resolve ambiguity in researcher identification caused by name changes, cultural differences in name presentation, and the inconsistent use of name abbreviations that is too often a source of confusion for those who must rely on the published scientific record.

By becoming signatories to the ORCID Open Letter, these two chemical societies are voicing their intent to collect ORCID iDs for all submitting authors through use of the ORCID API, and to display such identifiers in the articles published in their respective society journals. The integration of such activities within the publishers' workflows means authors will benefit from automated linkages between their ORCID record and unique identifiers embedded within their published research articles, ensuring their contributions are appropriately recognised and credited.

During the publishing process, ACS and the Royal Society of Chemistry will automatically deposit publications to Crossref, which in turn will coordinate with ORCID to link and update the publishing activity populated to authors' respective ORCID profiles, thus attributing each published work to the correct researcher.

American Chemical Society

What makes influential science? Telling a good story

In a study published in the journal *PLOS ONE* (doi: 10.1371/journal.pone.0167983), researchers from the University of Washington looked at the abstracts from more than 700 scientific papers about climate change to find out what makes a paper influential in its field. But instead of focusing on content, they looked at writing style, which is normally more the province of humanities professors than of scientists.

Their idea was that papers written in a more narrative style – those that tell a story – might be more influential than those with a drier, more expository style. The researchers – led by Annie Hillier, a recent graduate from the UW's School of Marine and Environmental Affairs, and professors Ryan Kelly and Terrie Klinger – wondered whether this theory would hold up in the realm of peer-reviewed scientific literature.

Remarkably, it did. The most highly cited papers tended to include elements such as sensory language, a greater degree of language indicating cause-and-effect and a direct appeal to the reader for a particular follow-up action. Perhaps even more surprising, the researchers noted, was the finding that the highest rated journals tended to feature articles that had more narrative content.

The researchers used a crowdsourcing website to evaluate the narrative content of the journal articles. Online contributors were asked a series of questions about each abstract to measure whether papers had a narrative style, including elements such as language that appeals to one's senses and emotions.

The researchers hope this work might lead to advances in scientific communication, improving the odds that science might lead the way to better decisions in the policy realm.

University of Washington

With the integration of author ORCID iDs in our publishing workflows, we will ensure that researchers receive proper credit for their accomplishments.

Sarah Tegen, Vice President of Global Editorial and Author Services at ACS Publications, American Chemical Society



We don't know if the really top journals pick the most readable articles, and that's why those articles are more influential, or if the more narrative papers would be influential no matter what journal they are in.

Ryan Kelly, School of Marine and Environmental Affairs, University of Washington

Names and symbols for four newly discovered elements

On 28 November 2016, the International Union of Pure and Applied Chemistry (IUPAC) approved the names and symbols for four elements.

Following a five-month period of public review, the names earlier proposed by the discoverers have been approved by the IUPAC Bureau. The following names and symbols are officially assigned:

- nihonium and symbol Nh for the element 113
- moscovium and symbol Mc for the element 115
- tennessine and symbol Ts for the element 117
- oganesson and symbol Og for the element 118.

In concordance with and following the earlier reports that the claims for discovery of these elements have been fulfilled, the discoverers were invited to propose names. Keeping with tradition, the newly discovered elements have been named after a place or geographical region, or a scientist. The ending of the names also reflects and maintains historical and chemical consistency: '-ium' for elements 113 and 115 and as for all new elements of groups 1-16; '-ine' for element 117 and belonging to group 17; and '-on' for element 118 element belonging to group 18. The recommendations will be published in the IUPAC journal Pure and Applied Chemistry.

The name nihonium was proposed by the discoverers at RIKEN Nishina Center for Accelerator-Based Science (Japan); the name came from Nihon, which is one of the two ways to say 'Japan' in Japanese, and literally means 'the Land of Rising Sun'.

Moscovium and tennessine were proposed by the discoverers at the Joint Institute for Nuclear Research, Dubna (Russia), Oak Ridge National Laboratory (US), Vanderbilt University (US) and Lawrence Livermore National Laboratory (US). Both are in line with tradition honouring a place or geographical region. Moscovium is in recognition of the Moscow region and honours the ancient Russian

land that is the home of the Joint
Institute for Nuclear Research, where the
discovery experiments were conducted
using the Dubna gas-filled recoil separator
in combination with the heavy ion
accelerator capabilities of the Flerov
Laboratory of Nuclear Reactions.
Tennessine is in recognition of the
contribution of the Tennessee region of the
US, including Oak Ridge National
Laboratory, Vanderbilt University and the
University of Tennessee at Knoxville, to
superheavy element research.

Lastly, and in line with the tradition of honouring a scientist, the name oganesson was proposed by the collaborating teams of discoverers at the Joint Institute for Nuclear Research, Dubna (Russia), and Lawrence Livermore National Laboratory (US) and recognises Professor Yuri Oganessian (born 1933) for his pioneering contributions to transactinoid elements research. His many achievements include the discovery of superheavy elements and significant advances in the nuclear physics of superheavy nuclei, including experimental evidence for the 'island of stability.'

Comments from the general public, during the five-month period were many. Apart from many full agreements, comments were received suggesting other names, in some cases accompanied by petitions from large groups of people. However, these suggestions could not be

Keeping with tradition, the newly discovered elements have been named after a place or geographical region, or a scientist.

accepted, given the fact that under the current quidelines only the discoverers have the right to propose names and symbols. Questions were also received about pronunciation of the names and the translations into other languages. Members of the chemistry community also raised the concern that Ts is one of the two commonly used abbreviations for the tosyl group. Recognising, however, that many two-letter abbreviations have multiple meanings - even in chemistry, and for example Ac and Pr - the conclusion was made that the context in which the symbols are used makes the meaning unambiquous.

'Overall, it was a real pleasure to realise that so many people are interested in the naming of the new elements, including high-school students, making essays about possible names and telling how proud they were to have been able to participate in the discussions,' said Professor Jan Reedijk, President of the Inorganic Chemistry Division. He added 'It is a long process from initial discovery to the final naming, and IUPAC is thankful for the cooperation of everyone involved. For now, we can all cherish our periodic table completed down to the seventh row.'

'The names of the new elements reflect the realities of our present time,' said IUPAC President Professor Natalia Tarasova, 'Universality of science, honouring places from three continents, where the elements have been discovered – Japan, Russia the United States – and the pivotal role of human capital in the development of science, honouring an outstanding scientist – Professor Yuri Oganessian.'

The exploration of new elements continues, and scientists are searching for elements beyond the seventh row of the periodic table. IUPAC and the International Union of Pure and Applied Physics (IUPAP) are establishing a new joint working group which task will be to examine the criteria used to verify claims for the discovery of new elements.

IUPAC

Why diamond nanothread could prove priceless for manufacturing

Would you dress in diamond nanothreads? It's not as far-fetched as you might think. And you'll have a Brisbane-based carbon chemist and engineer to thank for it.

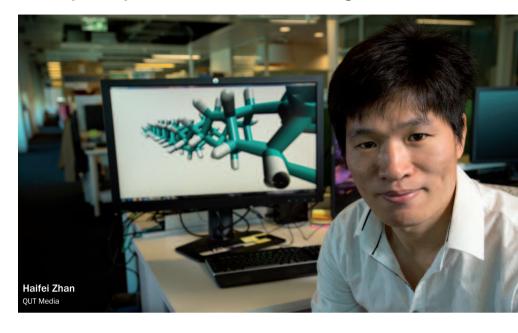
Dr Haifei Zhan is leading a global effort to work out how many ways humanity can use a newly invented material with enormous potential – diamond nanothread (DNT).

First created by Pennsylvania State University, one-dimensional DNT is similar to carbon nanotubes, hollow cylindrical tubes 10 000 times smaller than human hair, stronger than steel – but brittle.

'DNT, by comparison, is even thinner, incorporating kinks of hydrogen in the carbon's hollow structure, called Stone-Wale (SW) transformation defects, which I've discovered reduces brittleness and adds flexibility,' said Zhan, from QUT's School of Chemistry, Physics and Mechanical Engineering.

'That structure makes DNT a great candidate for a range of uses. It's possible DNT may become as ubiquitous as plastic in the future, used in everything from clothing to cars.

DNT does not look like a rock diamond. Rather, its name refers to the way the carbon atoms are packed



together, similar to diamond, giving it its phenomenal strength.

Zhan has been modelling the properties of DNT since it was invented, using large-scale molecular dynamics simulations and high-performance computing. He was the first to realise the SW defects were the key to DNT's versatility.

'My simulations have shown that the SW defects act like hinges, connecting straight sections of DNT. And by changing the spacing of those defects, we can a change – or tune – the flexibility of the DNT.'

'Once the manufacturing costs are viable, DNT would likely be used primarily in mechanical applications, combined with other materials to make ultrastrong, lightweight composites and components – such as plane fuselages,' Dr Zhan said.

The research is published in *Nanoscale* (doi: 10.1039/C6NR02414A).

University of Queensland

(a)
(b)

... its name refers to the way the carbon atoms are packed together, similar to diamond, giving it its phenomenal strength.

Atomic structures of three representative nanothreads: (a) achiral nanothread; (b) stiff chiral nanothread; (c) soft chiral nanothread. Right images are the cross-sectional view.

March 2017 Chemistry in Australia

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Pairing two stars of chemistry

Researchers at the Technical University of Munich have succeeded in linking graphene with another important chemical group, the porphyrins. Porphyrins are well known because of their striking functional properties, which, for example, play a central role in chlorophyll during photosynthesis. These new hybrid structures could also be used in the field of molecular electronics, in catalysis or even as sensors.

Graphene is flexible, extremely thin and transparent, while at the same time it has very high tensile strength and conducts electricity, ideal prerequisites for a wide variety of application areas. However, using graphene to capture solar energy or as a gas sensor requires other specific properties as well. These properties can be achieved by fusing functional molecules with the carbon layer.

In previous research, scientists were primarily concerned with wet-chemical methods for attaching the molecules to the surface of the material. Together with his colleagues, Molecular Engineering at Functional Interfaces Professor Wilhelm Auwärter decided to take a different approach. They were able to link porphyrin molecules to graphene in a controlled manner in an ultra-high vacuum, using the catalytic properties of a silver surface on which the graphene layer rested. When heated, the porphyrin molecules lose hydrogen atoms at their periphery and can thus form new bonds with the graphene edges.

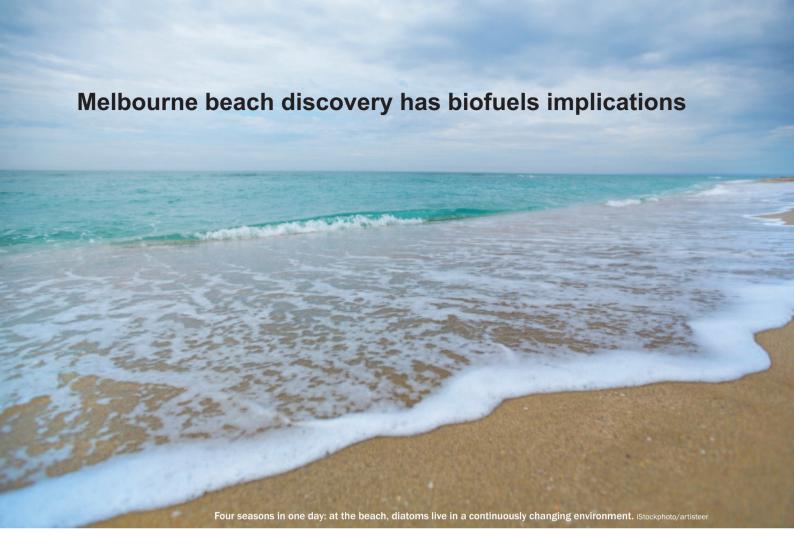
'This method creates a clean and controllable environment,' explained Auwärter. 'We can see exactly how the molecules bond and what types of bonds occur.' Here the researchers use the latest in modern atomic force microscopy to depict the chemical structure of individual molecules, the atomic 'skeletons', so to speak.

For the first time, the scientists have succeeded in attaching functional molecules to the edges of graphene covalently, i.e. with a stable chemical bond. 'We want to modify only the edges of the material; this way the graphene's positive properties are not destroyed, said Auwärter.

The researchers chose the porphyrin molecules as the partner for graphene because of their special properties. 'For example, porphyrins are responsible for transporting oxygen in haemoglobin, he continued. The molecules change their properties depending on which metals are at their centre and can take on various different tasks, e.g. specifically bonding with gas molecules such as oxygen and carbon dioxide.

In the future, this new method may make it possible to bond other molecules to graphene as well. The researchers also want to take even better control of the reaction, achieving targeted modifications by attaching molecules to carbon nanostructures such as graphene ribbons. These nanostructures are of central importance in electronic applications.

Technical University Munich



The popular Middle Park beach in Victoria is under the international spotlight following a world-first study by Monash University chemists who have discovered how sand 'holds its breath'.

The discovery, published in *Nature Geoscience* (doi: 10.1038/ngeo2843), has astonishing implications and potential

... micro-algal dark fermentation is the dominant metabolic pathway, which is the first time this has been documented in an environmental setting. uses in the biofuels industry, according to lead authors Associate Professor Perran Cook and PhD student Michael Bourke, from the Water Studies Centre, School of Chemistry.

Sand is full of algae called diatoms, but this environment is mixed about continuously so these organisms might get light one minute then be buried in the sediment with no oxygen the next.

'This is a new mechanism by which this type of algae survive under these conditions,' said Cook.

'Our work has found that they ferment, like yeast ferments sugar to alcohol.

'In this case, the products are hydrogen and "fats", for example oleate, which is a component of olive oil.'

Sand often has high concentrations of algae, which are highly productive and an important food source for food webs in the bay. It is important to understand how these organisms survive in the harsh environment in which they live.

In this work, scientists present the first study of the importance of anoxic micro-algal metabolism through fermentation in permeable sediments. They combined flow-through reactor experiments with microbiological approaches to determine the dominant contributors and pathways of dissolved inorganic carbon production in permeable sediments.

They show that micro-algal dark fermentation is the dominant metabolic pathway. This is the first time this has been documented in an environmental setting.

'The finding that hydrogen is a byproduct of this metabolism has important implications for the types of bacteria present in the sediment,' said Cook.

'It is well known that bacteria in the sediment can "eat" hydrogen; however, these hydrogen-eating bacteria may be more common than we previously thought.'

Monash University

Properties of xanthohumol may treat metabolic syndrome

Researchers at Oregon State University, US, have made a fundamental advance in understanding xanthohumol, a compound found in hops that's of significant interest to prevent or treat the lipid and metabolic disorders that are a primary killer of people in the developed world.

The scientists identified for the first time more precisely how xanthohumol works, and why it may have such significant promise in addressing the high cholesterol, blood sugar, obesity and other issues that are collectively referred to as 'metabolic syndrome'.

The research was based on mass

spectrometry in combination with a chemical labelling technique. In it, the scientists concluded that several prenylflavonoids, particularly xanthohumol, clearly are a ligand, or have a binding mechanism that promotes the activity of the farnesoid X receptor (FXR). FXR, in turn, is a master regulator of lipid and glucose metabolism.

This understanding of the FXR receptor at the molecular level, researchers said, could, in theory, facilitate the use of compounds that take advantage of it – such as xanthohumol – or development of other compounds with

a similar chemical structure that work even better.

The FXR receptor is a part of normal lipid and glucose metabolism, working in collaboration with appropriate diet, weight, exercise and other healthy activities. However, its function can be eroded by intake of too much fat and sugar. Restoring that function may help address metabolic problems.

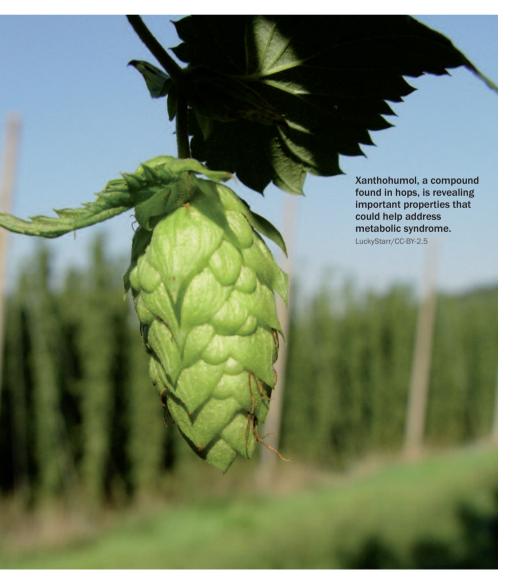
Previous research by OSU scientists involved studying laboratory animals that were on a high-fat diet. When they were given a high dosage of xanthohumol, it reduced their LDL, or 'bad' cholesterol, by 80%, their insulin level by 42%, and their level of IL-6, a biomarker of inflammation, by 78%.

Weight gain was also constrained, compared to animals not given xanthohumol. The levels of xanthohumol used in the research far exceeded any amount that could be obtained by normal dietary intake, but could be easily obtained through supplements.

In that study, researchers pointed out that direct healthcare costs arising from obesity or related disorders account for up to 10% of US healthcare expenditures.

Oregon State University

... the scientists concluded that several prenylflavonoids, particularly xanthohumol, clearly are a ligand, or have a binding mechanism that promotes the activity of the farnesoid X receptor (FXR).



High aldehyde levels in vapours from some flavoured e-liquids

Traditional cigarettes pose a well-established risk to smokers' health, but the effects of electronic cigarettes are still being determined. Helping to flesh out this picture, researchers are reporting in *Environmental Science & Technology* (doi: 10.1021/acs.est.6b05145) what happens to e-liquid flavourings when they're heated inside e-cigarettes or electronic nicotine-delivery systems. The study found that when converted into a vapour, some flavourings break down into toxic compounds at levels that exceed occupational safety standards.

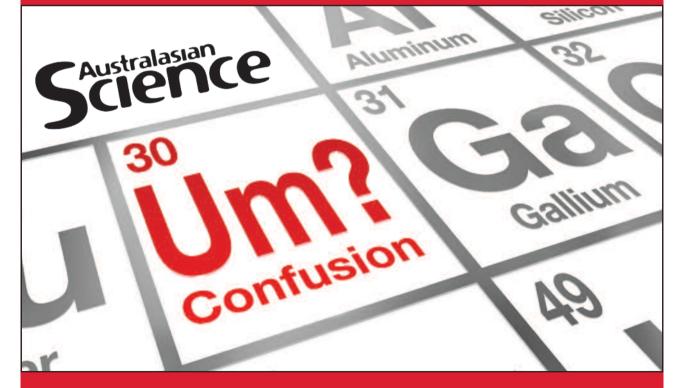
Since electronic cigarettes were first introduced to the US market in 2003, health officials have been tracking usage and studying potential health effects. A 2015 survey by the National Center for Health Statistics reported that 3.7% of adults used the devices regularly, and 12.6% had tried them at least once. Some studies have identified the ingredients in e-liquid flavourings, but very little research has been done to determine what happens to them when they are transformed

inside the device. A growing body of research on e-cigs has shown that the heat that converts e-liquids into vapour decomposes its contents, producing aldehydes and other toxic compounds that can potentially cause health problems. Andrey Khlystov and colleagues wanted to investigate the specific role that flavourings play in these reactions.

The researchers analysed vapours created from both unflavoured and flavoured e-liquids loaded into three popular types of e-cigarettes. The tests for 12 different aldehydes showed that the amount of potentially harmful compounds varied widely across e-liquid brands and flavours. However, the study also showed that in general, one puff of flavoured vapour contained levels of aldehydes exceeding the safe thresholds for occupational exposure – set by the American Conference of Governmental Industrial Hygienists – by factors of 1.5 to 270. Vapours from unflavoured e-liquids contained aldehydes at significantly lower levels.

American Chemical Society

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Safety storage of class 3 solvents with 90-minute fire-rated cabinets

The Australian laboratory design code AS2982 recommends that no more than 30 litres of class 3 flammable solvent be stored in a single under-bench safety cabinet. Lab safety standard AS2243.10 recommends a minimum of 3 metres between any class 3 safety cabinet and escape doors, and a 10-metre separation between aggregate dangerous goods quantities of 250 litres or more. The Australian flammables goods standard AS1940 recommends a maximum of 250 litres of flammable goods in safety cabinets, per 250 m² in multi-level buildings.

All these regulations refer to double-skinned metal cabinets manufactured according to AS1940, which require no formal testing of fire-resistance properties. For this reason, managers of labs and other large facilities are turning to dangerous-goods consultants to investigate a risk-based method of flammable storage to challenge these restraints and raise the level of safety in Australian labs. Often, the specified solution is a central fire-rated store with integrated spill containment, ventilation, explosion-proof lighting, access control etc., in effect a 'concrete bunker', which can be very expensive and creates a lot of inefficiencies for users.

Fortunately, this issue has been addressed well in other parts of the world, resulting in the development and regulation of cabinets with a guaranteed fire rating, such as those manufactured to EN14470 by Asecos in Germany.

If the EN approach is used as a guide, 90-minute fire-rated cabinets can be stored adjacent to each other because they are wholly isolated from the fire and from each other for 90 minutes in a fire incident.

Efficiency is immediately improved, as time spent fetching flammable liquids from the central storage room to the workplace is minimised and all hazardous materials for daily use

can be readily available safely and conveniently in the lab. An added benefit is the elimination of risks associated with moving flammable goods around the building through traffic areas such as corridors and lifts.

Safety cabinets in accordance with EN14470-1 for flammable liquids guarantee the highest fire protection available today, minimise the potential for explosions and prevent an existing fire from spreading. They will provide sufficient time for personnel to safely leave the building and for firefighters to rescue people from the building and extinguish a fire.



A double-walled steel cabinet provides 3–10 minutes of protection before the interior has heated to 200°C. A type 90 safety storage cabinet provides 90 minutes of protection before the interior reaches 200°C. That's almost 10 times more safety in the event of fire than with a double-walled steel cabinet designed to AS1940.

In the event of a fire, the cabinet must ensure that, over a period defined by the manufacturer (type 90 = 90 minutes), its contents do not present an additional risk that the fire will spread. The cabinet doors must close entirely, starting from any position (maximum closing time 20 seconds).

The cabinets must have openings for air inlet and outlet (for connection of the cabinet to an exhaust system). The ventilation openings must close automatically at a temperature of 70°C.

Each model must be independently verified by tests on a design sample. The cabinet will then be classed as type 15, 30, 60 or 90, according to the time that elapses before the temperature rises by 180°C.

Australian labs and industry are also taking advantage of 90-minute fire-rated gas cylinder stores designed to EN14470-2, for safe storage, provision and handling of gas cylinders in indoor areas. It is usually recommended to store gas cylinders in outdoor areas. In practice, this is often not possible or is expensive. EN14470-2 offers an economical and flexible option for the installation of gas cylinders in indoor areas.

While the Australian standards mentioned are a starting point for users looking for compliant solutions, EN14470-1 and EN14470-2 are providing some welcome and relevant guidance to Australian dangerous goods consultants and clients who are adopting a risk-based approach to dangerous goods storage to increase both efficiency and safety.

For more information, visit http://g3lab.com/haz._goods.html.



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For all enquiries, please email info@racicongress.com.



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ACCC6

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AIMECS 2017

11th AFMC International Medicinal Chemistry



Carbon 2017

World Conference on Carbon



Chemeca 2017

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Tetrahedron

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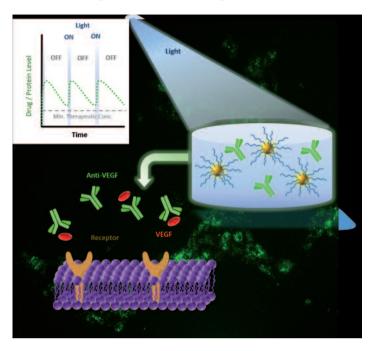
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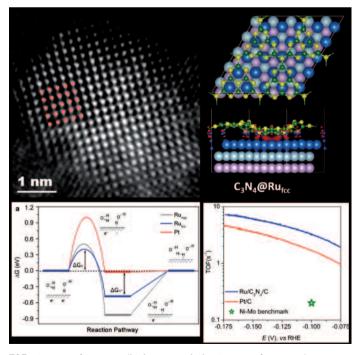
Saving vision with light



Protein-based drugs are increasingly being used to treat disease, but are quickly broken down in the body. As a result, delivery into the body generally involves direct injection, which is undesirable for medical conditions that require ongoing treatment. Implantation of a drug depot that can release multiple doses of a drug is an attractive potential solution. In a collaboration with two Chinese research institutes, researchers at CSIRO have recently demonstrated the light-modulated release of therapeutic proteins from an injectable depot (Basuki J.S., Qie F., Mulet X., Suryadinata R., Vashi A.V., Peng Y.Y., Li L., Hao X., Tan T., Hughes T.C. Angew. Chem. Int. Ed. 2017, doi: 10.1002/ange.201610618). The facile drug-delivery system consists of agarose (a non-toxic biopolymer), polymer-coated gold nanoparticles and unmodified therapeutic proteins. It exploits reversible changes in drug diffusion induced by the reversible softening of the thermoplastic agarose matrix caused by localised heating by light. The team showed that the released proteins retained a high degree of structural integrity and biological activity. Furthermore, the team established the potential of the technique for treating aged macular degeneration by demonstrating the controlled release by visible light of biomolecular vascular endothelial growth factor (VEGF) inhibitors, which reduced the growth of vascular endothelial cells in vitro.

Unusual catalyst boosts hydrogen production

The apparent rate of a surface reaction on a heterogeneous catalyst generally depends strongly on the catalyst's geometric properties and electronic structure, which act together to determine the adsorption of reaction intermediates and activation barriers. This complexity hinders the design and selection of the most appropriate catalyst for a specific reaction. Using the simple yet industrially relevant hydrogen evolution reaction (HER) as a model, Professor Shizhang Qiao and co-workers at the University of Adelaide have successfully linked the apparent catalytic activity of an unusual ruthenium (Ru) catalyst with its extrinsic crystallinity and intrinsic adsorption energetics (Zheng Y., Jiao Y., Zhu Y., Li L.H., Han Y., Chen Y., Jaroniec M., Qiao S.-Z. J. Am. Chem. Soc. 2016, 138, 16 174-81). The new electrocatalyst generates hydrogen 2.5 times faster than platinum - the benchmark HER catalyst yet costs only 1/25 as much. In fact, the new catalyst is among the most active HER electrocatalysts reported so far in alkaline solutions. A combination of experimental characterisation and density functional theory computation revealed that the extraordinary activity of this cost-effective Ru catalyst originates from the anomalous face-centred-cubic (fcc) crystallographic structure of the Ru nanoparticles formed on the catalyst's graphitic-C₂N₄/C support, which contrasts with the usual hexagonal close-packed structure of bulk Ru. This unusual fcc structure possesses favourable adsorption energetics for key reaction intermediates and reaction kinetics for the HER process.



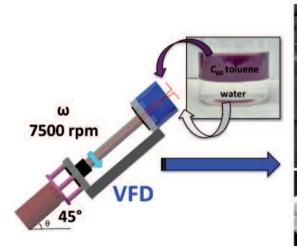
TOF = turnover frequency (hydrogen evolution turnover frequency)
RHE = reversible hydrogen electrode

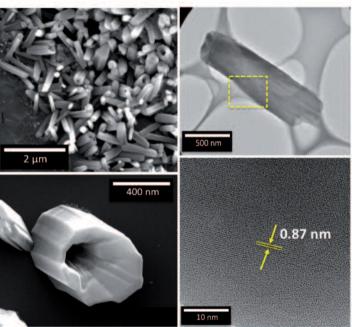
Surfactant-free fullerene nanotubule fabrication

The soccer-ball-shaped buckminsterfullerene (C₆₀) molecule has potential applications in diverse fields. Exquisite control of its self-assembly into specific geometries and dimensionalities is pivotal to tailoring properties of the resulting material. With the aim of fabricating a nanocarbon material using a green-chemistry approach, researchers from Flinders University have employed shear stress within dynamic thin films in a microfluidic device to control the self-

assembly of C₆₀ into nanotubules in the face-centred-cubic phase (Vimalanathan K., Shrestha R.G., Zhang Z., Zou J., Nakayama T., Raston C.L. *Angew. Chem. Int. Ed.* 2017, doi: 10.1002/anie.201608673). The micrometre-length nanotubules were devoid of trapped solvents, were fabricated in the absence of surfactants and, most importantly, were produced without the need for downstream processing. The high shear-stress

conditions were also instrumental in forming pores on the nanotubule surface, resulting in a material with a much higher response to small-molecule sensing than a similar material fabricated by batch processing. The use of shear stress under continuous flow to control the self-assembly and fabrication of nanocarbon materials is a paradigm shift in materials science and has potential for uptake in industry.







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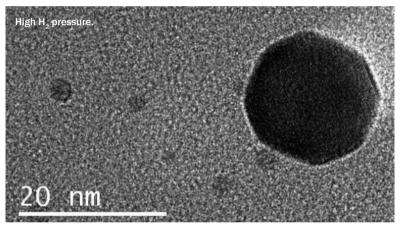
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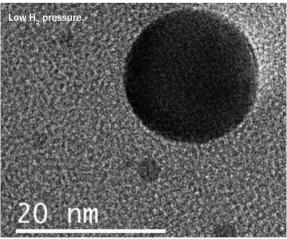


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Catalysts under pressure

There is a huge gap between the conditions under which real industrial catalysts operate and those under which their surface chemistry is usually studied in the lab. Real catalysts often work in a gas atmosphere under pressure, in some cases high pressure, while most surface studies are performed under ultrahigh vacuum, which is often essential for obtaining high-quality images, using techniques such as scanning tunnelling microscopy and transmission electron microscopy (TEM). As a result, information about how catalysts evolve under pressure is lacking. Dr Chenghua Sun from Monash University and his Chinese collaborators have used a combination of computational modelling and in situ TEM under atmospheric pressure to fill this gap (Jiang Y., Li H., Wu Z., Ye W., Zhang H., Wang Y., Sun C., Zhang Z. Angew. Chem. Int. Ed. 2016, 55, 12427-30). The key component of in situ TEM is the gas reactor holder, which is filled with the reaction gas and equipped with sealed windows through which an electron beam can pass. The team demonstrated that PdCu nanoparticles, which are widely used in hydrogen-related reactions, can change shape from spheres to truncated cubes under high hydrogen pressure. Calculations showed that this evolution essentially results from dynamic changes to surface stability associated with hydrogen adsorption.





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.

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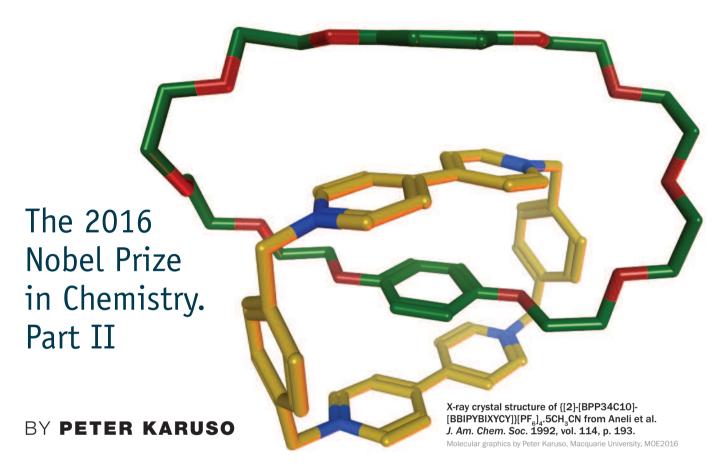
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Rise of the machines



The Nobel Laureates in Chemistry for 2016 have designed and synthesised molecular systems that can be taken out of equilibrium and into higher-energy states in which their movements can be controlled. Molecular machines will likely lead to nanorobots, sensors, storage devices and perhaps even artificial life.

he publication of *The nature* of the chemical bond by Linus Pauling in 1939 set the agenda in chemistry for the following 50 years. Its emphasis on covalent and ionic/electrostatic bonds dominated the machinations and work of chemists until Jean-Pierre Sauvage succeeded in efficiently linking two ring-shaped molecules together to form a chain, called a catenane, in 1983 (see February issue, p. 14). The

normal covalent bonds, where the atoms share electrons, were replaced by 'mechanical bonds' in catenanes, just like links in a chain.

Sauvage went on to make many other topological molecules such as knots, Borromean rings and trefoils that not only extended the nature of chemical bonds but crossed the boundary between science and art. However, to make a machine, molecules that can perform a task, the

molecules must be able to move relative to each other in a controlled way. Sauvage had demonstrated the rudimentary movement of [2] catenanes but the second step was taken by Fraser Stoddart by developing rotaxanes (from the Latin for wheel (rota) and axle (axis)) – the treading of a molecular ring onto an axle and demonstrating that the ring could be made to move back and forth on the axle.

Sir Fraser Stoddart

Fraser Stoddart was born on Victoria Day (24 May), 1942 at Edgelaw Farm, south of Edinburgh, Scotland. The son of a lowland tenant farmer, he grew up in a home without electricity or any modern conveniences in the post-war period when everything from food to clothes and petrol was rationed. With a need to improvise, Stoddart became obsessed first by jigsaw puzzles and then by the most sophisticated toy of the time – Meccano. These taught him pattern recognition and engineering respectively – highly desirable traits in a chemist.

In 1960, Stoddart went off to Edinburgh University, like many bright young Scots brought up on farms, to study medicine. The path to medicine involved first interacting with the sciences and so he started by studying chemistry, physics and mathematics. Soon, medicine started to pale into insignificance as a passion for research started to develop through his studies. Fraser soon realised that among the sciences, chemistry would give him the best opportunity to be creative.

He started a PhD in 1964 for Sir Edmund Hirst (Forbes Chair of Organic Chemistry at Edinburgh) and graduated at the end of 1966. In that time, he interacted with his supervisor exactly twice, once when he began his research in 1964 and then at his thesis defence, where Hirst left Stoddart with the words 'Whatever you do in research, Stoddart, make sure you work on big problems'.

With those words, Stoddart went off to Queens University in Canada in early 1967, determined to work on a 'big problem'. At the time, Pedersen's seminal paper on crown ethers appeared in *JACS* and it inspired Stoddart to base his research on the synthesis of chiral crown ethers, based on sugars. In 1970, he returned to the UK on an ICI research fellowship and took a lecturer position at Sheffield University, then later joined the ICI corporate laboratories (Runcorn) in



1978 on a three-year secondment. There he became aware of research on Paraquat and Diquat – commercial herbicides – and was convinced by Eric Goodings to look at crown ether complexation of organic cations (like Diquat) instead of transition metals. Runcorn was the place to do out-of-the-box things in the 1970s. Much of what Stoddart subsequently achieved as a scientist, he has said, can be traced back in large measure to those three years with ICI.

In 1981, Stoddart returned to Sheffield University and there used DB30C10, a crown ether synthesised in Donald Cram's group in 1977, to complex Diquat. The X-ray structure, published in 1987 (Chem. Commun. 1987, p. 1064), revealed that the guest (Paraguat) threads provocatively through the crown ether in a fashion that would later be called a [2]pseudorotaxane. The stage was now set to make the first electronic donor/acceptor [2]catenane. Jean-Pierre Sauvage had earlier (1983) published the metal-templated synthesis of [2]catenane; now Stoddart

pushed the first synthesis of a [2]catenane based on electrostatic attractions between DB30C10 and cyclobis(paraquat-p-phenylene), which surprisingly went in 70% yield at room temperature and crystallised out of the reaction flask! An X-ray structure can be found on page 18. Stoddart realised that this compound was the basis for the first bistable mechanical switch.

Despite this success, Stoddart's time at Sheffield was far from pleasant, as every success only seemed to engender envy and resentment in his senior and influential colleagues. His vocal criticism of state control and bureaucratic entanglement of universities did not win him any friends in high places either, but did increase his visibility and self-confidence.

In 1990, he departed Sheffield for the University of Birmingham. There, in 1991, he took a big leap forward through the first demonstration of 'translational isomerism' (*JACS* 1991, vol. 113, p. 5131). Stoddart and his group had synthesised a rotaxane by cyclising bis(paraquat-p-phenylene)

bromide around a linear version of a crown ether, stoppered at either end with bulky triisopropylsilane groups. The cyclised paraquat cyclophane (to be named 'the blue box' as a π -acceptor) was able to move from one π -donor dihydroquinone to the other. In 1994, one dihydroquinone was replaced by benzidine and the other by biphenol to make the first chemically switchable rotaxane (*Nature* 1994, vol. 369, p. 133).

Stoddart felt as though he was at the entrance of a gold mine and would regularly challenge his students to 'come back in the morning with 39 new ideas' – they often did and the

1990s was a very productive time and Birmingham University was incredibly supportive of chemistry, spending more than £10 million (~A\$25 million in 1993) on chemistry during the 1990s. Many other universities followed suit and this led to a long-awaited turnaround for chemistry infrastructure in the UK. However, in July 1997, Stoddart left the UK for the US (University of California, Los Angeles, Chemistry).

What drove him away from the UK was in part the bureaucracy and implications surrounding the Research Assessment Exercise (ERA in Australia) and the teaching equivalent

(AUQA/TEQSA audits) that he saw as a horrific waste of time and money and creating the wrong culture in university management, one where weaknesses are identified, leaving individuals, departments and universities on the fringes exposed. Another reason he left the UK was to get better medical care for his wife, who was diagnosed with breast cancer in 1992. The reason the UK lags behind the US in cancer treatment, according to Stoddart, is that young doctors in the UK are not trained in a way to equip them for the future or for tackling multi-dimensional big problems - like cancer. In the US, medical students are obliged to spend

four years reading for a science degree, as are dentists, engineers and many other disciplines.

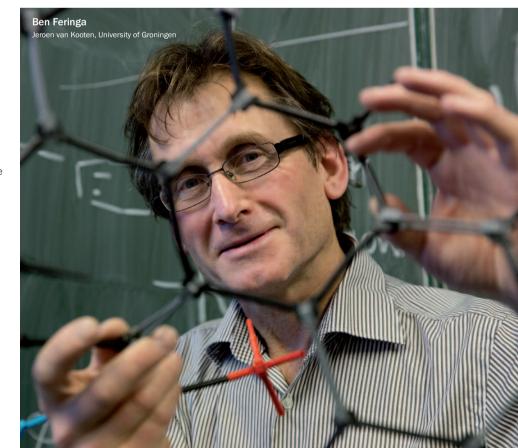
When Stoddart arrived at UCLA, he held the Saul Winstein Chair in Organic Chemistry. Winstein had been the intellectual giant in physical organic chemistry (see January-February 2011 issue, p. 22) but died tragically in his swimming pool from a heart attack at a relatively young age in 1969. A chair was endowed in his name and Donald Cram (Nobel Prize 1987 - along with Jean-Marie Lehn, Sauvage's PhD supervisor), a legend in his own time, became its first holder. When Don started to downsize his research effort in the 1990s. Stoddart was offered the chair.

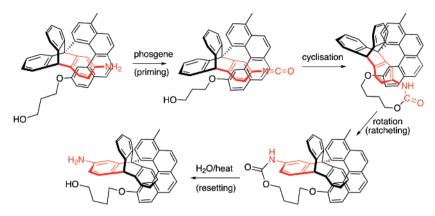
At UCLA, Stoddart began to think about multivalency in relation to rotaxanes. While the 1994 chemically switchable [2]rotaxane was revolutionary, it was not perfect. When deprotonated, the benzidine had only a 5:1 preference for the blue box (bisparaguat tertra-cation) over the biphenol. To improve the switch, in 2004 Stoddart's group made what became known as the 'molecular elevator' (Science 2004, vol. 303, p. 1845), which had three joined rotaxanes, running on three joined axles. The multivalency of three rotaxanes in one provided a 100% effective switch capable of exerting a force of 200 pN. Stoddart's group went on to move these switches and actuators onto solid surfaces to produce micro electronic devices, memory, pumps and motors. Motors are essential to any molecular machine and this aspect was being pursued in parallel to Stoddart, in Holland by Ben Feringa.

Ben Feringa

Bernard L. Feringa was also born on a farm, in the Netherlands on the border with Germany at Barger-Compascuum. He is a direct descendent of Johann Gerhard Bekel, the first (German) settler of the high moors in Holland. He attended the

University of Groningen to study chemistry and as an undergraduate worked in the lab of Hans Wijnberg (1928–2011). He obtained his Masters in 1974 and went on to a PhD with Wijnberg ('Asymmetric oxidation of phenols. Atropisomerism and optical activity', 1978).





T. Ross Kelly (Boston College) demonstrated a chemically driven 120° rotation in 1999.

Wiinberg was trained in the American academic tradition and has had a huge influence on the Faculty of Maths and Science at Groningen with its non-hierarchical structures and emphasis on entrepreneurship. Wijnberg was also highly innovative and instilled a need to tackle big questions in his students. Feringa did not do a postdoc but opted instead for an industry position and worked as a research scientist for Shell in Amsterdam and the UK from 1978 to 1984. In 1984, he took a lectureship position at the University of Groningen and succeeded Wijnberg as professor in 1988.

During his PhD, Feringa published a paper that would lead to the Nobel Prize in 2016 (*JACS* 1977, vol. 99, p. 602). The paper discusses the

synthesis and purification of atropisomers about a C=C double bond, that could be purified, gave distinct CD and ORD spectra but interconverted.

Photoswitchable double bonds have been known for a long time. For example it was known since 1937 that azobenzene could be switched from cis to trans and back again using light. The major challenge was how to make this isomerisation unidirectional and not just back and forth. As motors are fundamental to any molecular machine, these 'drive' the overall construction. Nature is luckily full of molecular motors such as flagella that are multicomponent but also singlecomponent motors such as myosin (muscle contraction), actin (polymerisation generates force),

F₀F₁-ATP synthase (proton pumps), DNA helicase (separates doublestranded DNA) and many more.

However, biological motors are very complex and we understand few of the precise details of how they actually work. At best, the characteristics of biological machines can give us broad ideas about how to construct molecular-level devices that exploit mechanical motion, but, until now, nonequilibrium statistical mechanics, not biology, has inspired the basic mechanisms for synthetic molecular machines. While many non-directional molecular motors have been reported. the first unidirectional motor was reported by Ross Kelly (Nature 1999, vol. 401, p. 150), who had been working on the construction of molecular motors since 1994. The system used the chemical reaction between (high-energy) phosgene and an amine as the source of energy. Once the isocyanate is formed, Brownian motion will eventually bring the hydroxyl close enough to react and then the helicene will rotate 120°. Hydrolysis of the urethane produces the starting material but there is no mechanism for the next 120° rotation required to continue the cycle.

Although this system can only carry out one-third of a full rotation, it demonstrated the principles required for a rotary system under chemical control and represented a major advance in the realisation of molecular level machine. In the same issue of Nature, Ben Feringa (1999, vol. 401, p. 152) reported a rotary motor that was not based on rotation around a single bond but based on an isomerisable double bond. Using this overcrowded alkene allowed the first synthetic molecular rotor capable of achieving a full and repetitive 360° unidirectional rotation. Irradiation (≥280 nm) causes chiral clockwise rotation of the upper half. However, this form is not stable at temperatures above -55°C because the methyl substituents on the cyclohexyl ring are placed in unfavourable equatorial



positions. At ambient temperatures, therefore, the system relaxes through a second, thermally activated helix inversion. Irradiation results in a second photoisomerisation and helix inversion followed by thermal relaxation to complete the cycle.

Over the next few years, the Feringa group improved the design of the motor and in 2014 achieved a 12 MHz rotation frequency (*Photochem. Photobiol. Sci.* 2014, vol. 13, p. 241). Several groups have developed similar motors and even attached four motors to a chassis to make nanocars – two motors that turn clockwise and two that turn anticlockwise.

The first nanocar race will take place this year in Toulouse, France. Six teams led by Gwénaël Rapenne, Rémy Pawlak, Saw-Wai Hla, Francesca Moresco, Waka Nakanishi and James M. Tour will compete (http://nanocarrace.cnrs.fr/course_en.php).

It would not be appropriate to finish this article without mentioning the contribution of James Tour to this field of research. His 2003 synthesis of anthropomorphic molecules - the 'nanoputians', a portmanteau of nanometre and lilliputian (J. Org. Chem. 2003, vol. 68, p. 8750), have no chemical or practical use but were synthesised to increase students' comprehension of chemistry and materials science, provide teachers with tools to teach nanoscale science and emerging molecular technologies, to demonstrate the overlap between art and science to facilitate learning, and to generate interest in nanotechnology.

Perhaps the best way to appreciate the potential of 2016's Nobel Prize research is to recognise that molecular machines are part of every significant biological process. Indeed, in contrast to biology, there is no task that can be performed by molecular machines that you cannot do more easily or

better some other way. However, when we do get to molecular machines that are better than biology, and it is a highly incremental process, we will be standing on the shoulders of three giants who gave us the tools required.

James M. Tour's synthesis of the first nanoputian.

Il faut respecter le temps long de la recherché.

[One must respect how long research takes.]

(Jean-Pierre Sauvage, 5 October 2016)

Peter Karuso FRACI CChem FRSN is Professor of Chemistry at Macquarie University, Sydney. Part I appeared in the February issue.

Light, soap and magnets turn graphene into

Some clever chemistry is employing magnetism and a light-sensitive soap to turn simple graphene into a supermaterial with applications in water purification and electronic devices.

t's almost impossible to pick up a scientific publication at the moment without reading something about graphene or one of its carbon cousins, including nanotubes and buckyballs. Graphene itself is simply an individual layer of the common mineral graphite – the black material in pencil lead – pure carbon atoms bonded together in an ultrastrong hexagonal pattern.

A significant proportion of graphene's appeal is that it retains graphite's electrical conductivity due to a phenomenon known as delocalisation, where some of the electrons that each carbon atom brings are shared throughout the structure and act as charge carriers. In fact, perfect sheets of graphene are exceptional conductors of both electricity and heat, making them an exciting proposition for the next generation of electronic devices.

However, it's still a major

technological challenge to make large quantities of graphene. The forces that hold the layers together are strong, and to overcome them requires a lot of mechanical energy. This was first memorably achieved by literally peeling layers off using tape, although this method doesn't scale well to produce larger amounts. An alternative to the mechanical approach is to use some clever chemistry, and this is where graphene oxide comes into the picture.

Graphene oxide is a version of graphene that has been oxidised – the sheets have been decorated with oxygen-containing functional groups. This is normally achieved chemically through the use of strong acids and oxidants, and has two important effects.

First, the conductivity of graphene is lost when all of the bonds to oxygen are formed, which is a problem if you want to make transistors and electronic devices. Second, adding all of that oxygen means that the sheets formed are hydrophilic.

Water is therefore able to penetrate between the layers, breaking apart the graphite structure from within and removing the need for mechanical peeling of the sheets.

We can, however, reverse the oxidation process by adding a chemical reducing agent to graphene oxide. A common choice for the reductant is hydrazine, an unusual and very unstable compound of hydrogen and nitrogen that's widely used in rocket fuels (although it's much safer when dissolved in water). This chemical can aggressively strip away the oxygen, returning graphene oxide to something much more like pure graphene, and offering a much less mechanically demanding route to 'graphene'.

However, the restoration is not perfect. Some defects and oxygen or nitrogen atoms remain in the sheets, and the conductivity never quite returns to that of pristine graphene or graphite. The material thus produced is usually known as 'reduced graphene oxide' to make this distinction clear.

However, graphene oxide and reduced graphene oxide have a slew of useful properties of their own, mostly because they can be dispersed

easily in water. As they retain a great deal of their carbon character, these materials love both water and oils, so they can be used instead of conventional emulsifiers to disperse oil in water.

Emulsions made using particles to stabilise their interfaces are known as Pickering or Ramsden emulsions, and are renowned for their extraordinary stability and shelf-life. Where graphenes are used as stabilisers, such emulsions might find applications in recovering crude oil from offshore reserves, and cleaning up oily spills from soil and water.

Perhaps even more usefully, graphene oxide is a brilliant adsorbent. This means that a wide array of molecules stick to graphene oxide in water, from pharmaceuticals, toxins and dyes to heavy metal ions like mercury and cadmium. This is not really surprising, as the most commonly used adsorbent in water treatment, activated carbon, looks chemically a lot like graphene oxide, with many of the same groups and bonds present. However, the benefit of graphene oxide is that peeling apart graphite into single layers that are one atom thick provides the greatest surface area possible - you get maximum adsorption capacity for your carbon buck!

So it sounds as though graphene oxide is the next supermaterial for water treatment – it's easy to make, captures all manner of toxins, and offers an astonishing surface area for every gram of carbon used.

But there's one tiny problem. The sheets created by the oxidation process are generally just a few microns across and only one atom thick. While this means they're easy to disperse stably in water, and hence can rapidly capture toxins and contaminants, getting them back is a challenge.

The usual methods for recovering tiny particles, such as filtration or centrifugation, don't work well because the graphene oxide sheets are simply too small.

Adding sticky polymers to 'glue' the sheets together and grab them works well, but this means that they can't be recycled and reused.

An appealing strategy to overcome this stumbling block is to find a way that external fields or stimuli can be used to capture graphene oxide, bringing it - and any adsorbed contaminants or toxins crashing out of water for easy collection and treatment. One way to achieve this is to use tiny iron oxide particles that also stick to the graphene oxide sheets. These particles are readily made to be magnetic, so

applying an external magnetic field gathers up the particle-laden carbon materials.

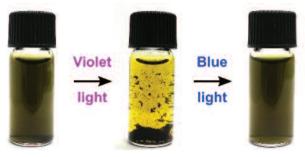
Handily, the surface charge of the iron oxide particles can be reversed with pH. At neutral conditions, the particles have an opposite charge to the graphene oxide sheets. Since opposite charges attract, they stick strongly.

After the magnet is applied and the graphene oxide – rendered magnetic by the adsorbed iron oxide particles – has been captured, adjusting the pH to slightly basic switches the iron oxide charge to negative. This means that the particles have the same charge as the graphene oxide sheets and spontaneously jump off, so that both materials can be collected, treated and recycled back into the process.

However, it's not just solid particles that can be used to capture graphenes. By using a small amount of a light-sensitive soap, the same effect can be achieved. The soap molecules contain a chemical group called azobenzene, which has the unique property of being able to change its shape and properties when illuminated with light



Left: an atomic force microscope image of graphene oxide sheets decorated with iron oxide nanoparticles. Right: the addition of iron oxide particles at a suitable pH allows magnetic capture of graphene oxide in the sample on the right. A control sample is on the left



The addition of a magnetic soap to reduced graphene oxide allows light to capture and redisperse the material.

of a specific wavelength.

Blue light makes the soap stick to carbon nanomaterials, increasing their stability in water. Violet light causes the soap to dissolve into the water, decreasing the graphene's stability and separating it for collection and treatment.

The handy part is that the soap's properties are completely reversible, so the system can be switched back and forth repeatedly with no loss of function

Whether you use light or magnets to capture them, it's clear that graphene and its family of related carbon nanomaterials are here to stay. They each have a unique set of properties that makes them valuable and appealing as the next generation of materials for water treatment and electronic devices.

We are now at a pivotal point where industry is realising the potential of this 'black gold', so you may start seeing more of the graphene family in your daily life!

Rico Tabor is a senior lecturer at Monash University's School of Chemistry. This article is reproduced from *Australasian Science* (austscience.com).

'Science business'

Centenary Che Congress

Dave Sammut speaks with Sharon Todd, SCI's Executive Director, about the organisation, its activities and its plans to participate in the 2017 Congress.

he 2017 RACI Congress marks a milestone in the history of our organisation. We will be celebrating 100 years serving the chemical profession and the community more widely. This July event will bring together scholars and professionals from around the world, with the combination of nine separate conferences and events into one substantive experience.

SCI (www.soci.org) will be one prominent participant in the Congress. In its own words 'SCI is a unique community – being "where science meets business" – and therefore its proposed contribution to the congress will focus on this uniqueness – bringing together both business and science'.

SCI's Executive Director Sharon Todd is an experienced senior executive with over 25 years in the chemical industry. She achieved her

SCI's motto, Scientia et Opera, depicted here on the Chemical Industry Medal. The medal is awarded annually by SCI for 'for contributions toward the growth of the chemical industry'.



first career role, with Albright & Wilson plc., through an SCI careers and networking event, working for 15 years in a variety of commercial roles, including Director of Strategy for ICI's Acrylics business. In 2001, she was appointed to the Board of Innospec Inc. as Executive Vice President responsible for Corporate Development, and in 2002 became Managing Director of the Performance Chemicals Division. Both roles were focused on driving growth through acquisition.

Sharon ran her own consultancy and interim management business for eight years, focusing on business development, strategic repositioning of businesses and mergers and acquisitions. This has involved working with start-ups, university spin-outs and large corporates - most recently with Synthomer plc. as Director of Corporate Development.

Sharon has diplomas from both the Chartered Institute of Marketing and the Institute of Directors. She has been involved with a number of industry trade associations including the Chemical Industries Association, and is currently a Non Executive Director of Chemicals North West, an industry-led, chemical cluster support organisation for the £10 billion North West chemical sector, the largest in the UK.

How did SCI begin?

SCI was established in 1881 as the Society of Chemical Industry. The founder members were scientists, inventors and entrepreneurs, people with a passion for science and for creating societal value through science. We are obviously a learned society, but our prime objective is the promotion of applied science into industry for the benefit of society.

Active early members included William Lever, who went on to form Lever Bros, now Unilever. Other members included Henry Tate, of Tate and Lyle, George Matthey (Johnson Matthey), Ernest Solvay (Solvay), Arthur Albright (Albright & Wilson,



Ms Sharon Todd. Executive Director of SCI since June 2015.

now Solvay), members from both the Proctor and Gamble families and Ludwig Mond, founder of ICI plc.

SCI was established as a forum to promote and foster innovation – through networking, educating and informing. Its motto 'Scientia et Opera' translates as 'Science and Industry'.

SCI has a global network with members in over 100 countries. It is different from many other professional societies, placing an emphasis on a multiscience and multidisciplinary approach to take science out of the lab into everyday products..

SCI's Australian branch grew out of the former Society of Chemical Industry of Victoria (SCIV), which was established in 1900, and the RACI emerged after a meeting of the SCIV in 1916.

The industrial great ICI was originally established by SCI members who networked through the SCI. SCI has always provided a forum for members to help each other by sharing and building on ideas. The early members were an instrumental body of people who built an innovation ecosystem, and helped to shape government policy through that network.

How has SCI changed under your leadership?

I have spent my career on the business side of industry in a global context. For me, then, any change has been on renewing the focus on industry and rebuilding industry linkages, and using applied science to drive the step changes in products and processes.

Over the course of my career, I have seen fundamental changes in industry and significant restructuring. As industry has become more fragmented (particularly in the Western world), from SCI's perspective it has become more challenging to keep some of the links going. It is important to maintain those links and to build a strategy to support industry in the future.

How does SCI's 'science meets business' vision translate into direct action?

SCI runs over 250 events per annum across a diverse range of topics, from 18 separate technical groups across a broad range of chemical topics. It is active in education and skills development, as well as providing expert advice in support of the development of Government policy in the UK and 'promoting informed debate' of important scientific issues through public forums. We strongly believe that personal networks are important. On the skills and education side, we run a wide range of events, including careers events to showcase opportunities in both large and small industry and a series of activities around the College of Scholars, promoting young people in particular PhDs – for both academic and industry careers. Additionally, we

have a range of networking and training activities for young and early career people and an ambassadors' program, and we've recently launched a mentoring program, because we have a natural mentoring community.

We also run registered training courses in packaging, licensing, publishing, and the necessary areas of biology ... Skills and education is a very important focus for us.

In the policy area, we seek to support informed debate on topical issues. For instance, we provide an independent scientific view and expert advisory services to the UK Government on the areas of decarbonisation technologies for industry, or climate change targets. Mostly, we tend to provide advice on areas related to innovation and enabling the flow of science from the lab into industry.

What do you see as the biggest challenges to the chemical industries over the next five or ten years?

There are global megatrends that everyone understands and knows so well – the burgeoning population and how to feed them; how to protect the planet; how to make sure that people's lives are better, that they are healthy and have improved wellbeing. We have also a low-growth global economy, a debt-laden economy, and now a dislocation in the Western communities from the political processes. In this context, science and innovation have a critical role to play in improving societal welfare.

Part of the solution to low growth has to involve science-based innovation. Organisations like SCI need to come to the fore and promote the ideas around how to bring innovations to market more quickly. We have to help define the innovations that are going to lead to step changes; and help promote the linkages between academia and industry.

What will SCI offer at the 2017 Congress?

We'll be doing a typical SCI agenda. Our event will have an overview of what is going on in the global marketplace, the broader trends and their impacts on industry and academia. We have experts who will talk about start-up companies, issues and challenges in commercialising new technologies and creating successful businesses. There will also be sessions on patenting, the challenges and opportunities in developing commercial patent portfolios, and publishing.

Will you be travelling while you are in Australia?

I would love to. I've travelled to many places around the world, but I've never been to Australia. At 14, my grandfather misrepresented his age to come to Australia. He lived in Australia for many years as an adventurer out in the bush, and I'd quite like to retrace some of his footsteps – if time allows.

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.

The RACI Congress will run 23–27 July in Melbourne. SCI is a partner organisation of the Congress and will run both presentation and training sessions. For more information visit www.racicongress.com.





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Women in chemistry speaking at RACI Centenary Congress, 23–28 July 2017

There are now less than five months to the start of the RACI Centenary Congress 2017 – the biggest chemical congress ever to be held in Australia.

The Congress is being hosted in collaboration with nine prestigious chemistry conferences that together make up a five-day Festival of Chemistry that will attract 3500 delegates across the breadth of the chemical sciences and technologies. The novel congress concept involves all of the partner conferences running concurrently during the week, allowing delegates to access sessions across a wide variety of chemistry disciplines.

Each day will commence with a common Congress plenary speaker for all delegates followed by the various conferences running their individual programs. All of the Congress themes are confirmed and are available by accessing the Congress website (www.racicongress.com).

A single Congress fee will allow delegates to attend any conference or session within the Festival of Chemistry. No one will be limited to a single conference stream.

In addition to the two previously confirmed Nobel Laureates – Professors Ada E. Yonath and Robert Grubbs – the conference committee are pleased to announce four extraordinary female plenary speakers who are all world leaders in their respective fields.

Professor Laura L. Kiessling holds the Steenbock Chair in Chemistry and is the Laurens Anderson Professor of Biochemistry at the University of Wisconsin–Madison, US. She also serves as the Director of the Keck Center for Chemical Genomics and the Chemistry–Biology Interface Training Program.

Her interests focus on elucidating and exploiting the mechanisms of cell surface recognition processes, especially those involving protein—carbohydrate interactions. Her research addresses questions regarding the assembly of glycans, their biological roles, and how to co-opt or inhibit glycan interactions.

Professor Kiessling's other honours and awards include the Alfred Bader Award in Bioorganic Chemistry, the ACS Claude S. Hudson Award, the Murray Goodman Award, a Guggenheim Fellowship, and a MacArthur Foundation Fellowship. She is a Fellow of the American Academy of Arts and Sciences and a Member of the National Academy of





Professor Frances H. Arnold is the Dick and Barbara Dickinson Professor at the California Institute of Technology, US.

Her research focuses on protein engineering by directed evolution, with applications in alternative energy, chemicals and medicine. Professor Arnold chairs the Advisory Panel of the David and Lucile Packard Foundation Fellowships in Science and Engineering program and serves as a judge for the Queen Elizabeth Prize in Engineering.

Professor Arnold's honours include the Millennium Technology Prize (2016), the Eni Prize in Renewable and Nonconventional Energy (2013), the US National Medal of Technology and Innovation (2011), and the Charles Stark Draper Prize of the US National Academy of Engineering (2011).

She was inducted into the US National Inventors Hall of Fame in 2014 and has been elected to membership in all three US National Academies, of Science, Medicine and Engineering.



Professor Molly M. Stevens is currently Professor of Biomedical Materials and Regenerative Medicine and the Research Director for Biomedical Material Sciences in the Department of Materials, Department of Bioengineering and the Institute of Biomedical Engineering at Imperial College London.

Professor Steven's research focuses on designing and developing innovative bio-inspired materials for applications in regenerative medicine, tissue engineering and biosensing.

Her research has been recognised by more than 20 major awards, including the 2016 Clemson Award for Basic Research from the Society for Biomaterials, the EU-40 Prize for best material scientist under the age of 40, a listing in *The Times* as one of the top 10 scientists under 40 and the European Life Sciences 2014 Research Group of the Year Award.



Professor Nieng Yan received her BSc from the Department of Biological Sciences and Biotechnology, Tsinghua University, Beijing, China, in 2000. She then pursued her PhD in the Department of Molecular Biology at Princeton University, US, under the supervision of Professor Yigong Shi between 2000 and 2004.

She was the regional winner of the Young Scientist Award (North America) cosponsored by Science/AAAS and GE Healthcare in 2005 for her thesis on the structural and mechanistic study of programmed cell death. She continued her postdoctoral training at Princeton University, focusing on the structural characterisation of intramembrane proteases.

In 2007, she joined the faculty of School of Medicine, Tsinghua University. Her lab mainly focuses on the structural and functional study of membrane transport proteins. In 2012 and 2013, she was promoted to tenured professor and Bayer Endowed Chair Professor, respectively.

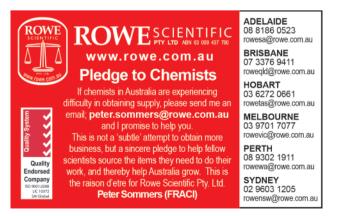
Professor Yan is an HHMI international early career scientist, Cheung Kong Scholar, and the recipient of the 2015 Protein Society Young Investigator Award and the Raymond and Beverly Sackler International Prize in Biophysics. Other confirmed plenary speakers include:

- Professor Oliver Einsle, Institute of Biochemistry, Spemann Graduate School of Biology and Medicine Freiburg, Germany
- Professor Andrew B. Holmes, Melbourne Laureate Professor Emeritus President of the Australian Academy of Science, Australia
- Dr Andrew Makarov, Director of Research in Life Sciences
 Mass Spectrometry, Thermo Fisher Scientific, Bremen, Germany.

Don't leave it until the last minute – submit your registration now to make sure you secure the reduced early bird registration rate.

Key dates	
Abstract submissions	Now open
Registrations	Now open
Short abstract submissions (Carbon 2017 only)	Closed
All abstract submissions (excluding Carbon 2017)	Closes 23 March
Early bird registration	Closes 23 April
Extended abstract submission (Carbon 2017 only)	Closes 30 April





New Fellow



Professor Michelle Coote is a graduate of the University of New South Wales, where she completed a BSc(Hons) in industrial chemistry (1995), followed by a PhD in polymer chemistry (2000) with Professor Tom Davis. Following postdoctoral work in polymer physics with Professor Randal

Richards at the University of Durham, UK, she joined the Research School of Chemistry, Australian National University, in 2001, initially as a postdoctoral fellow with Professor Leo Radom. She established her own research group in 2004 and was promoted to professor in 2011, the first female Professor of Chemistry at ANU.

She has published more than 200 papers in the fields of polymer chemistry, physical organic chemistry and computational quantum chemistry, and is a member of the ARC Centre of Excellence for Electromaterials Science. At present, her main research interests are the harnessing of electric fields for chemical catalysis and the development of techniques for controlling the stereochemistry of radical polymerisation.

Coote has been a member of RACI for more than 25 years and is currently Chair of the Polymer Division and Immediate Past Chair of the Physical Division. She has received many awards, including the 2001 IUPAC prize for young scientists, the RACI Cornforth Medal (2000), Rennie Medal (2006) David Sangster Polymer Science and Technology Achievement Award (2010) and H.G. Smith Medal (2016), the Le Fevre Memorial Prize of the Australian Academy of Science (2010) and the Pople Medal of the Asia–Pacific Association for Theoretical and Computational Chemistry (2015).

In 2014, she was elected to the Fellowship of the Australian Academy of Science as one of the youngest chemists in their history. She was recently appointed as the first Australian associate editor of the *Journal of the American Chemical Society*, following terms as an associate editor of *Scientific Reports* and the *Australian Journal of Chemistry*.

She lives with her husband and their two boys, two cats, six chickens, several fish, and many thousands of bees in country NSW, and enjoys gardening and reading in her spare time.

Geoff HawthorneCSIRO polymer chemist

Geoff Hawthorne was a genuine 'quiet achiever'. He contributed to many of CSIRO's notable polymer chemistry projects, such as the polymer banknote project and the development of high-temperature-resistant resins, but was little known outside the laboratory.

In his reference for Geoff, his MSc supervisor at the University of Melbourne, Professor William Davies noted that Geoff '... has the rather reserved and aloof manner not uncommon among such ardent research chemists.' Davies went on to say: 'He can be surly if "mothered" (chemically speaking) too much, but he will be an admirable member of a research team if his power of independent research is respected.' Geoff's supervisor knew his student well! Throughout his career Geoff had to be persuaded to let a promotion case go forward for fear that it would take time away from his laboratory bench. He did become a principal research scientist but two of the current authors could never persuade him to be considered for promotion to the rank of senior principal research scientist.

David Geoffrey Hawthorne was born in Kerang, Victoria, on 25 October 1935. In his last year at Scotch College, Melbourne, his chemistry teacher told him that parttime laboratory assistants at the University of Melbourne learnt far more about practical chemistry than full-time students and persuaded him to become such an assistant. He commenced these activities in 1953 and finally graduated with a PhD in 1965. He worked for a few months as a research scientist at Moulded Products in Mentone (just before it changed its name to Nylex) before joining the CSIRO Division of Applied Mineralogy in October 1965 as an experimental scientist to work on mineral-organic complexes with Dr George Walker.

Two years before Geoff joined the Division, Dr Walker had recruited Dr David Solomon to initiate work on the interaction of polymers with minerals and so Geoff joined an active group at Fishermens Bend. Dr Walker died during a cardiac operation in February 1970 and from then Geoff worked with Dr Solomon. David was already working on the (then highly secret) polymer banknote project and in July 1970 his whole group was transferred to the Division of Applied Chemistry.

For the polymer banknote project, Geoff undertook the development of materials and methods for the incorporation of moiré devices into the banknotes. He was also involved in work on moiré design and the discovery and development of improved spectroscopic label transfer foils. He was given a specimen \$10 commemorative note by the Reserve Bank in recognition of his contribution to the project.

Geoff was an important contributor to new work on the mechanism of cyclopolymerisation of diallyamine monomers. This showed that the previous structures proposed for these commercially important polymers were incorrect. In the course of this work, he introduced the use of ESR spectroscopy to the polymer group and was for many years the Division's expert on that technique.

He was one of the original scientists to work with Dr Solomon and then Dr Ezio Rizzardo on nitroxide-mediated living free radical polymerisation and shared the 1990 CSIRO Medal for this work.

His outstanding technical expertise was particularly valuable in improving and keeping running a number of temperamental polymer characterisation instruments. His blunt demeanour was good at frightening the young and clumsy from damaging such equipment but he was always willing to help train others in new techniques.

Geoff joined the RACI in 1961 at the completion of his MSc and was elected a Fellow in 1978. He was very much involved in the Polymer Division.

He was an active member of The Steam Locomotive Society of Victoria. To participate fully in the Society's activities, he went to night school with one of us at the former Chisholm TAFE to hone up his practical skills in fitting and turning. Geoff embraced setting up his own workshop with characteristic thoroughness. His long-term project to build a large-scale C38 locomotive will now have to be completed by someone else.

Geoff died 20 October 2016. He is survived by his three sons, David, John and Philip, and his grandchildren Lucy and Sam.

J.H. Hodgkin FRACI CChem, **T.C. Morton** and **T.H. Spurling** FRACI CChem

William Percy Wilkinson Analytical chemist, ampelographer and provocateur

Percy Wilkinson was an important figure in the early days of Australian chemistry, who has been largely ignored by historians of Australian science. In our centenary year, this obituary belatedly recognises his contribution.

William Percy Wilkinson, analytical chemist, ampelographer and provocateur, was born on 13 May 1868 in Cathkin, Victoria, and died in Melbourne on 14 March 1947. His parents were William Wilkinson, a manager of a sheep station near Cathkin, and Bessie Percy Wilkinson.

Percy completed his secondary education at St James's Grammar School, which was associated with St James Old Cathedral and was on the corner of Bourke and William Streets in Melbourne. He passed his preliminary examination for the Pharmacy Board of Victoria in 1886 and the intermediate examination in 1888 but never practised as a pharmacist. He was elected a Fellow of the Institute of Chemistry (in London) in 1913 and the post-nominal FIC was the only one he used. He commenced work as the Assistant Victorian Analyst in 1890. Percy Wilkinson married Alice Blackett, the younger daughter of C.R. Blackett (the Victorian Analyst at the time) in 1899. Blackett remained the Victorian Government Analyst until a few days before his death in 1902. Percy Wilkinson succeeded his father-in-law in the position and occupied that until he became the first Commonwealth Analyst in 1908. He retired from that position in 1933.

In the early years of the Commonwealth, income from customs

and excise made up around 75% of the Commonwealth's revenue and the Commonwealth Analyst was a senior appointment in the Department of Trade and Customs. In that position, Percy established what was known as the Commonwealth Laboratory in 1908. This two-storey building in Flinders Lane, Melbourne, behind what is now the Immigration Museum, was demolished in the 1960s and the site is now the Tribute Garden of the Immigration Museum.

One of his first studies in the Victorian Government Analyst laboratory was a chemical examination of constituents of eucalyptus oils. In 1893, he reported on the examination of 87 samples of essential oil from 17 different species of Eucalyptus. This work pre-dated the more recognised work of H.G. Smith by about four years.

He was intensely interested in wines and winemaking and in 1901 published his first book Studies on wine-sterilizing machines. He published papers on ampelography, which is the field of botany concerned with the identification and classification of grapevines, and he predicted the controversy about the names of wine in his fourth and final book, The nomenclature of Australian wines: in relation to historical commercial usage of European wine names, international conventions for the protection of industrial property, and recent European commercial treaties, published in 1919.

In 1912, he embarked on an extensive overseas tour to Europe, Japan and the United States. While in the US he

represented Australia at the Eighth Triennial International Congress of Applied Chemistry along with 1200 other chemists from around the world.

Given his position and experience and importance to the Commonwealth, it is surprising that he didn't play a more prominent role in the discussions around the formation of an Institute of Science and Industry that commenced after Prime Minister Hughes's speech in Melbourne in December 1915. Although he was a member of the Advisory Council of Science and Industry set up in 1916 to advise the Prime Minister, his name does not appear on the record of those who signed the final report to the Prime Minister. As the authors of the history of the early years of CSIRO noted, Percy Wilkinson 'consistently pursued a policy of non-co-operation with the Advisory Council, probably seeing in the proposed new Institute some challenge to his own laboratory in the Customs Department'. Further, Masson referred to him as one who would 'smash our organisation if he could'.

Percy Wilkinson continued his distinguished career as the Commonwealth Analyst until he turned 65 in 1933. The Commonwealth Laboratory underwent several reorganisations in subsequent years with its functions today being largely within the National Measurement Institute. His legacy as a founder of chemical metrology through the Commonwealth Laboratory is secure.

T.H. Spurling FRACI CChem and **J.M. Webb** FRACI CChem

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What your pee and poo colour says about your health

Out of the blue I passed bright red pee. I freaked, thinking it was a sign of terminal disease. Then I remembered the roasted beetroot tarts served at the party the night before – so delicious, I'd eaten three!

Beetroot, artificial colours, vitamin supplements and medications can change the colour of your urine or bowel motions. Knowing which colour changes are due to food or medicines can save you worry, or provide an early alert to get to the doctor.



Beeturia

Beeturia is the term for passing red urine after eating beetroot. The red colour comes from a pigment called betalain, also in some flower petals, fruit, leaves, stems and roots. Concentrated beetroot extract, called Beet Red or additive number 162 on food labels, can be added to 'pink' foods, such as ice-cream.

Whether betalain turns your pee red or not depends on the type of beetroot, amount eaten and how it's prepared, because betalain is destroyed by heat, light and acid.

How much betalain enters your digestive tract depends on stomach acid and stomach emptying rate (people taking medications to reduce stomach acid may be prone to beeturia). Once in the bloodstream, betalain pigments are filtered out by the kidneys. Most is eliminated 2–8 hours after eating.

Persistent red urine can be due to blood loss, infection, enlarged prostate, cancer, cysts, kidney stones or after a long-distance run. If you see red and have not been eating beetroot, see your doctor.

What should your pee look like?

Normal pee should be the colour of straw. If your pee is so colourless that it looks like water, you probably drank more than you needed.

You should never see purple pee, but hospital staff might. 'Purple urine bag' syndrome happens in patients with catheters and infections or complications.

Very dark yellow pee usually means you are a bit dehydrated and need to drink more water.

Compare your pee colour to the Cleveland Clinic's scale opposite.

Strange pee colours due to food, drugs or disease

Pee the colour of syrup or molasses needs medical investigation. While it could be due to extreme dehydration, it can be a sign of liver diseases such as hepatitis and cirrhosis, where a build-up of bilirubin spills into your pee. Bilirubin is a breakdown product of red blood cells; it's also responsible for poo's normal brown colour.

Pee can turn bright orange or yellow when taking beta-carotene or vitamin B supplements, especially large doses of riboflavin (vitamin B2). These supplements are water soluble. What your body can't use or store gets filtered out via your kidneys and into pee.

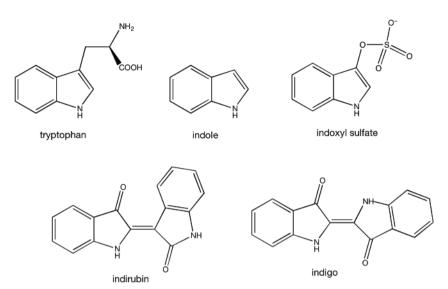
Medications including phenazopyridine (for urinary tract infections), rifampin (antibiotic for treating tuberculosis and Legionnaire's disease), warfarin (blood thinner) and some laxatives can also change pee colour.

If you pass blue or green pee, it's most likely due to food colouring or methylene blue used in some diagnostic test procedures and some drugs.

But a range of medications can also trigger blue or green urine. These include antihistamines, anti-inflammatories, antibacterials, antidepressants, some nausea drugs or those for reducing stomach acid.

Rare genetic conditions Hartnup disease and blue diaper syndrome cause blue-green urine. So see your doctor if it persists or it happens in an infant.

You should never see purple pee, but hospital staff might. 'Purple urine bag' syndrome happens in patients with catheters and infections or complications. The catheter or bag turns purple due to a chemical reaction between protein breakdown products in urine and the plastic.



Tryptophan from food is metabolised by bacteria in the gastrointestinal tract to produce indole. This is absorbed into the blood by the intestine and goes from there to the liver, where it becomes indoxyl sulfate. This is excreted in the urine. It has been suggested that in purple urine bag syndrome, bacteria in the urinary catheter convert the indoxyl sulfate to indirubin and indigo.

Occasionally, pee can be frothy. It's a normal reaction if protein intake is high and pee comes out fast. It is more likely if you consume protein powders or protein supplements. Excess protein can't be stored in the body so the nitrogen component (responsible for the froth) gets removed and the kidneys excrete it as urea.

See your doctor if the frothiness doesn't go away or gets worse, as protein can leak into pee if you have kidney disease.

Poo colours of the rainbow

Normal poo colour ranges from light yellow to brown to black. The colour is due to a mix of bile, which starts off green in the gall bladder, and bilirubin a yellow breakdown product from red blood cells.

Poo can turn green after consuming food and drink containing blue or green food colouring, or if food travels too fast through the gut and some bile is still present.

Poo that is yellow, greasy and smells really bad signals food malabsorption. If this colour is associated with weight loss in an adult or poor growth in a child, see a doctor to rule out gut infections such as giardia or medical conditions like coeliac disease.

Very pale or clay-coloured poo can happen when taking some anti-diarrhoeal medications, or when digestive problems affect the liver, gut, pancreas or gall bladder.

At the other extreme of the colour spectrum, black poo could be a serious medical issue due to bleeding in the stomach or upper gut. Or it could be a harmless side-effect from taking iron supplements, or eating lots of licorice.

Red poo can also be a serious medical issue due to bleeding in the lower gut, or from haemorrhoids, or harmless after having large amounts of red food colouring.

If you don't know what colour your pee or poo is, take a look. If you see a colour that's out of the ordinary and you haven't eaten anything unusual, take a picture and make an appointment to show your GP.

Clare Collins is Professor in Nutrition and Dietetics, University of Newcastle. Kristine Pezdirc is Research Associate and Postdoctoral Researcher, University of Newcastle. Megan Rollois is Postdoctoral Research Fellow, Nutrition & Dietetics, University of Newcastle. First published at www.theconversation.com and adapted with permission.





Your body isn't getting enough water.
Drink some now.

SYRUP OR BROWN ALE.

Or severe dehydration. Drink water and see your doctor if it persists.

PINK TO REDDISH.

Have you eaten beets, blueberries or rhubarb recently? If not, you may have blood in your urine. It could be nothing. Or it could be a sign of kidney disease, tumors, urinary tract irfections, prostate problems or something else. Maybe even lead or mercury poisoning. Contact your doctor.

ORANGE.

You may not be drinking enough water. Or you could have a liver or bile duct condition, Or it could be food dye. Contact your doctor.

BLUE OR GREEN.

Okay, this is different. There is a rare genetic desage that can turn your urine blue or green. Also certain bacteria can infect the urinary tract. But it's probably a food dye in something you ate. Or a medication. You won't die from it, but see your doctor if it persists.

PURPLE.

There's no such thing as purple urine.

FOAMING OR FIZZING.

A harmless hydraulic effect, if occasional. But could indicate excess protein in your d et or a kidney problem. See a doctor if framing happens all the time

OUTSIDE INFLUENCES:

Stuff you take can change the color of your urine. For instance, some medications, laxatives, chemotherapy drugs and dyes doctors give you to diagnose urinary tract infections can make your urine carker than normal. Are you taking any of these things?



INAL WORD:

You can tell a lot from looking at your urine. But you an tell a lot more from the kind of sophisticated urinalysis you should be getting along with a regular khysical examination from your doctor. Blood in the urine, a serious sign, is often invisible to the naked ye. The level of sugars in your urine may indicate urisk for diabetes. When you're at your doctor's fflice, don't be afraid to pee in the cup. It's one of ne best things you can do for your health.

clevelandclinic.org/HealthHub

SOURCE: "Unine – Abnormal Color" MedinePlus Medical Encyclopedia, National Institutes of Health

Hydrogen: fuel of the (far-distant) future?



Toyota's fuel cell vehicle 'Mirai', Yokohama, Japan. iStockohoto/ioel-t

In the community and politics, there is a tendency to conflate technically demonstrated projects with economically viable projects. Many technologies can be technically demonstrated, especially if money is no object, but they will always remain not commercially viable. The hydrogen economy is a good example.

Across the research and development community, there is a fascination for the use of hydrogen as a transport fuel, especially for cars fitted with fuel cells. The attraction comes from two drivers. The first is that hydrogen combustion does not emit carbon and thus the use of hydrogen is an alternative to battery-powered vehicles for decarbonising the transport fleet. The second is that internal combustion engines are not very thermally efficient while theoretically at least fuel cells have a much higher efficiency. Today, there are many examples of demonstration programs, many supported by the vehicle manufacturers, for hydrogen fuel cells and the required infrastructure. A small demonstration program has recently been announced by the ACT Government, supported by Hyundai and Siemens and others associated with the renewable fuels industry.

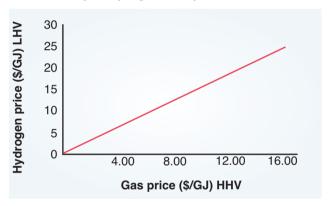
Three steps are required for the effective use of hydrogenfuelled vehicles, each requiring significant innovation before practical use can come to fruition:

- 1 hydrogen production at a competitive cost
- 2 hydrogen distribution to the filling point
- 3 operation and storage of hydrogen at the filling point and in the vehicle.

Hydrogen is widely used in the hydrocarbon processing industry, including oil refining where it is produced as a byproduct of dehydrogenation processes, such as naphtha reforming to produce aromatics for fuels and chemicals. These processes are supplemented by steam reforming of natural gas

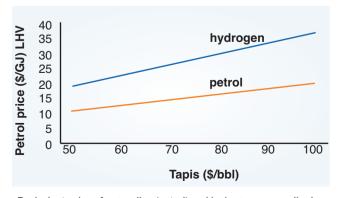
(or partial oxidation of natural gas). The coproduced carbon monoxide is converted to more hydrogen by the water-gas-shift process and the coproduced carbon dioxide is extracted by an absorption process. Nowadays, many plants separate pure hydrogen from this product stream by using membrane or PSA separators. The natural gas route is considered the most efficient and cheapest method for producing hydrogen.

One concept for hydrogen distribution is to have a large centrally placed production facility that distributes the hydrogen to retail forecourt sites. Such a central facility would produce about 400 kt/year of hydrogen, enough to provide over 2 million vehicle fills. The large facility would maximise the benefits from economies of scale and my estimates for the production cost from such a facility is shown in the following graph (data extracted from US National Academy of Science reports). Gas priced below US\$4/GJ (HHV basis on which gas is usually sold) would produce hydrogen below \$7/GJ (LHV basis, which is the way the hydrogen is used).



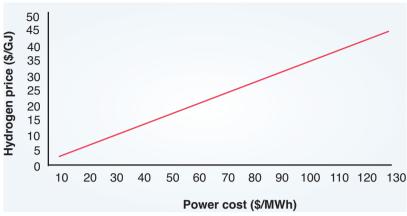
Estimated hydrogen production cost from gas in a large central facility.

How this stacks up against gasoline (petrol) prices is shown in the next graph, which illustrates the change in the traded price of petrol expressed in energy units (US\$/GJ, LHV basis) on the Singapore market as the price of crude oil (Tapis blend) changes. If we assume that a vehicle fuel cell has an efficiency



Equivalent values for gasoline (petrol) and hydrogen versus oil price (Tapis).

Because of its innate properties, for a reasonable operational mileage, hydrogen has to be stored on board the vehicle at very high pressure, typically 350 bar or even 700 bar.



Marginal hydrogen production cost using electrolysis.

of 55% and petrol engine of 30%, then the price equivalent cost of hydrogen is shown on the top line. Thus with prevailing oil prices at \$60/bbl, the petrol price is US\$12.50/GJ and the hydrogen equivalent price is US\$23/GJ, which is achieved with gas prices below US\$14/GJ (see graph above). Since gas prices (even in Australia) are well below this, all seems well and good. Unfortunately, there are a couple of issues that spoil this rather rosy picture.

One is the basic assumption that a fuel cell vehicle will operate at significantly higher efficiency than a modern petrol or diesel hybrid vehicle. In practice, when losses from the fuel cell to the electric drive and drive chain are taken into account, there may not be much difference. This would reduce the target production cost for hydrogen to a similar order for petrol or diesel unless the consumer is happy, or forced, to pay more for the privilege of a hydrogen vehicle.

Because of its innate properties, for a reasonable operational mileage, hydrogen has to be stored on board the vehicle at very high pressure, typically 350 bar or even 700 bar. These are very high pressures for an application as common as vehicle refuelling.

Hydrogen at these pressures is very dangerous. Leaks can spontaneously ignite. The flame is at more than 2000°C, which melts metal structures holding the pipeline or storage facility together. I once worked on a hydrogen plant that operated at over 200 bar and was built in 1936. All the pipe-work was extremely thick; it was made by the Woolwich Arsenal, which had the specialist equipment to manufacture it. To prevent destruction from hydrogen leaks, the whole plant was clad in more than 4 inches of blue asbestos and stood behind a thick brick wall to further protect operators. Only senior qualified graduate engineers were allowed to tackle leaks behind the wall, much to the fear of the tradesmen, because often the engineers would feign ignorance of which way to turn the 6-inch diameter bolts to tighten gaskets. I would hope the mechanical engineering design has improved since then.

Hydrogen production facilities tend to operate at about 30 bar for steam methane reforming (and 100 bar for partial oxidation). A rough estimate is that to intensify the pressure

from 30 to 350 bar in a central facility producing hydrogen, it would require 85 MW; and to compress to 700 bar, it would require about 125 MW. This would represent a serious cost penalty, especially if the power was from wind or solar generators.

What about different approaches? The marginal (no capital considered) cost of production of hydrogen by electrolysis is illustrated in the graph above. Wind and solar generation costs are generally in excess of \$100/MWh (unsubsidised basis) and production by this route is clearly very costly compared to conventional fuels. This is further exacerbated by electrolysis generally occurring at or near atmospheric pressure, which will incur vast compression costs to bring the product to a 350 bar filling pressure. This issue has been addressed by some developers trying to use electrolysis at high pressure (Honda).

In the research stage are several routes to produce hydrogen by solar irradiation, missing out the photovoltaic and electrolysis steps. This is very much a research activity and as yet is well away from a demonstration facility, let alone commercialisation.

There are also developments in using small-scale PV for distributed hydrogen generation (household make-your-own hydrogen). How proponents solve the problem of providing homes with 350 bar hydrogen compressors is somewhat unclear.

The pressure problem can be overcome by moving to liquid hydrogen storage. Insulation size would restrict this to larger vehicles and does not address the compressor cost for cooling the gas to below the critical point (-240°C).

Across the board, the hydrogen economy is replete with research and demonstration projects pushing boundaries with innovative solutions. Unfortunately, as this analysis shows, the hydrogen economy for Australia is still a long way off. Hydrogen may be destined to be the fuel of the future but will always remain so.



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Searching for the sweet spot

I first mentioned the concept of the 'sweet spot' in my October 2012 column (p. 39). At the time, I indicated that this sensory factor was deserving of another column and I have finally got around to writing it. The sweet spot concept is a great example of how experience of winemakers can form the basis of an intriguing research project.

Perhaps the sweet spot issue has come about as a consequence of increasing alcohol (i.e. ethanol) concentration in wine in recent years and the need to reduce this concentration without affecting or removing other components from the wine. A survey performed by the Australian Wine Research Institute (AWRI) found that the mean ethanol concentration for red wines increased from less than 12.5% in 1984 to 14.5% in 2005, before decreasing to 13.6% in 2014 (Gooden et al. Aust. J. Grape Wine Res. 2015, vol. 21, pp. 741-53). I have seen some red wines with an ethanol concentration higher than 16%. Global warming has been suggested as one factor for this increase, although for some time winemakers have been seeking 'phenolic ripeness', which results in grape harvesting occurring later in the growing season with the consequence of a high grape sugar level and thus more ethanol after fermentation. As ethanol can have a dominating influence on the taste of wine, technologies for the reduction in ethanol post-fermentation were introduced (also see my October 2012 column). This ethanol reduction step could well contribute to the decrease in the mean peak in 2005: the AWRI survey looked at finished or bottled wines.

If ethanol reduction is to be carried out, the question is by how much. This is where the 'sweet spot' comes in. Perhaps the best description of the sweet spot is the ethanol concentration where all components in the wine are in balance. This is identified by tasting wines for which the ethanol concentration is incremented usually in steps of 0.1%. Tasters will then assess the wines to ascertain the 'favourite'. In my only experience with this process, my selected wine differed from the 'clear favourite' by 0.2%, but as the others were responsible for the commercial product, I graciously gave way to their decision!

David Wollan of Memstar is a fan of the sweet spot concept as it is closely related to his commercial interest in lowering the ethanol concentration of wine. David is of the view that while winemakers recognise and can identify the sweet spot, present research knowledge is not sufficient to provide a scientific basis on which to base predictions regarding the sweet spot. The ARC Training Centre for Innovative Wine Production has incorporated the sweet spot as one of its activities (see bit.ly/2hoA8eF; projects 10a and 10b). David and Duc-Truc Pham are the researchers involved in this activity and the difficulty they face is simply that tasters do not seem able to discriminate between wines that differ by less than 0.4%



ethanol. This creates a little difficulty as the sweet spot is predicated on the basis of 0.1% difference.

The impact of ethanol on sensory perception of wine has received considerable attention in recent times, although generally on wines that have been manipulated, either by ethanol removal or by fortification, practices that could themselves alter the sensory characteristics. Dr Hildegarde Heymann of University of California, Davis, is one of the research leaders in this field and her group has examined sensory profiles of Cabernet Sauvignon with ethanol concentrations between 12 and 16%. These were all commercial wines in bottle and ranged in price from US\$6 to US\$100. Critically important to the results was the order of tasting. That is, the rating a taster would develop when tasting from low to high ethanol was different from the rating when tasting in the reverse direction. When the wines were randomised in terms of ethanol concentration, another rating was obtained (see King et al. Food Qual. Pref. 2013, vol. 28, pp. 235-43). These observations are reinforced in other work from Hildegarde's group. To add to this order of tasting complexity, a recent study from the ARC Training Centre for Innovative Wine Production has shown that the loss of ethanol by evaporation from uncovered wine glasses, resulting in a change in the relative proportion of ethanol and water, can be significant. This loss can impact on sensory perception of the wine (Wollan et al. J. Agric. Food Chem. 2016, vol. 64, pp. 7569-75).

The sensory approach to identifying the sweet spot is thus fraught with difficulty. One factor that appears not to have been considered is the change in the hydrophilic/hydrophobic balance as the ethanol/water balance changes. In essence, to follow a hobby horse of mine, molecular aggregation processes will be dependent on the changing hydrophobicity of the wine and this may well affect the sensory response. Techniques such as dynamic light scattering and diffusion NMR spectroscopy may well provide insight into the changing solution chemistry that could impact on sensory perception. 'Wine for thought' perhaps!



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Saved by the patent grace period?

Paul Whenman, Partner and Registered Patent and Trade Marks Attorney, FB Rice



Your paper on novel electrode assemblies was published almost ten months ago in a leading refereed journal. Recently, you ran into a former colleague at a conference who expressed interest in your paper. In particular, she asked if a patent application had been filed as she was aware of other groups involved in the same area of research that 'always filed patent applications' to protect

possible commercial uses.

Since your group was always on the lookout for additional funding through licencing, you wondered why a patent application had not been filed. In particular, the performance achieved by your electrodes was clearly superior to others reported in the literature. As your colleague had pointed out, it is 'Patents 101' that you can't patent something that has already been disclosed. Nevertheless, for future work, you decide on your return to the lab to take up patenting policies with your supervisor.

Although your group did discuss patenting from time to time, you were unsure about the existence of any consistent approach or indeed if a patenting policy existed. In this case, you assumed that your supervisor had decided not to proceed to file a patent application.

Somewhat surprisingly, your supervisor has told you that he was aware of competing groups and knew they frequently filed patent applications. Since your group's work was close to these competing groups, he considered it a waste of resources to file patent applications. Furthermore, he thought it was now too late to file although he confessed to hearing about a US researcher filing after

publication. Since your supervisor's interest is revitalised on learning the extent to which competing groups are patenting, as well as the potential for commercial application and hence funding, he suggests you review the patent policy and investigate the possibility of filing after publication.

Your research reveals there is a general rule that publication of an invention prior to filing a patent application destroys the novelty of an invention. However, a number of countries allow for filing after publication subject to specific country-by-country rules. The university's patent attorney refers to this after-publication filing as a 'grace period' filing.

On investigating further, you find that of relevance to the group's electrode work, South Korea, Canada, the US and Australia all provide a grace period for filing of up to one year after publication. However, other significant countries, including Europe, China and India, do not generally provide a grace period.

To take advantage of the grace period, you are advised it is important to ensure that the disclosure and invention claimed in the grace period patent application is commensurate with that of the published paper.

As the patent attorney points out, the grace period is a stop-gap measure with limited application. Best practice always is to review work pre-publication and if required, file a patent application prior to any publication. In this case, since your paper was published within the grace period it is provided to the patent attorney to draft and file a patent application.

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

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Science as a human endeavour

Science is continually changing as new knowledge is discovered. However, many students believe that scientific knowledge is immutable and that there is always a single, correct 'textbook' answer to every scientific question. This is contrary to the expected learning outcomes in the Australian Curriculum, which state: 'Science involves the construction of explanations based on evidence and science knowledge can be changed as new evidence becomes available.' Similarly, at university level, the Learning and Teaching Academic Standards (LTAS) Threshold Learning Outcomes for Science state that 'current scientific knowledge is both contestable and testable by further inquiry', and that 'scientific knowledge is dynamic'.

Part of the reason for the misconception that modern scientific knowledge is unchanging is that many textbooks present a misleading view of John Dewey's 'scientific method'. In *How we think*, Dewey contrasts empirical thinking and scientific thinking, giving an example of the latter as formulating ideas and testing those ideas using controlled experiments. Textbooks typically apply Dewey's 'scientific method' to astrophysics, in which there were major revisions of cosmological models from Earth-centric models to various sun-centric views of the solar system, and different understandings of gravity by Aristotle, Galileo, Newton and Einstein, amongst others. Each paradigm shift has been a major revision of pre-existing knowledge.

Since Dewey's scientific method was intended to be an example of the methods (plural) of science, it is incorrect for textbooks to present it as *the* scientific method.

The most recent example of this textbook scientific method is Einstein's general relativity, 100 years ago. The synthesis of new pharmaceuticals, advances in nanotechnology and genetic modification are all examples of discoveries of new knowledge, without necessarily displacing pre-existing knowledge.

A notable recent Australian exemplar of the textbook scientific method, involving the revision of pre-existing knowledge, is the 2005 Nobel Prize in Physiology or Medicine awarded to Marshall and Warren. Prior to their work, it was believed that bacteria could not survive in the stomach, and that stomach inflammation and ulcers were due to stress or lifestyle factors. Marshall and Warren showed that inflammation and ulcers were due to the bacterium *Helicobacter pylori*, and they could cure these diseases by killing the bacterium. Their discoveries rewrote medical textbooks. While the Marshall and Warren story is discussed in the biology sections of school science textbooks, it is not discussed as

an example of a scientific method. The textbook scientific method is outdated and divorced from modern reality.

A second shortcoming of the textbook scientific method has been discussed previously in this column (April 2012 issue, p. 39). Since Dewey's scientific method was intended to be an example of the methods (plural) of science, it is incorrect for textbooks to present it as *the* scientific method. The LTAS statements and Australian Curriculum are quite explicit about this, always referring to 'scientific methods' and the 'methods of science'. By promoting only one scientific method, textbooks implicitly devalue all other aspects of scientific endeavour.

Human endeavours are full of both human triumphs and human imperfections. The latter can include personal rivalries and jealousies, vested interests, political or religious ideologies and zealotries, and other frailties. While textbooks celebrate the triumph of Einstein's relativity as an improvement over Newtonian physics, the truth is that many in the scientific community did not accept relativity for many years. Einstein's first paper on relativity was published in 1905, his main papers on general relativity were published in 1915–17, and there was experimental verification in 1919 that the bending of light during a solar eclipse was consistent with general relativity and inconsistent with other theories. Einstein received 62 nominations for the Nobel Prize in Physics between 1910 and 1922, but was awarded the Nobel Prize only when the committee specifically excluded the work on relativity from consideration.

The idea of resistance to change was expounded by Kuhn in The structure of scientific revolutions. Even when a new, improved scientific idea has been put forward and verified, there is huge emotional and other investments in the older established idea that prevent or delay the acceptance of the new idea. Nuclear fission in the 1930s and 1940s provided undeniable evidence for relativity. Fictional works like Game of thrones are captivating and compelling because they show both human tribulations and human depravities. The stories of science are also filled with conflict of interest, human drama and intrigue. Even though 97-98% of the climate researchers most actively publishing in the field support the tenets of tenets of anthropogenic climate change, and the relative climate expertise and scientific prominence of the researchers unconvinced of anthropogenic climate change are substantially below that of the convinced researchers, there is still widespread resistance to and nonacceptance of anthropogenic climate change. Similarly, there is still significant resistance to evolution, even though it is accepted by most.

Perhaps students will be more interested in learning about science as a human endeavour, when that human endeavour is presented more realistically, warts and all.



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Accentuating the negative

I have been engaging in a mild bout of decluttering, and so browsing in the collection of old science books that are scattered on my bookshelves. Is the book a gem that gives me a glimpse of how chemistry was seen and done during the last 150 years, or is it junk that should go into the recycling bin? It might be available in a library or repository, where I could get it if I wanted it, but how would I know that it was interesting if I wasn't able to inspect it?

These thoughts were in my mind as I flipped through A class book of physical chemistry (1934) by T. Martin Lowry (Professor of Physical Chemistry at Cambridge) and Samuel Sugden (Professor of Chemistry at Birkbeck College of the University of London). Surely such luminaries - remember Brönsted-Lowry theory and Sugden's parachor (a long-forgotten function of molecular weight, surface tension and density of liquid and vapour) - would have something interesting to say to me.

If it appeared in modern digital communication, the term 'negative catalysis' would be seen as an example of 'click bait' ...

I found it in the chapter on 'The Mechanism of Chemical Change' and its section on negative catalysis. If it appeared in modern digital communication, the term 'negative catalysis' would be seen as an example of 'click bait' or at least the catchy headlines that one finds in British newspapers. A lure it might have been, but I was easily lured into reading a couple of pages that began with the confession that the substances under consideration are catalyst poisons. The example chosen by the authors to exemplify this phenomenon is the decomposition of hydrogen peroxide catalysed by colloidal platinum or by the enzyme haemase:

$$2H_{2}O_{2} \rightarrow 2H_{2}O + O_{2}$$

The concentrations (molar) of various catalyst poisons required to reduce the rate of decomposition to one-half are given in the following table.

Poison	Catalyst		
	Colloidal Pt	Haemase	
H ₂ S	3 × 10 ⁻⁶	1×10 ⁻⁶	
HCN	5 × 10 ⁻⁸	1×10^{-6}	
HgCl ₂	5 × 10 ⁻⁷	5 × 10 ⁻⁷	
Aniline	2 × 10 ⁻⁴	2.5×10^{-3}	
CO	Very poisonous	No poisoning	
HCl	3×10^{-4}	1 × 10 ⁻⁵	
HNO ₃	No poisoning	4×10^{-6}	

Many industrial processes depend on catalysis, the authors note, and since only very small amounts of poison are enough to reduce the effectiveness of catalysts and slow down the reactions, the raw materials need to be highly purified so as to remove all or most of any catalyst poison. The example they cite is the catalytic oxidation of sulfur dioxide over platinum, which is seriously affected by traces of arsenic in the sulfur or the pyrites from which the SO, was generated.

Now the argument got onto more familiar ground for me. In the old lead chamber process for production of sulfuric acid, in which nitrogen dioxide (we know now that it was mostly N₂O₂) was the oxidant, some arsenic oxide in the gas stream did not affect the reaction. This meant there was sometimes a little arsenic in the sulfuric acid, and where contaminated acid was used to accelerate the malting of the grain this arsenic ended

up in the beer and some heavy drinkers were poisoned. The contact process, as it was known, switched to vanadium pentoxide as catalyst for the oxidation reaction and sulfur dioxide from a purer source such as sulfur itself was required because even this catalyst was affected by arsenic.

I first heard the word 'vanadium' when I worked one summer in a sulfuric acid factory and, since it was a novelty, I took a little of the catalyst to my home laboratory for exploration. Boiling with dilute acid served to extract a little vanadium from the carrier material and I got a yellow solution containing V5+ ions. A piece of zinc metal added to the solution was sufficient to reduce the vanadium cations and I saw the succession of colours - blue (V4+), green (V3+) and finally



V5+, V4+, V3+, V2+.

violet (V2+) - that assured me that it was indeed vanadium that I had met for the first time.

All these years later, it was a comfort to me to know that Sugden's first published paper (1921) was about reduction by metals in acid solution, even though he was reducing ferric ions and not the more exotic vanadium. His second was about the determination of surface tension by the rise of a liquid in a capillary tube and this, of course, led on to the parachor.



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cryptic chemistry

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1 2 3 4 5 6 7 8 9 10 10 12 12 12 13 14 15 15 15 15 17 16 17 17 17 19 20 20 20 24 24 24 25 26 10 26 10 26 10 26 10

Across

- 9 Mexico went carbonless to produce R₂C=NOH. (5)
- 10 & 17 Across Incisive steps see transformation of individuals that can only survive within a narrow range of environmental conditions. (9,7)
- **11** Revolutionary film for one of us. (7)
- **12** Os, O_3 and O_8 . (7)
- **13** Vitamers of vitamin A concerning tin oxide papers. (9)
- **15** Sulfur, lithium and sodium are over *N*-phenyl imines. (5)
- 16 Throw boot, Spooner. That burns! (7)
- 17 See 10 Across.
- **18** Finally, the corn to ethanol conversions are 14 Down with aldehydes or ketones. (5)
- **19** Expert, and yet lens shot emission of sulfur and C₂H₂. (9)
- 21 Lines of muddy carpets. (7)
- 23 Closers break methylphenols. (7)
- **25** $C_4H_4S = 9053815210.$ (9)
- 26 53: agreement is optimal. (5)

Down

- 1 Agree to take in dog. (6)
- **2 & 24 Down** Vulnerable and completely unresolved. (4,4)
- 3 Allocates names. (10)
- 4 Sulfur analogues of RN=C=O are singularly 6 Down as chocolate melts emitting chlorine. (15)
- **5** Variance in scenic tones is fluctuating. (15)
- 6 Insignificant two elements. (4)
- 7 $C_5H_{11}N/I_2/Ne$ ripped open. (10)
- 8 Carries on with 15681416 and what is proposed for 117. (8)
- 14 Readily interconvert with a constitutional isomer from titre.com.au! (10)
- **15** CH_3CO nice about something to do with 19 Across. (10)
- **16** Coal tar distillate 67576852. (8)
- 20 Included in Type A Silylmetalation without difficulty. (6)
- 22 Kind characters in print. (4)
- 24 See 2 Down.

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



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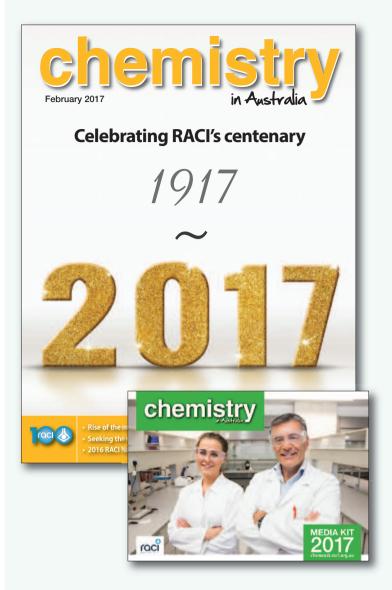
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