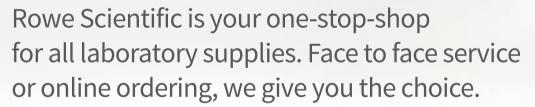




- Introducing chemical education highlights
- Brynn Hibbert, IUPAC Analytical Division representative
- Australia's chemical industries: a social network analysis



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# chemistry in Australia

## **January/February 2019**





#### cover story

#### Chemical evolution: the 2018 Nobel Prize in Chemistry

Darwin's concept of evolution revolutionised biology some 150 years ago and remains a central paradigm of biology. This year's Nobel Prize in Chemistry recognises the application of evolutionary principles at the molecular level, directing molecules to rapidly evolve useful functions.

14

#### 20 The life of Brynn

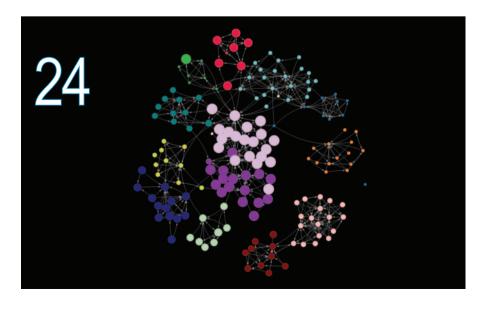
In this International Year of the Periodic Table, Dave Sammut and Chantelle Craig profile Australia's representative to the IUPAC Analytical Division, Emeritus Professor Brynn Hibbert.

#### 24 Networks, workforce development and resilience

Industry networks are surprisingly fragile, and Australia's chemical industries are no exception. Tom Spurling and colleagues explain the importance of social network analysis.

#### 28 Profile: Mapping molecules

A scientist once told me that identifying the optimal interaction between molecules is like finding a needle in a haystack. Professor Brian Smith is an expert at just that.



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chemaust.raci.org.au

#### Highlighting chemistry education research

It was with great pleasure that I accepted the invitation to contribute the guest editorial for this issue. I am particularly excited to be the instigator and editor of the new Chemistry Education Research section of the magazine (p. 12). Chemistry education as a research field has been growing in Australia for some time. Recently, this area has enjoyed increased interest from not only established chemistry researchers, but also students undertaking honours and postgraduate studies in chemistry education. One potential benefit I can see from this exposure is the opportunities for collaboration between chemistry education researchers and chemistry researchers, which can benefit all parties involved. These opportunities can yield exciting outcomes for chemistry education researchers, chemistry researchers and students undertaking studies in chemistry – an example of which I will share.

During my honours year in chemistry education, I found the combination of teaching and research thrilling, and went on to complete PhD studies in chemistry education at the University of Tasmania. In parallel, I undertook a Graduate Diploma of Education (Senior Years) at the Queensland University of Technology. During this time, I also taught at both the University of Tasmania and a local high school. Despite the differences between teaching in secondary and tertiary institutions, I saw that linking of the educational content with aspects of chemistry research was particularly successful in engaging students across both environments. This is by no means a new concept but one that we should regularly revisit as the needs and interests of our students continually change. With these issues in mind, the placement of Chemistry Education Highlights beside the chemical science research section of Chemistry in Australia recognises the mutual benefits between research in chemistry education and chemical science. Research exploring how we teach chemistry can benefit disciplinary chemistry itself, and vice versa.

During my PhD studies at the University of Tasmania, I explored the development of new chemistry laboratory experiments to better prepare students for postgraduate study. One of these, involving a cross-coupling reaction, allowed students to investigate a variety of concepts and develop a number of core skills across synthetic and analytical chemistry.

Ultimately, this experiment provided a novel approach to examining key principles of the palladium-catalysed Suzuki–Miyaura reaction in the undergraduate laboratory (Pullen R., Olding A., Smith J.A., Bissember A.C. *J. Chem. Ed.* 2018, doi: 10.021/acs.jchemed.7b00964). During early iterations, staff and students observed that aryl iodides exhibited very poor reactivity compared to the corresponding bromides. A follow-up study led by Dr Alex Bissember (which also featured undergraduate researcher Angus Olding) determined that this phenomenon derived from the unexpected poor turnover of a fundamental palladium species on the active catalytic cycle (Ho C.C., Olding A., Smith J.A., Bissember A.C. *Organometallics* 2018, vol. 37(11), pp. 1745–50).

This recent example reflects that research in chemical science and chemistry education go hand in hand. Further support for this important relationship may take the form of reinforcing and promoting greater recognition of the value of educating future chemists, in addition to inspiring students by presenting them with engaging examples of chemistry research. As experts in our fields, it is essential that we continue to improve approaches to educating future generations of scientists, and disseminating and sharing research in this area is a key step towards these aspirations.

I invite RACI members and readers of this magazine to contact me to share summaries of your recently published articles that are consistent with the scope of Chemistry Education Research. The guidelines, including contact information for submissions, appear with the new section on p. 13.



Reyne Pullen MRACI CChem is currently working as a postdoctoral research fellow at the University of New South Wales, where he is contributing to the significant redevelopment and redesign of the first-year chemistry curriculum. He has previously undertaken chemistry education research at Monash University and the University of Tasmania, and participated in various science communication and outreach activities in Tasmania.



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Contributors' views are not necessarily endorsed by the RACI, and no responsibility is accepted for accuracy of contributions. Visit the website's resource centre at chemaust.raci.org.au for information about submissions.

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#### Judging evidence

In the Sept/Oct issue of *Chemistry in Australia*, I received special mention as one of those nasty experts who give expert witnesses a bad name. Not only that, I had previously been attacked by four judges of the Supreme Court of New South Wales for being a bad expert witness, so my reputation is legally in tatters. Previously, I had been an associate professor in physics for many years but had just retired so my reputation in legal circles didn't actually matter to me. Since then, I have published about 120 scientific papers as an honorary member of staff, so my reputation has been partly restored by the physics community. It was never actually in doubt, until those four judges decided to examine my physics.

One of the rules of the legal system in Australia and elsewhere is that expert witnesses are not allowed to express an opinion in court that is outside their field of expertise. It is a perfectly reasonable rule. However, one of the failings of the legal system is that members of the legal profession are entitled to express opinions about scientific matters even if they know nothing about the subject. As a result, some very strange opinions are often expressed in court, and some ill-informed decisions are often handed down. Nevertheless, if a judge of the Supreme Court hands down a decision, then it is usually taken as gospel, unless someone decides to appeal. In my case there was no appeal, so there the matter has stood.

Legal experts around the country often quote my case as an example of bad science, and it still pops up now and then even in odd places such as *Chemistry in Australia*. It happened enough times that I wrote an article in the *Australian Journal of Forensic Sciences* in December 2014 (pp. 368–82). It is called 'Misinterpretation of expert evidence'. I listed six or seven examples where the judges got it wrong. They even said that Newton's first law of motion cannot be correct, although they used different words to say so. There was not enough space in the article to list all of their mistakes. I counted 170 of them in their judgement.

More recently, one of the judges decided that my measurement of the width of female shoulders was invalid. I measured 16 of my students and they were all about 40 centimetres across the shoulders. However, the judge ruled that I shouldn't have done that because I didn't have the qualifications. Apparently, a PhD in physics does not qualify a person to use a ruler, at least in New South Wales. I gave evidence in court that a woman 40 centimetres across the shoulders could not enter a 30-centimetre wide hole head first and at high speed without serious injury to her shoulders. A medical expert confirmed my opinion. But it was my unqualified use of the ruler that irked the judge.

The Sept/Oct article refers to a complaint that I did not notify the police of a mistake in the landing spot. That was one of the 170 mistakes made by the judges. It was the police who notified me that they misidentified the landing spot, so I needed to repeat all my measurements and calculations.

**Rod Cross** 

#### Call to RACI citizens

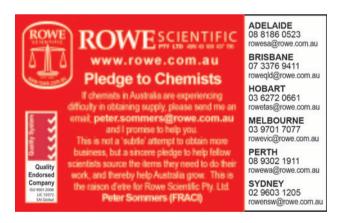
The RACI needs to be involved with the wider community. I suggest a citizen science project (citizenscience.org.au).

While writing an article on a way of jazzing up the relevance of some dry physical chemistry I selected the topic of fragrances. This led to a revelation as to the constipation in Australia's regulatory regimes in dealing with products perfumed with Huon pine (100%).

Its major fragrant component, methyl eugenol, had been tested (among many) by Doug Waterhouse at CSIRO during World War II as a probable insect repellent for our troops in the tropics. It worked wonderfully as a repellent but had to be discarded because of its toxicity (csiropedia.csiro.au/aerogard).

Now 100% Huon-pine-stuffed teddy bears are sold to the unsuspecting public and apparently also to unsuspecting regulators (of which there is a multitude, both federal and state). Given that products are advertised and sold on the internet, we RACI citizens need to monitor the markets for non-acute chemical safety issues. Read labels and adverts, use your knowledge of chemistry to check for more information, find the relevant enforcement authority (good luck), and have all this assessed and collated, with the results publicised in *Chemistry in Australia*.

Ben Selinger FRACI CChem



#### Pushing 'print' on large-scale piezoelectric materials

Researchers have developed a revolutionary method to 'print' large-scale sheets of two-dimensional piezoelectric material, opening new opportunities for piezo-sensors and energy harvesting (*Nature Communications*, doi: 10.1038/s41467-018-06124-1).

Importantly, the inexpensive process allows the integration of piezoelectric components directly onto silicon chips. Until now, no 2D piezoelectric material has been manufactured in large sheets, making it impossible to integrate into silicon chips or use in large-scale surface manufacturing.

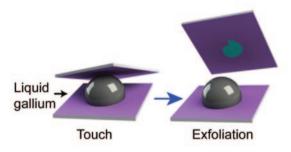
This limitation meant that piezo accelerometer devices – such as vehicle air-bag triggers or the devices that recognise orientation changes in mobile phones – have required separate, expensive components to be embedded onto silicon substrates, adding significant manufacturing costs.

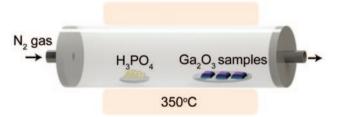
Now, FLEET researchers at RMIT University in Melbourne have demonstrated a method to produce large-scale 2D gallium phosphate sheets, allowing this material to be formed at large scales in low-cost, low-temperature manufacturing processes onto silicon substrates, or any other surface.

Gallium phosphate (GaPO<sub>4</sub>) is an important piezoelectric material commonly used in pressure sensors and microgramscale mass measurement, particularly at high temperatures or in other harsh environments.

'As so often in science, this work builds on past successes', lead researcher Professor Kourosh Kalantar-zadeh explains. 'We adopted the liquid-metal material deposition technique we developed recently to create 2D films of GaPO<sub>4</sub> through an easy, two-step process.'

Kalantar-zadeh, now Professor of Chemical Engineering at University of New South Wales, led the team that developed the





Upper: van der Waals 2D printing of  ${\rm Ga_2O_3}$  nanosheet from liquid metal gallium. Lower: chemical vapour phase reaction system for transforming  ${\rm Ga_2O_3}$  to  ${\rm GaPO_4}$  nanosheets.

new method while Professor of Electronic Engineering at RMIT University. The work was materialised as a result of significant contribution from RMIT's Dr Torben Daeneke and extreme persistence and focus shown by the first author of the work, PhD researcher Nitu Syed.

The revolutionary new method allows easy, inexpensive growth of large-area (several centimetres), wide-bandgap, 2D  ${\rm GaPO}_4$  nanosheets of unit cell thickness. It is the first demonstration of strong, out-of-plane piezoelectricity of the popular piezoelectric material.

The two-step process is:

- exfoliate self-limiting gallium oxide from the surface of liquid gallium made possible by the lack of affinity between oxide and the bulk of the liquid metal
- 'print' that film onto a substrate and transform it into 2D GaPO4 by exposure to phosphate vapour.

The new process is simple, scalable, low-temperature and cost effective, significantly expanding the range of materials available to industry at such scales and guality.

The process is suitable for the synthesis of free-standing GaPO<sub>4</sub> nanosheets. The low-temperature synthesis method is compatible with a variety of electronic device fabrication procedures, providing a route for the development of future 2D piezoelectric materials.

This simple, industry-compatible procedure to print large surface area 2D piezoelectric films onto any substrate offers tremendous opportunities for the development of piezo-sensors and energy harvesters.

Piezoelectric materials are materials that can convert applied mechanical force or strain into electrical energy. Such materials form the basis of sound and pressure sensors, embedded devices that are powered by vibration or bending, and even the simple 'piezo' lighter used for gas barbecues and stovetops.

Piezoelectric materials can also take advantage of the small voltages generated by tiny mechanical displacement, vibration, bending or stretching to power miniaturised devices.

Gallium phosphate is a quartz-like crystal used in piezoelectric applications such as pressure sensors since the late 1980s, and particularly valued in high-temperature applications. Because it does not naturally crystallise in a stratified structure and hence cannot be exfoliated by conventional methods, its use to date has been limited to applications that rely on carving the crystal from its bulk.

Test materials were synthesised in RMIT's Micro Nano Research Facility by using van der Waals exfoliation followed by a chemical vapour phosphatisation. Measurements included piezo-force microscopy, which confirmed a high out-of-plane piezoelectric coefficient of 8–10 pm/V, confirmed by density functional theory calculations. This is sufficiently high to provide promise in 2D-material based piezotronic sensing and energy harvesting.

ARC Centre for Excellence in Future Low-Energy Electronics Technologies

#### Ezio Rizzardo Polymer Scholarship

The inaugural Ezio Rizzardo Polymer Scholarship has been awarded to Queensland University of Technology student Naomi Paxton.

The scholarship acknowledges the potential impact of an outstanding PhD candidate in polymer science or engineering. It provides \$10 000 per year over three years, plus a \$5000 travel fund.

It has been established to honour Professor Ezio Rizzardo AC FRS FRACI CChem FTSE FAA, one of Australia's pre-eminent polymer scientists and a major contributor to the science and management of the CRC for Polymers during its 22-year life. The scholarship is open to domestic students at one of the 14 participant universities of the former CRC.

Paxton impressed the selection committee with her academic record and involvement in STEM outreach activities.

Committee chair, Dr Peter Coldrey FTSE, said Paxton had not only demonstrated excellence in her undergraduate degree but had presented a research proposal with the potential to make a high-impact contribution to both polymer science and engineering.

'Naomi also clearly demonstrated her ability to communicate her scientific ideas and accomplishments to a broad audience. She is a worthy winner.'

At QUT, she received both a Science and Engineering Dean's Scholarship and a Vice-Chancellor's Academic Scholarship in 2012, completing her BAppSci, majoring in physics and mathematics, in just 2.5 years.

In 2015, she was one of 20 students internationally to complete the Dual International Biofabrication Masters degree, combining her background in physics with polymer chemistry, engineering, biology and materials science.

She completed two highly successful research projects, melt electrospinning polycaprolactone scaffolds for bone regeneration and optimising hydrogel formulations for bioprinting cartilage.

Her research applies principles in polymer science in 3D printing and works closely with industry partner, Melbourne-based medical device company Anatomics to explore the fabrication of high-density, polyethylene, patient-specific surgical implants.

She has been a committed STEM ambassador and science communicator, involving herself in STEM engagement activities since 2012. Since 2013, she has presented at five conferences.

Members of the CRC for Polymers agreed to contribute a substantial sum to establish the scholarship. It is administered by the Australian Academy of Technology and Engineering and the selection committee comprises Academy Fellows who are polymer specialists.

Australian Academy of Technology and Engineering

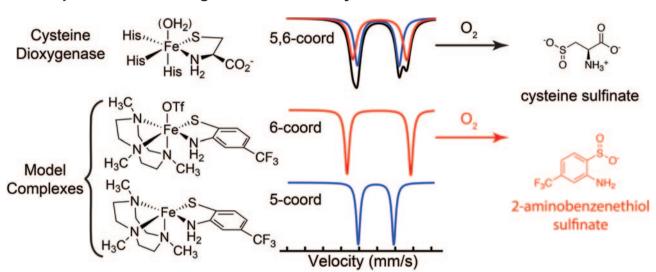




# Kicking goals: the first highly enantioselective application of the deoxy-Breslow intermediate

The Breslow intermediate is prominent in many organocatalytic reactions. Limitations of the Breslow intermediate have prompted investigation into related species and led to the discovery of the deoxy-Breslow intermediate. While this intermediate has been implicated in new transformations, until recently it had not been used to generate highly enantioenriched products. Now, Lydia Scott, Yuji Nakano, Changhe Zhang and David Lupton at Monash University have uncovered the utility of the deoxy-Breslow intermediate in the highly enantioselective cyclisation of electron-deficient 1,5-dienes (Scott L., Nakano Y., Zhang C., Lupton D.W. *Angew. Chem. Int. Ed.* 2018, **57**, 10 299–303). This transformation was applied to 17 dienes and allowed the synthesis of enantioenriched, highly functionalised cyclopentenes in excellent yields (all >65%) and with good enantioselectivity

#### Better picture of binding in essential enzyme



Cysteine dioxygenase is an enzyme important in cysteine homeostasis. The octahedral ferrous iron is coordinated by three histidine residues from the protein and is chelated by the cysteine substrate via the thiol and amine, leaving the last coordination site free for dioxygen to bind. Previous studies by the Jameson group, now based at Bio21 at the University of Melbourne, produced Mössbauer spectra suggesting that this

free site is actually partially occupied by a water molecule, contrary to related enzymes. Collaborating with researchers from Johns Hopkins University, USA, the Jameson group has now confirmed that water partially occupies the dioxygen site but does not appear to prevent dioxygen binding (Gordon J.B., McGale J.P., Prendergast J.R., Shirani-Sarmazeh Z., Siegler M.A., Jameson G.N.L., Goldberg D.P. J. Am. Chem. Soc. 2018,

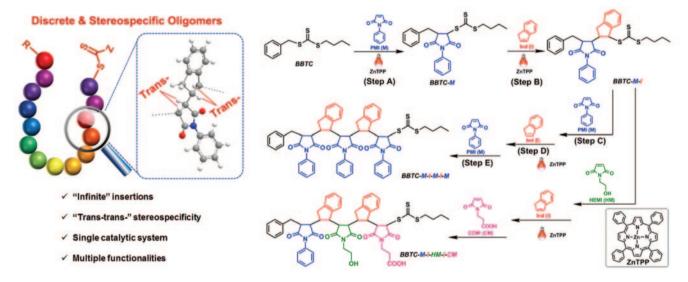
**140**, 14 807–22). The team achieved this new insight by comparing the spectroscopic signals of the protein with small molecule complexes that mimic the coordination geometry. In contrast to the enzyme, the complexes could sulfinate an unnatural substrate

(2-aminobenzenethiol), showing the importance of correct coordination to the iron centre.

#### Discrete and stereospecific oligomers as natural biopolymer mimics

Natural biopolymers such as DNA and proteins have uniform microstructures with defined molecular weight, precise monomer sequence, and stereoregularity along the polymer main chain, which endows them with unique biological functions. Mimicking natural biopolymers, Jiangtao (Jason) Xu and co-workers at the University of New South Wales and their collaborators from the Australian National University, CSIRO, University of California, Santa Barbara, USA, and Nagoya University, Japan, recently established a new method to prepare discrete and stereospecific oligomers using sequential and alternating photoinduced RAFT single-unit monomer insertion (Photo-RAFT SUMI) (Huang Z., Noble B.B., Corrigan N., Chu Y., Satoh K., Thomas D.S.,

Hawker C.J., Moad G., Kamigaito M., Coote M.L., Boyer C., Xu J. J. Am. Chem. Soc. 2018, 40, 13392–406). This technique employs two families of cyclic monomers, indene and N-substituted maleimide, which can be inserted into RAFT agents alternately, one unit at a time, allowing the monomer sequence to be controlled through sequential and alternating monomer addition. Meanwhile, the stereochemistry of cyclic monomer insertion into the RAFT agents is trans-selective along the main chain due to steric hindrance from the repeating monomer units. This study demonstrates the concept of using synthetic polymers to reproduce structurally perfect natural polymers in order to understand the mechanism of specific functions.

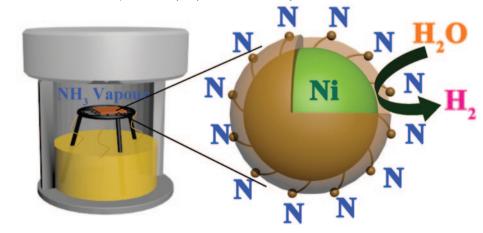


#### Nickel-heteroatom bridge sites boost hydrogen fuel generation

Water electrolysis is one of the simplest approaches for hydrogen fuel production and so developing good hydrogen evolution reaction (HER) catalysts is critical for large-scale hydrogen generation. Metallic nickel-based materials are known to exhibit excellent electrocatalytic water electrolysis activity. However, the strong interaction between adsorbed H\* and metallic nickel leads to poor reaction kinetics. Recently, a team led by Chuan Zhao at the University of New South Wales developed a controllable surface modification approach to tune the H\* adsorption behaviour on metallic Ni via the formation of Ni-heteroatom (N or S) bridge sites (Li Y., Tan X., Chen S., Bo X., Ren H., Smith S.C., Zhao C. Angew. Chem. Int. Ed. 2018, https://doi.org/10.1002/

anie.201808629). A mechanistic study revealed that the strong electronegativity of heteroatoms such as nitrogen can result in electron transfer from Ni to N. Thus, fewer electrons localised on Ni sites closest to the adsorbed N atom leads to weaker H adsorption on Ni(111)

and enhanced HER activity. This research not only provides a promising way to realise notable HER performance based on metallic Ni, but also sheds light on the crucial role of heteroatom surface modifications at active bridging sites in water electrolysis.



#### Cryptic chlorination in biosynthesis

Marine microorganisms have evolved vanadium-dependent chloroperoxidase (VCPO) enzymes that are capable of oxidising chloride anions in the ocean into an electrophilic source of 'Cl+'. This allows chlorine to be introduced into organic molecules in the biosynthesis of chlorinated natural products. Recent work conducted by researchers at the University of Adelaide and the Scripps Institution of Oceanography, USA, has shown that marine *Streptomyces* bacteria also use VCPO enzymes to oxidise

aromatic ring systems by cryptic chlorination in the biosynthesis of the naphterpin and marinone families of meroterpenoid natural products (Murray L.A.M, McKinnie S.M.K, Pepper H.P., Erni R., Miles Z.D., Cruickshank M.C., Lopez-Perez B., Moore B.S., George J.H. *Angew. Chem. Int. Ed.* 2018, **57**, 11 009–14). The biosynthetic sequence is initiated by VCPO-mediated oxidative dearomatisation and dichlorination, followed by an  $\alpha$ -hydroxyketone rearrangement.

Subsequent loss of chloride-anion leaving groups allows the formation of a highly oxidised naphthoquinone core. The entire biosynthetic pathway was mimicked in biomimetic total syntheses of 7-demethylnaphterpin and debromomarinone. Several proposed biosynthetic intermediates were also synthesised and used as substrates and synthetic standards to help elucidate the function of two new VCPO enzymes, MarH1 and MarH3, that initiate marinone biosynthesis.

## Stories from the Periodic Table

Do you have a story connected to a certain element?

1 <b>H</b>																	He
3 <b>Li</b> 6941	Be 9.012											5 <b>B</b>	6 C	7 <b>N</b>	0	F 18.00	Ne 20.10
Na 22.90	Mg					7						13 <b>AI</b> 26.90	14 Si 28.09	15 P 20.97	5 S 2 8	CI 25.45	Ar 22.95
19 <b>K</b>	Ca	Sc 44.86	722 Ti	23 <b>V</b> 50:54	Cr	Mn	26 Fe	Co	28 Ni 58.70	Cu	Zn	Ga	32 Ge	As 74.82	Se	35 Br	36 <b>Kr</b>
37 <b>Rb</b>	38 Sr	39 <b>Y</b>	Zr	Nb	Mo	TC	Ru	Rh	46 Pd	Ag	48 Cd	In	\$n	51 Sb	Te	53   126.90	Xe
55 Cs	56 Ba	57-71	72 <b>Hf</b>	73 Ta	74 W	75 Re	76 Os	77  r 192.2	78 Pt	79 <b>Au</b>	Hg	81 TI 2014	Pb	83 Bi	₽°o	Åt	к̈́n
Fr	ĸa	89-103	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Č'n	Nh	FI	Mc	Lv	Ts	Ög
			La	58 Ce	59 Pr	Nd	Pm	Sm	Eu	<b>d</b> Gd ₃	Tb	66 <b>Dy</b>	67 Ho	68 Er	Tm	70 Yb	71 Lu 175.0
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Round	Submissions Close	Best Story Winner Announced	Audience Poll	Audience Poll Winner Announced	
1	15 December 2018	8 March 2019	April 2019	19 April 2019	
2	31 March 2019	7 June 2019	July 2019	19 July 2019	
3	30 June 2019	6 September 2019	October 2019	18 October 2019	
4	30 September 2019	15 November 2019	-	-	

Whether it's from your work, studies or everyday life, the RACI wants to hear your personal connection to this element.

Over the course of the International Year of the Periodic Table in 2019, the RACI will publish these stories on the RACI website and social media to highlight the personal connections that people have to science, and to chemistry.

Story submissions will be accepted in four rounds. Each round will feature a best story, as well as an audience favourite story (excepting round four (4)).

Submissions from residents in Australia or New Zealand will be entered into a competition for the chance to meet and mingle with the leadership in Australian chemistry at the RACI National Awards Dinner in November 2019. The winners will also have their stories and/or biographies published in Chemistry in Australia and will each receive a copy of A Century of Bonds.

Submissions in text (up to 500 words) or video (up to four minutes) will be accepted and are to be sent to communications@raci.org.au.

For full competition details visit raci.org.au

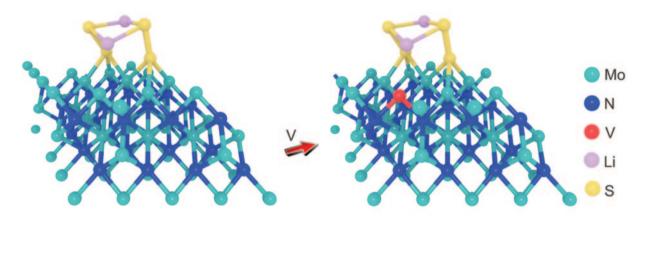


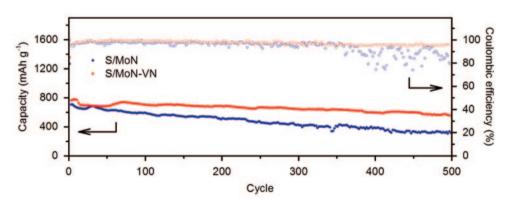
#### 2D materials for better lithium-sulfur batteries

Lithium-sulfur batteries hold great promise for next-generation energy storage. But they suffer from rapid capacity decay. The chemical interactions between the sulfur host and polysulfides in these batteries are also poorly understood at the atomic level, impeding improvements in battery performance. Recently, a team led by Shizhang Qiao from the University of Adelaide and Haihui Wang at South China University of Technology, China, reported the fabrication of a novel 2D MoN-VN

heterostructure as a model sulfur host in lithium–sulfur batteries with improved capacity decay characteristics (Ye C., Jiao Y., Jin H., Slattery A.D., Davey K., Wang H., Qiao S.-Z. *Angew. Chem. Int. Ed.* 2018, https://doi.org/10.1002/anie.201810579). The researchers used calculations to show that the electronic structure of MoN can be tailored by incorporating vanadium, leading to enhanced polysulfide adsorption compared with 2D single-component MoN. Furthermore, they used in situ

synchrotron X-ray diffraction and electrochemical measurements to reveal efficient regulation and utilisation of the polysulfides in the MoN–VN heterostructure. The MoN–VN-based lithium–sulfur battery had a slow capacity decay of 0.068% per cycle over 500 cycles. This research provides insight into the mechanism of polysulfide adsorption in a heterostructured sulfurhost material and is expected to stimulate further development of hybrid materials for energy storage.



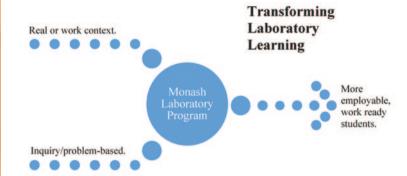


Compiled by **David Huang** MRACI CChem (david.huang@adelaide.edu.au). This section showcases the very best research carried out primarily in Australia. RACI members whose recent work has been published in high impact journals (e.g. *Nature*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*) are encouraged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



Alchemy is often thought of as a mis-step on the journey to modern chemistry. Contrary to this view, alchemy led to a number of important developments still relevant today, such as metal extractions, purification by distillation, and the invention and development of gunpowder. Chinese alchemists applied a proto-scientific method of trial and error to the development of blends of honey, potassium nitrate and sulfur. These mixtures were observed to burn with intense heat and flame, and ultimately led to the development of modern gunpowder formulations. Researchers at the University of Tasmania have set out to refine and formalise the deflagration (rapid combustion without detonation) of an early form of gunpowder for the purposes of a chemical demonstration (Wolfenden A.V., Kilah N.L. J. Chem. Ed. 2018, 95, 1350-3). This demonstration is intended as a suitable starting point for discussions to challenge student understanding and preconceptions of the role of alchemy in the history of chemistry, and specifically on the development and refinement of gunpowder. The deflagration is highly visually appealing and was very well received by the over 400 attendees of the RACI Tasmanian Branch event 'The Chemistry of Fireworks'.

#### **Transforming laboratory learning**



Recipe-based teaching laboratories, where students simply follow a given set of instructions are known for invoking little critical thought and have yet to been shown to help students learn theoretical concepts. To address this, the use of inquiry (i.e. where students answer questions rather than simply following steps) and contextualisation (i.e. connecting the material to real-world or industrial settings) is increasingly being used, with many examples existing in chemistry and beyond. However, it is unusual for this approach to be used across an entire chemistry program within a university. Current research at Monash University (George-Williams S.R., Soo J.T., Ziebell A.L., Thompson C.T., Overton T.L. Chem. Educ. Res. Pract. 2018, https://doi.org/10.1039/C7RP00233E) is tracking the effect of updating a large number of teaching laboratories over all year levels throughout all chemistry courses. It was found that students: (a) found the new experiences less easy and more challenging, (b) recognised the increased use of inquiry and context, (c) were less dependent on the laboratory manual, and (d) enjoyed the new laboratories for a large variety of reasons (e.g. real-world context or student driven). Further research is currently being undertaken into the overall effect of these changes on the students' readiness for the workforce.

## Are we preparing our chemistry undergraduates for career success?

How can we ensure chemistry graduates are best prepared to gain employment and succeed at work? Research shows that in addition to their scientific knowledge, graduates will need to both possess and be able to articulate a wide range of 'generic' skills. These include communication, teamwork, problemsolving, critical thinking, organisational, numeracy, adaptability, independent learning, computer/IT, commercial awareness and creativity/innovation. However, do chemistry students think they are gaining these skills at university

and do they recognise their importance?

Last year, research at Monash University and University of Warwick (UK) asked almost 1000 chemistry undergraduates, through open-ended questions, which skills they've developed during their degree and that employers are seeking (Hill M.A., Overton T.L., Thompson C.D., Kitson R.R.A., Coppo P. Chem. Educ. Res. Pract. 2018, doi: 10.1039/C8RP00105G). On average, students identified three skills from among laboratory, communication, thinking/problem-solving,

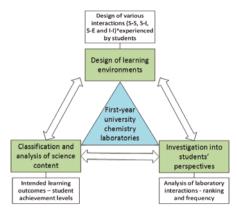


organisational/time management and teamwork, as both developed and valued by employers. However, they were unlikely to name any other skills. The researchers concluded that there was a need for better communication to chemistry undergraduates about the wide range of skills they are developing during their degree and/or to incorporate more skill-rich activities in the curriculum.

#### Characterising interactions in science laboratories

Laboratory classes are environments with a high degree of interactions and are an essential component of chemistry degree programs. The level and types of interactions experienced by students during laboratory classes influence the effectiveness of their learning. To better understand how these interactions influence learning, researchers at Curtin University have developed instruments to capture students' interactions with their environment (Wei J., Mocerino M., Treagust D.F., Lucey A.D., Zadnik M.G., Lindsay E.D., Carter D.J. Chem. Educ. Res. Pract. 2018, 19, 1186-98). A pre-lab survey was used to collect information

about students' expectations and ranking of the types interactions they would experience, while a post-lab survey was used to capture students' perspectives of the frequency of interactions experienced. The data was sorted into three levels of student achievement in order to relate students' responses with their laboratory grades. In the pre-lab survey, students ranked interactions with instructors as most important for their learning, while in the post-lab survey, they reported the most frequent interactions were between students. Furthermore, high-achieving students participated in interactions with other

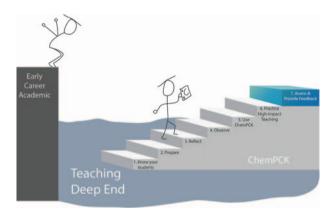


students and instructors more than weaker students. The team believe that findings from this study can help to improve laboratory curriculum and classroom design.

#### Pedagogical content knowledge

How do experts teach NMR spectroscopy or quantum mechanics? What strategies are best to help students understand the mole concept, acids and bases or curved arrows for organic mechanisms? Two studies of Teacher Professional Knowledge and Skill, including pedagogical content knowledge (PCK), published by Madeleine Schultz and Gwen Lawrie, elucidate how tertiary chemistry teachers help students understand these complex topics. PCK includes the choice of effective examples, representations and assessment for particular ideas, together with an understanding of student difficulties (see September 2014, p. 38, and August 2016, p. 24). During workshops held around Australia, insights, including participants' knowledge about their students' thinking, their teaching approaches and the variety of teaching strategies they use were collected (Schultz M., Lawrie G.A., Bailey C.H., Dargaville B.L. Chem. Educ. Res. Pract. 2018, 19, 508-19)

Over 300 teaching strategies were collated into an accessible, searchable database (chemnet.edu.au/chem-pck). RACI members are encouraged to adopt and adapt these strategies in their own teaching; new contributions are invited. Seven Steps to Transform Teaching are also available with detailed information on how academics can improve their teaching.



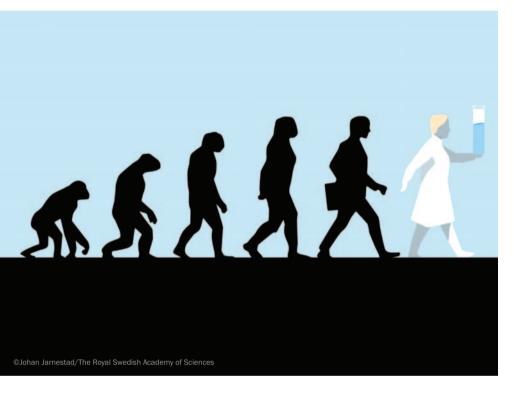
Interviews with ten expert chemistry teachers revealed their strategies for teaching specific topics (Lawrie G.A., Schultz M., Bailey C.H., Dargaville B.L. *Chem. Educ. Res. Pract.* 2018, doi: 10.1039/C8RP00187A). Common characteristics of experts included:

- seeking and receiving feedback from students;
- · encouraging active learning;
- focusing on concepts while reducing content;
- developing classroom strategies from experience; and
- purposeful reflective practice and a willingness to adapt.

  The findings of these two studies can inform professional development, particularly for those new to tertiary teaching.

Compiled by **Reyne Pullen** MRACI CChem (r.pullen@unsw.edu.au). This section showcases exciting chemistry education research carried out primarily in Australia. RACI members whose recent work has been published in prominent chemistry education journals (e.g. *Chem. Educ. Res. Pract., J. Chem. Educ., J. Res. Sci. Teach.*) are encouraged to contribute general summaries, of no more than 200 words, and an image to Reyne.

# Chemical evolution



The 2018 Nobel Prize in Chemistry

BY PETER KARUSO

Darwin's concept of evolution revolutionised biology some 150 years ago and remains a central paradigm of biology. This year's Nobel Prize in Chemistry recognises the application of evolutionary principles at the molecular level, directing molecules to rapidly evolve useful functions.

n the night of 10 December 2018 in Stockholm Sweden, half of the Nobel Prize in Chemistry was awarded to Frances H. Arnold (Caltech, USA) 'for the directed evolution of enzymes' and the other half was shared between George P. Smith (University of Missouri, USA) and Sir Gregory P. Winter (Cambridge, UK) 'for the phage display of peptides and antibodies'. Arnold was the first to artificially direct the evolution of enzymes and Smith and Winter developed 'phage display' for the directed evolution of antibodies, both harnessing the power of evolution for the benefit of chemistry.

## Directed evolution of catalysis and affinity

In biology, most proteins perform either a catalytic (e.g. enzymes) or an affinity (e.g. antibodies, receptors, carrier proteins) role. The proteins bind to either a ground state (affinity) or a transition state (enzyme) of another molecule, but it is essentially a recognition process. All these proteins have been shaped by evolution over the past 3.7 billion years (or so). In fact, there is no better place to see evolution at work than in the protein sequences of ubiquitous proteins such as the FK506 binding proteins (BMC Dev. Biol. 2018, vol. 18, p. 7). Gradual changes over geological timescales have led to all the species we see on Earth today. But, clearly, this process is too slow to produce catalysts for new reactions at the rates we need to find them to stoke the fires of industry or to find that magic cure for a sick relative.

The idea of 'directed evolution' of proteins was first proposed by Manfred Eigen as a theoretical idea. From 1953, he worked at the Max Planck Institute and became its Director in 1964. He received a Nobel Prize in Chemistry with Ronald Norrish and George Porter for the study of ultrafast reactions in 1967. The following year he turned his attention to the problem of self-organisation of matter and the evolution of biological macromolecules, and in 1984 proposed a method for the direct evolution of enzymes (Pure Appl. Chem. 1984, vol. 56, p. 967). He reasoned that it would be impossible to find improved variants of an enzyme in random libraries. The average protein has 250 amino acids, and if only 100 are 'mutated' that would be a library of 20100 members. So many, in fact, that there is not enough matter in the universe to make even one molecule of each. Instead, Eigen proposed several generations of mutagenesis and screening and predicted that it would be possible to evolve molecules to produce optimised enzymes.

An alternative, of course, is not to make the library but to model them in silico, as it were. This was proposed by a scientist at Genex Corp also in 1984 (World Biotech. Rep. 1984, vol. 2, p. 233) - Robert C. Ladner. Ladner went on to found Protein Engineering Corp. where he patented a way to facilitate the 'directed evolution of novel binding proteins' (US6979538B2) by encoding the library in bacteriophage and expressing these on their surface and then separating the binding phage and introducing errors in the DNA to evolve the best binding variants.

#### Frances H. Arnold



Frances Hamilton Arnold was born on 25 July 1956 in Pittsburgh, daughter of the famous nuclear physicist William Howard Arnold. She attended the city's Taylor Allderdice High School and moved out of home by age 17, hitchhiked to Washington DC to protest the Vietnam War and skipped school to work as a taxi driver and as a cocktail waitress by night. She got into Princeton, not on her grades (which were average), but on near-perfect standardised test scores and a compelling essay explaining her lack of interest in the traditional high school curriculum. While at Princeton, she continued to drive cabs and made several solo trips to South America and Europe on the proceeds. She graduated in mechanical engineering (1979) as one of fewer than five

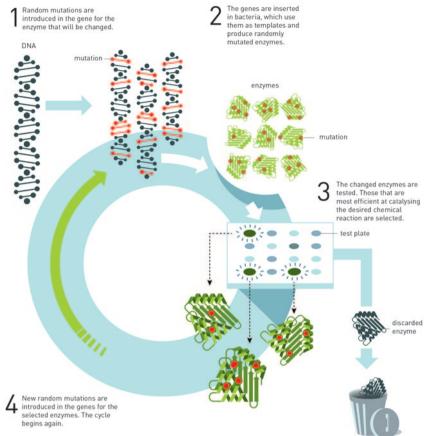
women and then went to work for the Solar Energy Research Institute (SERI) in Colorado, envisaging a future free of fossil fuels.

However, the oil crisis finished,
Americans drove big cars again and
Frances' brother (Eddy Arnold,
professor of chemistry at Rutgers)
encouraged her to 'try chemistry'
instead of solar research. So she left
SERI in 1980 destined for a PhD in
chemical engineering at Berkeley. Just in
time, as it turned out. A year later Ronald
Reagan cut SERI's budget by 90% and
almost everyone there lost their job.

At Berkeley, she realised that she didn't know any chemistry and had to take the entire undergraduate curriculum, which she completed in 12 months, and then began working on biofuels with Harvey Blanch. Reagan's cuts also saw Blanch's funding for biofuels cut to zero and so he moved into biotechnology.

Arnold finally obtained her PhD in 1985 on affinity chromatography. She continued to work for 18 months at Berkeley for Ignacio Tinoco until obtaining a position at CalTech in late 1986. While at Caltech she brought Manfred Eigen's vision to a technically elegant reality. Arnold developed rapid iterative methods that mimicked the slow random mutagenesis and selection found in nature. Coupled with innovative screening techniques to select mutations that addressed targeted properties, this resulted in the discovery of enzymes that worked in organic solvents (Proc. Nat. Acad. Sci. USA 1993, vol. 90, p. 5618), enzymes

Arnold developed rapid iterative methods that mimicked the slow random mutagenesis and selection found in nature.



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that catalyse reactions invented by chemists and not known in nature, such as olefin cyclopropanation (*Science* 2013, vol. 339, p. 307), and enzymes that catalyse the formation of bonds not found in nature, such as C–Si bonds, through carbene insertion into Si–H bonds (*Science* 2016, vol. 354, p. 1048). C–Si bonds are useful in medicinal chemistry and a wide variety of consumer products, but are unknown in biological systems.

The discovery of enzymatic olefin cyclopropanation started with a literature report of haem mimics performing cyclopropanation in organic solvents. Screening of haem proteins for this activity led to the discovery of a bacterial cytochrome

P450 that displayed a low level of promiscuous (cyclopropanation) activity when fed diazocarbenes and a suitable olefin. Directed evolution involved DNA sequence library construction, mutating residues in or near the active site. This step is critical and relies on a detailed knowledge of the enzyme's structure. Not unexpectedly, the full sequence space for any enzyme is very sparsely populated in activity, which tends to be clustered in a few islands. The trick is to stay close to land. In the next step. screening of the library for the reaction you want allows you to narrow the field and re-mutate the most active variants from the first screen and then repeat the process. In just a few generations

of directed evolution, the Arnold group was able to improve the activity and selectivity of the enzyme so that it could produce, for example, a precursor for the heart drug ticagrelor with very high diastereo-and enantio-selectivity (see diagram below).

Another aspect of this work is to replace toxic heavy metals with green enzyme catalysis. For example, the industrial synthesis of sitagliptin, a selective DPP-4 inhibitor for the treatment of type 2 diabetes, is made via a key step that requires Rh<sup>1</sup>/t-Bu JOSIPHOS, an expensive heavy-metal-containing catalyst. The scientists at Merck were able to use 11 rounds of enzyme evolution on an artificial (*R*)-selective transaminase to produce an enzyme that did the same reaction in much higher enantioselectivity and without the use of toxic heavy metals.

Another way to navigate the sparse activity landscape of enzymes, and stay close to land, is to use related enzymes to guide mutations. This is called 'DNA shuffling' and was introduced by Pim Stemmer in 1994 (Nature 1994, vol. 370, p. 389). In this process, pieces of DNA for the same enzyme in several organisms are shuffled like a deck of cards. In this way, mutations are directed toward areas already known to produce active enzymes. The same process has been used for antibodies (called affinity maturation), and is much more efficient than random mutations at accessing wider chemical space. These methods have been facilitated by the advent of cheap DNA synthesis and sequencing and, it could be argued, would not have been possible without this (Gilbert and Sanger, Nobel Prize in Chemistry 1980; Ochoa and Kornberg, Nobel Prize in Physiology or Medicine 1959).

The other half of the Nobel Prize went to the directed evolution of 'affinity' (as opposed to 'activity'). which is facilitated by phage display, a method of physically coupling a phenotype (high-affinity binding protein) with a genotype (the DNA for that protein). Phage, or more properly 'bacteriophage' are the champions of the underdog. In the wild, when any species of bacteria threatens to take over a local environment, their viruses (phages) come in to decimate the Johnny-come-lately. With an estimated global population of 1031 and launching 10<sup>24</sup> successful infections per second, they have major effects on the global energy and nutrient cycles much of biology is about feeding the phages. They were also crucial to identifying DNA as the genetic material in 1952 (Alfred Hershey, Nobel Prize 1969), that DNA had a triplet code in 1961 (Francis Crick (Nobel Prize 1962), Leslie Barnett, Sydney Brenner (Nobel Prize 2002), and Richard Watts-Tobin) and later in uncovering the mechanism of gene regulation, protein folding, DNA binding and genetic recombination. Look anywhere in molecular biology and you will find indispensable phage enzymes at work.

#### George P. Smith

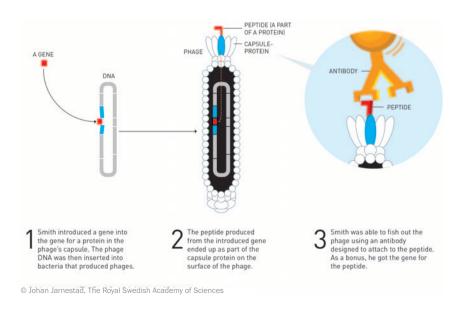


George Smith was born 10 March 1941 in Norwalk. Connecticut (USA), and obtained a BA in biology from Haverford College in 1961. He was fascinated by reptiles and hoped to become a herpetologist, but his mathematical way of thinking made him much more suited to molecular biology. His senior thesis project tried to answer the question of how the immune system can recognise anything foreign. His experiments were naive and unsuccessful and actually solved the next year by Edgar Haber (Harvard). After a year as a high school teacher and lab technician, Smith was accepted into a PhD program at Harvard with none other

than Edgar Haber, who was also hosting another (future) Nobel laureate at about the same time (Bob Lefkowitz). After a postdoc at Wisconsin with another future Nobel laureate (Oliver Smithies), he joined the faculty at the University of Missouri in 1975 and has remained there till this day.

Smith has a career total of about 50 papers. He got none from his PhD but several as a postdoc at Wisconsin, including in Science and Cell. Notably, his first paper as an assistant professor at the University of Missouri was also in Science – a sole author paper about the evolution of repeated DNA sequences. He became interested in phage and using these as cloning vectors. For example, he discovered a new filamentous phage cloning vector (Gene 1980, vol. 9, p. 127) in 1980. Here he was able to clone the tetracycline resistance gene into the fd phage and show that infected E. coli became tetracycline resistant. However, it was a two-year sabbatical (1983-4) at Duke University with Robert Webster that led to the Nobelwinning breakthrough. Webster recalls that Smith was able to demonstrate that it was possible to fuse a foreign protein to the pIII coat protein of phage fd (Science 1985, vol. 228, p. 1315). The

... Smith was able to demonstrate that it was possible to fuse a foreign protein to the plll coat protein of phage fd ...



chimeric protein pIII-EcoR1 was able to be packaged into the phage and was correctly displayed on the surface so that an EcoR1 antibody could be used to purify the phages displaying the enzyme by 108-fold in three rounds of 'biopanning'. Smith coined the term for affinity purification of phages displaying EcoR1 from a background wild-type phage, using a streptavidincoated Petri dish to which biotinylated EcoR1 antibody was adsorbed (Gene, 1988, vol. 73, p. 305). Coincidentally, the restriction enzyme EcoR1 and the antibody used by Smith to confirm the enzyme was functionally expressed on the surface of the phage particle were supplied by Paul Modrich (Nobel Prize in Chemistry 2015, for DNA repair) also at Duke. Smith immediately recognised the power of this and advanced the technique over the years. By 1990, he had published the first 'phage display' library. This library was composed of peptides, 'displayed' on the surface of filamentous phage particle; a different peptide for every phage particle as encoded by the DNA inside (40 million hexamers in this case). He was able to purify specific phages that bound to an immobilised antibody (Science 1990, vol. 249, p. 386).

Of course, there were many scientists working on phage at this time and in many ways Smith just

Winter took an scFv (single-chain variable fragment of an antibody) derived from mice immunised against chicken egg-white lysozyme and fused it to protein plll of fd phage ...

happened to be in the right place at the right time. On the other side of the Atlantic, Sir Gregory P. Winter reported the display of a folded and fully functional antibody fragment on filamentous phage also in 1990. This was something new and exciting because, for the first time, it decoupled an antibody from the animal that produced it.

#### Gregory P. Winter



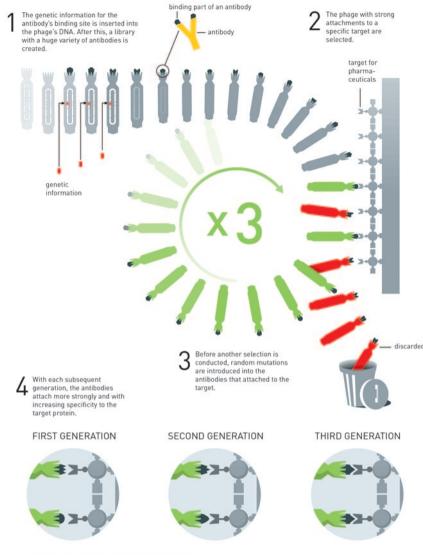
Greg Winter was born six weeks prematurely in Leicester, UK, in 1951, and was a sickly child. His parents moved to West Africa (Legon in Ghana), where Winter grew up, in part, to keep young Gregory warm, which was near impossible in post-war London. He thrived in Africa (despite contracting malaria and some other tropical diseases) and recalls that what launched him into science was the sight of a huge sea turtle brought to school by the first 'scientist' he had ever met. Gradually he discovered that the unknown frontiers he craved were not so much of the David Attenborough sort but those associated with the unseeable molecular world. Winter returned to the UK for high school at the Royal Grammar School, Newcastle upon Tyne. He went on to read natural sciences at the University of Cambridge, graduating from Trinity College, in 1973 (of which he became Master in 2012). Staying on at Cambridge, he was awarded a PhD in 1977 from the MRC, for studying tryptophanyl-tRNA synthetase from

Bacillus stearothermophilus. He was supervised by Brian S. Hartley and George Brownlee and, unlike Smith, wrote up five papers from his PhD. He left Cambridge (briefly) for a postdoc at Imperial College and then another at the Institute of Genetics at Cambridge before becoming a group leader at the MRC in 1981.

His first encounter with phage was in 1980 (Nucl. Acids Res. 1980, vol. 8, p. 1965), when he cloned influenza cDNA into bacteriophage M13. In 1982, he won a fellowship and travelled to Canada to pursue work on how mutations affected enzyme function. On his return to the UK, César Milstein (Nobel Prize 1984) suggested that Winter should work on antibodies, the development of which for human use was hampered because they were raised in animals, typically mice, so contained too much 'mouse'. What was needed to develop antibody drugs was a way to 'humanise' them so they would not produce an immune response. Winter responded with intense excitement about the possibilities of using site-directed mutagenesis to alter antibody structures. He postulated that antibodies were just scaffolds with only small sections required for antigen recognition.

He initially worked with Herman Waldmann, who was using antibodies raised in rats to treat leukaemia patients, and Sir Alan Fersht, who was a protein engineer. Together, they made a major leap forward by replacing large sections of rat antibody with the human equivalent and found the antibodies still worked as before. At about the same time, Winter was also using M13 phage display to dissect the tyrosyl-tRNA synthetase enzyme to see what sections were required and which were not. Applying this technique to humanising antibodies was a logical step forward but one Winter was also quick to realise had huge commercial potential.

In 1989, he set up Cambridge Antibody Technology (CAT) to



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commercialise this work. In the first paper, Winter took an scFv (single-chain variable fragment of an antibody) derived from mice immunised against chicken egg-white lysozyme and fused it to protein pIII of fd phage, taking inspiration from Smith's 1985 paper. They showed that the scFv-phages had high specificity and could be amplified  $10^6$  times over other phages in two rounds of affinity purification (*Nature* 1990, vol. 348, p. 552).

In collaboration with BASF, CAT developed adalimumab, which was bought by AbbVie and marketed as Humira. It was the first fully human antibody (against TNF $\alpha$ ) drug ever developed by using phage display and the world's largest selling drug in 2017 (US\$18 billion). It is used to treat inflammatory diseases such as rheumatoid arthritis and Crohn's disease and costs about US\$52 000 per year in the USA. It came off patent

in 2018 but biosimilars appeared in India in 2014 and are now globally available at US\$2400 per year.

The first biologic drug (chemically humanised insulin) became available in 1982, and by 2016, there were 64 fully human antibody drugs that had been developed by phage display in the clinic or in clinical trials. This may well only be the vanguard and the ensuing decades may see small molecules largely replaced with biologics, or the two drug discovery paradiams may merge as is being witnessed by the emergence of antibody-drug conjugates. In late 2018, there were four conjugates approved - brentuximab vedotin (Seattle Genetics), ado-trastuzumab entansine (Genetech/Roche) inotuzumab ozogamicin (Wyeth/Pfizer) and gemtuzumab ozogamicin (Wyeth/Pfizer).

Winter went on to found his second (Domantis in 2000) and third company (Bicycle Therapeutics in 2009) but still remained first and foremost an academic who thinks about practical problems. His thesis advisor once told him 'Bugger interesting, is it an important question?' Virtually the same advice was given to Fraser Stoddard by his PhD advisor at their second meeting (at his thesis defence).

The 2018 Nobel Prize in Chemistry recognises Arnold, Smith and Winter, all with very different trajectories, for 'hacking' evolution to generate better drug treatments faster, greener and more efficient chemical manufacturing processes and more economical biofuels. Thanks to these innovations, what nature takes millennia to do, chemists can achieve in weeks or months. I think, if nothing else, this year's Nobel Prize provides final proof for the molecular basis for Darwin's theory of evolution.

**Peter Karuso** FRACI CChem FRSN is Professor of Chemistry at Macquarie University, Sydney.

# The life of Brynn

In this International Year of the Periodic Table, **Dave Sammut** and **Chantelle Craig** profile Australia's representative to the IUPAC Analytical Division, Emeritus Professor Brynn Hibbert.



his year is a year of celebration for chemistry. For a profession that counts its history in centuries, this is a milestone year: 150 years since Dimitri Mendeleev first published his periodic table. The International Union of Pure and Applied Chemistry, IUPAC, will celebrate its own centenary by killing the kilogram – at least in corporeal form. January kicks off the International Year of the Periodic Table (see box p. 22). And on World Metrology Day (20 May), new definitions will come into force for the ampere, kelvin, mole and kilogram (see box p. 23).

These new definitions for the SI units are the culmination of years of international collaboration (and argument) among scientists who really know how to nitpick.

This is not another article about metrology – a topic so dry it can't even be read without a handy glass or

beaker of something wet close by. Instead, we'd like to profile Australia's representative to IUPAC's Analytical Division: the RACI's own Emeritus Professor Brynn Hibbert, recently appointed a Member of the Order of Australia (AM), renowned as a metrologist, expert witness, raconteur, all-round great guy, and a man who would never object to the proximity of a cold and frosty beverage.

We'll freely admit to being big fans of Hibbert. He was a close friend of Don Craig, Chantelle's father (who was himself a chemistry colleague at UNSW for 54 years), and has been an inspiration to Dave throughout his career. So, for this article, we set out to 'chew the adipose tissue' with Professor Hibbert.

The year ahead will be another busy one for Hibbert. July brings the centenary celebration for IUPAC. 'The French are good at putting on parties',



The Wanderer and His Shadow, Huihai Xie (1957–) (mixed media on canvas 137 × 198 cm). This portrait of Hibbert was a finalist in the 2000–2001 Doug Moran National Portrait Prize.

says Hibbert, 'I shall go along as [IUPAC's Interdivisional Committee on Terminology, Nomenclature and Symbols] ICTNS Secretary and the Australian rep and also probably one of the Australian delegates to the general assembly. It's actually brilliant! You've got the flag, and the voting card, and it's just like the Eurovision Song Contest ... or so I imagine. Australia trois points!'

Of his current role with the ICTNS, Hibbert jokes: 'I am in charge of the terminology of chemistry'. Wielding this power with grace, he assures us that he does not intend to revisit the spelling of 'sulfur'. Nor will we see IUPAC's disastrous attempts a few years ago to 'rectify' common usage terms in science, such as trying to stop the use of 'acetylene' for 'ethyne' and trying to force chemists to replace 'sample' (due to its mathematical concept of a number of items taken

from a population) with 'test portion'. As Hibbert observes: "They very quickly realised that nobody took a blind bit of notice'.

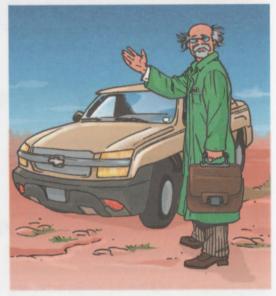
This sense of humour is characteristic of Hibbert, Personable and self-effacing, he jokes that his office at UNSW – shared with several other emeritus academics – should be called the 'Thanatocoenotic room', a geological term for a stratum in which a lot of old fossils have died together. Continuing his jokes - this time about his transfer to emeritus status -Hibbert decries that he never actually got to deliver his retirement speech, in which he set down the guiding principles of this life: that he 'had suffered fools gladly' and 'never left his comfort zone'.

Discussing his career, Hibbert says: 'I've always been distracted too easily, but I reckon that I've published with more people than any of my

colleagues.' He has certainly touched on a lot of areas, from his prized *Nature* cover article on fractals to his being featured as a character in a best-selling French-language book for children (in which the eponymous character investigates the cause of a fire, eventually determining it to have been caused by a (small) meteor).

Born in Yorkshire, England, to parents who had little education, Hibbert was raised in Bournemouth. Father Herbert was a retired grocer and mother Florence had run a hairdressing business. He recounts his mother saying to the children: 'I don't know what that university is, but thar's going to it'. His much older brother, whom he idolised, studied chemistry at Kings, 'and so I did', he states, 'That was it. No teenage angst'. And it was only later that his brother admitted that he never wanted to be a chemist. He wanted to be a historian. 'You bastard!'

Puis Brynn Hibbert enferma précieusement la paillette dans une éprouvette, et la rangea avec son matériel. Il fut reconduit à sa voiture, fit crisser ses pneus sur la terre ocre du bush, et salua la troupe d'un grand geste du bras à travers la fenêtre. Puis il disparut dans le lointain, emportant son trésor sur la route de Sydney.



Text: Nathan Editions. Art: Loic Malnati

Hibbert exclaimed, 'Then I'd have been an historian!'

Hibbert was awarded a scholarship to study at Kings. 'I flourished at chemistry. My passion for it is more because I can do it, and I can do it Then, Brynn Hibbert carefully sealed the speck in a test tube and stored it with the rest of his equipment. They took him back to his car. He made his tyres squeal on the ochre soil of the bush, and waved a salute to the band through the window. Then he disappeared into the distance, taking his treasure away on the road back to Sydney.

well, than because I have a burning thing to do this bit of chemistry or that.' He worked in academic roles after university, and his big break came with the opportunity to take up the newly created Chair of Analytical

Chemistry at the UNSW in 1987. 'I had this really good interview [in 1986]. It turns out I didn't know what ICP stood for, but never mind ... When they offered me the job, you could have knocked me down. And it was really

rather good because that week Chernobyl happened and I remember thinking that Australia is really a long way away from there.'

On teaching, Hibbert says 'A student once said that "I liked Professor Hibbert's lectures the best because he never mentioned chemistry". In fact, I did tell them quite a lot about chemistry and the fact that he didn't notice was really rather good, I thought. My attitude to teaching goes something like this: I do not believe education is tiptoeing down the garden of knowledge hand in hand with your

#### **International Year of the Periodic Table**

According to IUPAC, 'The United Nations has recognised the importance of raising global awareness of how chemistry promotes sustainable development and provides solutions to global challenges in energy, education, agriculture and health'.

Professor Mary Garson (Past President, RACI Queenland Branch) currently serves on IUPAC's Subcommittee on Biomolecular Chemistry, and is responsible for the global planning of IUPAC's centenary celebrations. She notes that the Periodic Table of Younger Chemists activity (https://iupac.org/

100/pt-of-chemist) features as 'iron' the RACI's

Dr Liz New (winner of multiple
awards, including NSW
Premier's Prize for Early
Career Researcher of
the Year, 2017).

Commencing in January 2019, the Periodic Table Challenge (https://iupac.org/100/pt-challenge) is aimed at secondary school students. After taking a quiz, students will be asked to identify an element that is special to them. They are then asked to make an artefact that demonstrates why this element is special for them. The artefact may be a picture, a physical object, a poster, a short story, a video, whatever they like.

At the time of writing, 20 countries have signed up to participate in the Global Breakfast Networking activity (https://iupac.org/100/global-breakfast)to be held on 12 February 2019, with expressions of interest from seven others

RACI is canvassing ideas for its own celebrations for the International Year of the Periodic Table. Keep an eye on your branch newsletters for opportunities to get involved.

students as you learn together. As it happens, I know heaps about chemistry and if you ask me nicely I'll tell you.'

One of Hibbert's early PhD students in Australia, Dr Karyn Weitzner, recalls how popular he was as an engaging lecturer and active supervisor. 'One of my biggest memories is that our school was old, run down and poorly funded', says Weitzner with a smile, 'We often had to run our experiments on jury-rigged equipment, barely holding together. Brynn would come into the lab, and in his enthusiasm touch something and break it, then cry "Oops, I've got to go" and quickly scurry out again'.

In our chat, Hibbert was enthusiastic about the substantial expansion of access to university. 'It's really good that tertiary education has come to the masses', he says, '... as long as we can still recognise the one or two super bright students in a year and make sure they do a good PhD, then that's good'.

How does Hibbert see the balance of pure versus applied research at univerities? 'Universities should be concentrating on pure research rather than applied, very much so, but of course pure research comes often from different angles. So, you can have an applied problem, that when you've solved it, can have wide-reaching consequences. Simply doing research for its own sake is okay – there is a continuum – providing that bedrock on which the applied advances are made is probably what universities do well.'

He was less enthusiastic about the modern shift in the focus of learning away from analytical techniques and towards individual applications (such as forensics). 'I reckon that we now teach perhaps a third of the chemistry that we used to teach. Now it's all about uses, and not methods', he says. 'When do they actually learn about the analytical chemistry?'

Hibbert's advice to the next generation of scientists is, according to him, 'boring': 'Work hard, because if you don't know anything you can't advance knowledge. So all this – "it's at the touch of a button and Google things" - it's only half of the story. It's about knowing an awful lot of stuff, and that means not just what you do, but everything around it. So, try and open

up to as much as you can and learn as much as you can. And never say "no". If anybody asks you to collaborate, say "yes" and things will work for you.'

We've run out of space to talk about Hibbert's role as Head of School at UNSW, his subsequent career as an expert witness in court proceedings (see Sep/Oct 2018, p. 18), nor his term as President of the Royal Society of NSW, nor Hibbert's wonderfully engaging public speaking. Suffice to say that should you ever have a chance to hear him speak, or to sit down with him for a chat, then this will be a part of your life very well spent.

In a discipline sometimes best characterised by its eccentrics, Brynn Hibbert is a wonderful example of the atypical, a three-sigma outlier.

There will come a day when Hibbert will need to retire from his active retirement. Asked about how he would like to be remembered when that day eventually comes, he responded succinctly: 'Mostly harmless'.

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

#### **RIP International Prototype Kilogram**

The redefinition of the SI units was discussed in the Nov/Dec 2018 issue (p. 28), and the final resolution was passed at the 26th meeting of the Conférence Générale des Poids et Mesures (CGPM) on 16 November 2018 – with a live broadcast to YouTube.

In the simple explanation from Brynn Hibbert, 'There is the big K [the International Prototype Kilogram, currently the international physical definition of the kilogram] and the 50-odd copies around the world. At the moment the big K weighs one kilogram with no uncertainty – after the approved cleaning method – end of story. After World Metrology Day, the big K will then be an object that weighs (we hope) roughly a kilogram, that we can measure, and the measurement will have uncertainty.'

The new measures will be based on the use of fundamental physical constants. 'I was reasonably against [the use of constants] for a long while,' admits Hibbert 'I was brought kicking and screaming to the fold. Some little bit of the universe may have a different speed of light – who knows?'

'There's quite a few people around the world who think it's the end of civilisation.'

Monsieur Kilogram, a character in NIST's League of SI Superheroes animated online series, is able to determine the mass of any object simply by holding it.  $_{\mbox{\scriptsize NIST}}$ 



# Networks, workforce development and resilience

BY TOM
SPURLING, COLIN
GALLAGHER,
DEAN LUSHER,
CHRIS SUCH AND
TIM DAVEY

Industry networks are surprisingly fragile, and Australia's chemical industries are no exception. Tom Spurling and colleagues explain the importance of social network analysis.

he change came down 'like a garage door', according to Chris Such. 'All of that international network disappeared instantly in 1997. Instantly, Chris, who joined Dulux in 1976 and rose to be the New Technology Manager of Dulux Australia, was commenting on the day that the international giant ICI PLC sold its Australian interests to the new company Orica. It was a lifetime's worth of collaborations - gone. 'So one of my jobs was to rebuild', said Such. 'We didn't have an external. international network because we were just here in Australia. This is the headquarters for the world, for Dulux Australia. So it was "How do you protect the future?" and that was about getting out and about and building some external networks, consider what the killer ideas we needed were, and how we were going to get there. So it's that blend of internal versus external, you know, a classic partnership-sort of model, given that we didn't have international collaborators so it would move heavily towards Australian-based collaborators.

Chris Such's insights illustrate an important characteristic of social networks of collaboration. They take a lot of time and effort to establish but can disappear or be destroyed very quickly. All companies have networks of suppliers, customers and technology providers. Who companies collaborate with is heavily dependent on the technology underpinning their business. Then it is about personal relationship management. Who is good at what the company needs and where are they?

Such's story points to a bigger picture - one in which Australia's chemical industry sector is contracting in the face of lower cost of manufacture in emerging economies, improved transportation, free trade, and the globalisation of many industries. Despite these pressures, high-value chemical products produced in Australia are used in global and domestic supply chains, and are poised to meet increasing demand from these markets. It remains the second largest manufacturing industry in Australia and provides industry 'value-add' of about \$12 billion. It



supplies inputs to 109 of the country's 111 industries. Moreover, contraction is not inevitable, with comparable advanced economies learning to swim upstream. Germany hosts three of the top-10 chemical companies in the world. Switzerland, with a smaller population and higher average wages, consistently ranks near the top of OECD tables for chemistry. Given the importance of the chemical industries to our economic, environmental and social wellbeing, a key question is whether Australia can follow suit over the coming decades. What will make the difference?

One of Australia's well-springs of resilience is our well-educated workforce. Our educational resources put us at a distinct advantage in identifying and developing new high-value niches. Accordingly, in its strategic roadmap, the national body for Australia's plastics and chemicals industries, Chemistry Australia, noted 'skilled and productive talent' as one of the sector's fundamental needs. Australia needs to be able to leverage this human capital, by combining it with social capital – our ability to make

the most of our social ties to others. Importantly, the resilience of the sector is not just about personal expertise of individual chemists – it's about how many forms of expertise are combined and recombined in innovative ways. Confronting challenges together, not merely side-by-side. Connecting ideas and expertise – just as Chris Such suggests – is a way forward. Understanding what makes the chemical industries resilient means

Understanding what makes the chemical industries resilient means understanding the many ways in which people are connected to one another ...

understanding the many ways in which people are connected to one another through cooperation, coordination and competition.

But with so many types of crisscrossing, complex social connections all around us, where do we look first? Where do we try to make a difference? Networks of collaboration and exchange tell a particularly important story within the chemical industry because of its unique supply chain position. The chemical industry supplies Australia's industries through its 5500 businesses, small, medium and large. Each of these companies needs to develop and maintain networks with their own suppliers, their customers and their technology providers. These technology providers might be another company, CSIRO or a university.

Understanding the nature of these networks, how they are initiated, maintained and expanded, and how they link up players with different resources, skills and priorities, is part of the program of the new ARC Industrial Transformation Training Centre for the Chemical Industries

#### Research themes within ATCI

ATCI research theme	Description	University researchers
Innovations in Advanced Materials and Process Chemistry	The advanced materials and process chemistry field plays an important role in most socioeconomic sectors such as agriculture, water, health, building construction, machine manufacturing and transport. The sector also impacts significantly on high-end applications and has made major contributions in the development of better energy and health products. However, in a global marketplace, companies are under constant pressure to develop new products that meet emerging market trends and consumer needs.	University of Melbourne, Chemistry: Dr Anastasios (Tash) Polyzos, Prof. Paul Donnelly, Assoc. Prof. Craig Hutton, Prof. Paul Mulvaney, Prof. Mark Rizzacasa, Dr Georgina Such, Prof. Jonathan White, Assoc. Prof. Uta Wille, Prof. Spencer Williams University of Melbourne, Chemical Engineering: Prof. Frank Caruso,
New Approaches to Medicinal and Biochemical Chemistry	Globally, small molecule drugs comprise around 90% of the market, and in Australia represent one of our major manufactured exports (\$3.9 billion in 2012–13). The industry employed approximately 16 500 people in manufacturing and spent around \$404 million on pharmaceutical manufacturing R&D in 2011–12. These industries demand broad graduate attributes: strong technical skills in synthetic chemistry, molecular design and modelling, and traditional and modern approaches to drug design and manufacturing.	Dr Francesca Cavalieri, Dr Luke Connal, Prof. Greg Qiao  University of NSW, Chemistry: Prof. Martina Stenzel, Dr Jonathon Beves, Prof. Luke Hunter, Assoc. Prof. Shelli McAlpine, Dr Thanh Vinh Nguyen, Assoc. Prof. John Stride, Prof. Ricard Tilley, Prof. Pall Thordarson

(ATCI). ATCI aims to foster a world-class environment of transformative innovative research in Australia's chemical and advanced manufacturing industry through sustained partnerships with universities. ATCI will link leaders from the chemical industries and peak industry bodies with research and teaching academics from the three partner universities. The centre will harness this combined expertise to lay foundations for transformative changes to industry training and research translation.

At a more hands-on level, ATCI is making fundamental moves to change the current research training landscape by establishing a new model of industry-led graduate research. The newly established Masters of Industrial Research (MIR) (Chemistry), offered at the University of Melbourne and University of New South Wales, meets the demand from the sector for short, nimble research projects that are industry-relevant, with shorter timeframes than a typical PhD

project, with a supportive and flexible IP arrangement at each university. Developed in close consultation with both Chemistry Australia and leading employers in the industry, this two-year course will allow graduates to develop employable skills and attributes while running a significant research project with a chemical company. Usually hosted at the company site, students will work hands-on with company staff as an industrial R&D chemist, for a minimum of 12±months. In developing their research projects, the students will have access to the expertise and facilities of the university research groups associated with the Centre. As part of the MIR, students will also enjoy wide resources for up-skilling that are designed to suit their specific project and professional development needs, including a range of online and on-campus elective course offerings delivered by the universities in partnership with the industry host.

Research themes within ATCI include Innovations in Advanced

Materials and Process Chemistry and New Approaches to Medicinal and Biochemical Chemistry (see table). Underpinning these are developments in the fields of analytical chemistry and material characterisation. A range of techniques will be available through

... ATCI is making fundamental moves to change the current research training landscape by establishing a new model of industryled graduate research.



this program, including NMR, IR and Raman spectroscopy, mass spectrometry, scanning and transmission electron microscopy, X-ray diffraction and atomic force microscopy.

Importantly, a further theme of ATCI is understanding the importance of social networks. In this regard, the role of Swinburne University of Technology in ATCI in social network analysis affords ATCU a fine-grained look into its own social structure, and a unique vantage point on the impact of ATCI activities (www.swinburne.edu.au/sna). These networks can be person-toperson, group-to-group or company-to-company, and represent various forms of advice, trust and collaboration, to name just a few possibilities. Social network analysis permits the mapping of social connections.

The graphic presents a network visualisation (or map) of the connectivity of leading international researchers in laboratories around the world who are working within the field of controlled living/radical polymerisation. The network data comes from interviews with key researchers in which they were asked about their advice-seeking on technical issues related to their work

on this topic. Each colour within the network represents a different international laboratory – of which there are many in this network. What we can clearly see is that there is strong advice-seeking within laboratories, but that technical advice-seeking connects these research labs around the world. It is this sharing of knowledge that offers advantages to the overall ecosystem.

Visualisation is highly useful, but not always the best way to investigate a network. It is possible to move beyond simply drawing network maps, and use statistical models for social networks to investigate the structure and implications of these networks. Which people are most sought out as experts in the field? Who are the key brokers that join this network together? Which laboratories are the most central (and thus most connected and influential) in this advice-seeking network?

Swinburne has world-leading capacity in social network analysis, providing statistical techniques to understand social networks with models that allow us to go beyond visualising networks. As part of ATCI, Swinburne researchers will use social network analysis tools to understand networks in the context of the chemical industries. Importantly, a key issue that

the ARC Training Centre hopes to understand is how networks affect collaboration and knowledge transfer between industry and academia, and how we can develop effective networks moving into the future.

The ARC Industrial Transformation Training Centre for the Chemical Industries is led by the University of Melbourne in collaboration with the University of New South Wales, Swinburne University of Technology and Chemistry Australia and partners CSIRO, Dulux, PPG, DCS Technical and Qenos. Further information is available at www.arc-chemind.org.

Tom Spurling FRACI CChem, Colin Gallagher and Dean Lusher are at Swinburne University of Technology Centre for Transformative Innovation. Tim Davey MRACI is at Dulux Australia and Chris Such is recently retired from Dulux Australia.



# **Mapping molecules**

#### BY GISELLE ROBERTS

A scientist once told me that identifying the optimal interaction between molecules is like finding a needle in a haystack. Professor Brian Smith, molecular modeller at the La Trobe Institute for Molecular Science at La Trobe University, is an expert at just that.

is research, a complex mix of computer simulations and mathematics, calculates the structure and properties of molecules, and predicts what they might do over time and in particular settings. It is critical work for drug discovery, providing unique data on what may turn out to be the next miracle molecule.

I sat down with Professor Smith to find out more about what molecular

modellers do, and how their research is transforming our understanding of health and disease.

Science meets technology
GISELLE ROBERTS: Brian, you have been
modelling molecules for over 30 years.
What do you do and what role does
modelling play in scientific research?
BRIAN SMITH: I use mathematical
models to describe molecules and their
interaction with proteins, peptides and

drugs. I have a particular focus on how they change over time. We all experience time. We wake up in the morning and we go to bed at night, and things happen from one point to another. Things happen to molecules too and my job involves charting their journey.

**GR:** And you use computers to do that. **BS:** Yes. Calculating molecular interactions over time requires enormous computational power. We use the

supercomputers at NCI Australia in conjunction with standard computers that have graphics processing units, the hardware that supports video games. It produces the special effects in a game, but can be repurposed to generate scientific data. I use that hardware and write computer programs to answer specific molecular questions, usually around predicting what sorts of compounds might make useful drugs. We run simulations until we feel that we have generated confidence in the information, analyse the data, and create a visual representation of that for further

**GR:** OK, so what are the advantages of modelling? Why not just track molecules in the lab using other experimental techniques?

analysis.

BS: We can obtain calculations that have a degree of accuracy that is unachievable by any other method. And we can interrogate very small timeframes on systems that have no experimental parallel. That said, a model is only an idea. It's in silico, or virtual, until it is validated. Modelling predicts how an interaction between molecules might occur, how it changes, and how to improve the interaction if that is what we are trying to do - which is particularly critical to drug discovery. We can also identify the shortest route of delivery, while running long simulations in an effort to understand the entire system.

#### New insulins

**GR:** In terms of drug discovery, I understand you are part of a team that is developing new forms of insulin to treat diabetes.

**BS:** Yes. Regulating blood sugar is key to managing insulin-related diseases such as diabetes. Insulin helps to stabilise blood sugar, but it treads a fine line between modulating the spike in glucose after a meal, while also maintaining an

effective base level. It tends to be slow and long lasting, which is not necessarily what you want as a diabetic. Instead, you want to be able to see a hamburger, buy it, and enjoy your meal without having to wait 30 minutes before the insulin is working properly.

GR: How can we overcome that?

BS: My group is part of an international team that is working to identify new forms of insulin that respond immediately without the long-lasting effects. Our part in the project has been to use computer models to explore the behaviour of these stable, fast-acting insulin-like molecules. We hope the project will lead to more effective therapies that can accurately reflect normal blood insulin activity. We've also identified more robust insulinlike molecules that do not require refrigeration. It could be transformative for diabetics.

**GR:** It must be exciting to contribute to projects that have such incredible translational outcomes.

**BS:** It is. Earlier in my career, I was part of a large consortium working on

anticancer drugs. One therapeutic from that research collaboration ended up on the market last year. My part in it was small, but it was nice to contribute to something that will help people.

**GR:** And, perhaps, in the future, your research may contribute to the development of more responsive forms of insulin.

**BS:** I hope so. To help somebody beyond academia is an incredible driver. The people I work with tackle big problems such as influenza, cancer, diabetes and malaria – diseases that affect millions of people every year. Any solution, big or small, has global impact. I love solving problems that scientists have no way of interrogating by any other method. It's also very rewarding to achieve an impact beyond a nice scientific paper, to make a difference to someone's quality of life in a broader sense.

**Dr Giselle Roberts** is Communications Coordinator at the La Trobe Institute for Molecular Science.

#### **Emeritus Professor Lloyd Earle Smythe**

#### Distinguished analytical chemist

Lloyd Smythe was born in Suva, Fiji, on 15 June 1922, and most of his primary and secondary schooling was at the Boys Grammar School, Suva. He studied chemistry at the University of Sydney from 1939 to 1943, graduating with first class honours. He then commenced employment with Beetle Elliott Plastics in Rozelle, working on synthetic urea formaldehyde resin adhesives used for production of the wooden Australian-made mosquito bomber. After the war, Smythe completed an MSc at the University of Sydney on the kinetics of the urea-formaldehyde reaction before being appointed as the youngest lecturer in chemistry, and was busy coping with the influx of returned servicemen entering university.

He married Ann Jean Gilbert of Mosman, New South Wales, in 1945 before returning to Fiji as Chemist, Department of Agriculture in 1947. He then moved to the University of Tasmania (UTAS) in 1949 as a lecturer in inorganic chemistry. Their daughter, Lesley Ann was born that year. Smythe completed his studies at UTAS for the newly established PhD degree (introduced in Australia in 1949) working on the project 'Kinetics and formation of substituted diamides of carbonic acid'. He was promoted to senior lecturer in 1953 and was also awarded the Carday-Morgan Fellowship of the London Chemical Society (the first such award to an Australian citizen) to undertake postdoctoral work with Professor H.J. Emelius FRS in 1955.

In 1956, Smythe accepted an appointment as principal research officer at the Australian Atomic Energy Commission to lead the newly formed Analytical Chemistry Group concerned with trace element and radiochemical analysis. He was promoted to senior principal research scientist. In 1968, he accepted an invitation for appointment as Foundation Professor of Analytical Chemistry at the University of NSW, and he then played a leading role in the recognition of analytical chemistry in Australia. I completed my BSc(Hons) and PhD degrees under his supervision over the period 1971–5 and the Department of Analytical Chemistry was a vibrant unit with internationally recognised expertise in analytical spectroscopy, gas and liquid chromatography, and electrochemical analysis. Smythe was Vice-President of the RACI in 1969 and President in 1970.

Smythe can be credited with the establishment in Australia of neutron activation analysis (NAA) and he was the first in Australia to use this technique in a murder trial. He was called by the defence of Terence Guirin, who had been accused of murdering a 25-year-old woman. NAA analysis of hair found in the victim's hand showed a probability of <0.1% that it belonged to Guirin. Nevertheless, the accused was given a life sentence!

He was involved in two very high-profile research projects. The first was a comprehensive study of the lead burden of Sydney schoolchildren. Blood from 1200 Sydney area schoolchildren was analysed over a three-year period and showed that the lead levels were unacceptably high and could



result in severe neurological damage. This lead was due primarily to air pollution from the exhausts of vehicles and Smythe's study eventually led to the reduction and later removal of lead in Australian petrols, despite a long battle with the 'lead lobby'. The second project concerned the accuracy of the newly introduced 'Breathalyser' used by police for the monitoring of alcohol in blood. Smythe pointed out that there were serious deficiencies in the precision and accuracy of the instrument when operated by police officers with limited training, so that accuracy was, at best, ±20%. Over my PhD studies we always had a Breathalyser in the lab and during Friday afternoon drinks, we had the opportunity to perform first-hand checks on our blood alcohol. After some successful court cases in which Breathalyser results were successfully challenged, the law in NSW was amended so that a Breathalyser reading by a police officer was prima facie evidence for conviction.

In 2001, Smythe was awarded a Member of the Order of Australia 'for service to science through education and research, particularly the development of the discipline of analytical chemistry'. He died aged 96 on 3 September 2018 at his home at Mt Eymard in Bowral and his wife of 73 years died five days later on 8 September. They were buried together at Bowral Cemetery.

Lloyd Smythe made a profound impact on Australian chemistry and he can be credited with the establishment of analytical chemistry as an accepted subdiscipline of chemistry in this country. He was an 'old school' professor: very distinguished looking, always wore a suit and tie, and always a true gentleman who was caring and polite to his staff and students. He leaves a great legacy to us all, especially those who were fortunate enough to work with him.

Paul R. Haddad FRACI CChem

#### 2018 RACI National Award winners



#### Applied Research Award

The Applied Research Award is given to a member of the RACI who has contributed significantly towards the development of, or innovation

through, applied research, or in industrial fields.

Professor Colin Raston's invention, the vortex fluidic device, performs greener chemical synthesis while also addressing limitations of conventional (batch processing) methods. The device has almost unlimited applications, from controlling chemical reactivity and selectivity in synthesis to materials processing. For example, by control over protein folding, the device is capable of 'unboiling an egg' - a feat for which Colin and his colleagues received the 2015 Iq Nobel Prize in Chemistry. Further practical applications have included precisely slicing carbon nanotubes in the absence of chemical stabilisers (doi: 10.1038/srep22865), fabrication of nontoxic carbon dots, synthesis of complex molecules in a single pass through the device, separation of proteins, and the acceleration of enzymatic reactions. Colin's work on thin film microfluidics also contributes to fundamental discovery by imagining the revolutionary impact on chemical manufacturing if chemical reactions could occur with extremely short diffusion path lengths (beyond diffusion control).

As Professor of Clean Technology at Flinders University, Colin hopes to help steer the planet onto a sustainable trajectory. He is a Fellow of the RACI, the Royal Society of Chemistry (UK) and the Australian Academy of Science, and contributes his expertise on the Advisory Board for *Green Chemistry* and the Board for *Scientific Reports*. Colin also served as President of the RACI in 1997.

#### Citation

The RACI Citation is intended to provide recognition to members who have, over a period of many years, made substantial contributions to chemistry, and especially to the progress of the profession.



Ashraf Ghanem, Associate Professor of Organic Chemistry at the University of Canberra, uses chemistry to prevent, diagnose and treat disease. Because of the link between the chiral nature of most biologically relevant molecules and their function, the key to testing and improving the efficacy of certain medications is the ability to switch from a mixture of chiral forms (racemic mixture) to a single enantiomer. Through the development of asymmetric and enantioselective catalysts, Ashraf can control this switch. Licensed in 2016 to Strem Chemicals, one of his patented catalysts is used worldwide to access Ritalin, a medication widely used to treat ADHD. Beyond treatment, Ashraf's work in the prevention of disease includes an ongoing project in collaboration with MyHealthTest to develop diagnostic tests that require only a drop of dried blood.

Strongly believing in fulfilling his 'academic social responsibility', Ashraf is a passionate ambassador for science. As President of the ACT Branch of the RACI for the past six years, he has become well known locally for his school visits and chemistry shows. Having brought the RACI crystal growing competition to the ACT in 2011, Ashraf has introduced thousands of students to the wonders of growing crystals.



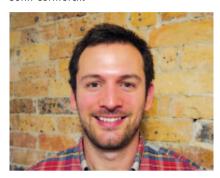
Dave Sammut is a world expert in an impossibly narrow branch of minerals processing chemistry, called chloride hydrometallurgy. As founder and Principal of DCS Technical, he develops new industrial processes for more efficient, cleaner and more economic alternatives to current technologies that recover metals from industrial wastes and mineral concentrates. He stands on the cusp of commercialising a technology that scientists have struggled with for 40 years.

Passionate about bringing science to the public, Dave is a regular contributor to *Chemistry in Australia*. Among the most recent of his 49 articles, are articles about science on vacation, expert witnesses and the strategic future of qallium.

One of Dave's foremost desires is to create a self-maintaining support system for the chemistry profession, wherein each generation helps the next. After years of match-making students with experienced chemistry professionals in New South Wales, Dave has recently taken on the position of RACI Mentoring Programme Coordinator and will be spearheading the national roll-out of the program in 2019.

#### Cornforth Medal

The Cornforth Medal is awarded to give recognition to outstanding achievement in chemistry and to promote chemical communication. The Medal, bearing the words 'For a Thesis on Chemical Research', commemorates the work of Australian-British Nobel Laureate Sir John Cornforth.



Dr Andrew Giltrap designs pathways to synthesise complex organic molecules found in nature. During his PhD studies, he completed the first total synthesis of teixobactin (doi:

10.1021/acs.orglett.6b01324), a molecule of great interest – especially at this time of increasing antibiotic resistance – due to its potential as a treatment for tuberculosis and MRSA, among other bacterial infections.

Highlights from Andrew's career so far involve a great concentration of Nobel Laureates. Having been selected to represent Australia at the 2017 Lindau Nobel Laureate meeting, he was one of 300 young scientists who gathered from around the world to meet and learn from 35 Nobel Laureates. Today he is elated to receive a medal bearing the likeness and name of great Australian-British organic chemist and Nobel Laureate, Sir John Cornforth.

Having completed his PhD in September 2017, Andrew continues to pursue total synthesis as a postdoctoral research associate at the University of Sydney. Andrew aims to one day establish his own research group, which he hopes to direct to gain a better understanding of disease through chemistry.

#### Distinguished Fellowship

A Distinguished Fellowship is the recognition of highly distinguished contributions to the chemistry profession in academia, government or industry and to the RACI.



Rather than using traditional laboratory-based techniques, Emeritus Professor **Leo Radom** from the University of Sydney studies molecules and their reactions by computer calculations. His computational quantum chemistry approach can describe and predict the structures of molecules and the mechanisms of chemical reactions.

Having entered computational quantum chemistry in its infancy, Leo has had the pleasure of watching the field blossom. A prominent contribution to the field is his co-authorship of the defining text *Ab initio molecular orbital theory*, together with (among others) Nobel Laureate John Pople. Leo was also instrumental in bringing to Australia in 2008 the Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), firmly placing the country on the map as an international centre of excellence in theoretical and computational chemistry.

Beyond his contributions to the field, Leo also holds an eminent position in the community. A Fellow of the Australian Academy of Science, the Royal Society of Chemistry (UK) and the Royal Society of NSW, a member of the International Academy of Quantum Molecular Science and now Distinguished Fellow of the RACI, he is President of both the Asia–Pacific and Australian Associations of Theoretical and Computational Chemists, having also served in the past as President of WATOC and the ACT Branch of the RACI.

## RACI Educator of the Year Award

The RACI Educator of the Year Award provides recognition to developing teachers from tutors to senior lecturers teaching in undergraduate or postgraduate university courses.



As Associate Dean of Education and Senior Lecturer (soon to be Associate Professor) at Monash University, Dr Chris Thompson's research focus is on the chemistry classroom. In 2013, Chris' overhaul of the first-year undergraduate chemistry course immediately doubled the number of students who proceeded to study chemistry in their second year, and who subsequently went on to complete chemistry majors. The key was higher engagement: in place of more lectures, the plan implemented demonstrations and in-class activities to make classes more interactive and exciting.

Chris' dream is to make the study of chemistry accessible to deaf students. Without a comprehensive vocabulary of chemistry terms in AUSLAN, deaf students fall away from the subject in secondary school. With the aid of the Australian Deaf Community, Chris is working to address this deficiency.

As Chair of the RACI Chemical Education Division in 2015–16 and since 2016 as Chair of the RACI Vic. Chemical Education Group, Chris has shared and continues to share his passion for and expertise in chemistry education with the community.

#### Fensham Medal for Outstanding Contribution to Chemical Education

The RACI Fensham Medal for Outstanding Contribution to Chemical Education is awarded to recognise outstanding contributions to the teaching of chemistry and science in general over an extended period. This award is named after Professor Peter Fensham AM, who popularised and advocated for the notion of 'Science for all'.



Associate Professor
Mauro Mocerino's
research is split
between organic
chemistry and chemistry
education. When he is
not developing potential
treatments for sleeping
sickness, Mauro
investigates the role of
active learning and

guided inquiry in both classrooms and in laboratories.

Recognising that demonstrators play a critical role in tertiary laboratory classes, he has been working since 1999 to establish professional development opportunities for sessional teaching staff. Beginning at his home institution of Curtin University, his training program has since spread to many universities in Australia and even overseas. To broaden the impact of this work, Mauro is currently working with the European Chemistry Thematic Network (as the only non-European in the working group) to develop a Massive Open Online Course for relatively inexperienced university-level laboratory teachers.

Mauro's work on training laboratory demonstrators was also recognised in 2013 with an Australian Award for Programs that Enhance Student Learning, administered by the Australian Government Department of Education and Training. Mauro is a Fellow of the RACI and the Royal Society of Chemistry (UK), and a member of the American Chemical Society. He has served as Chair of the RACI Chemical Education Division and on two occasions as Chair of the WA Chemical Education Group.

#### H. G. Smith Memorial Award

The H. G. Smith Memorial Award is given to a member of the RACI who, in the opinion of the RACI Board, has most contributed to the development of a branch of chemical science. The Medal depicts and commemorates Henry George Smith, who made significant contributions to organic chemistry in Australia with his work on natural products.



Like a molecular architect, Professor **Kate Jolliffe** directs the design of complex molecular structures. Her target molecules are designed for functions ranging from the self-assembly of nanotubes to therapeutic applications, and the transport of anions to sensing. A recent focus in her research has been the synthesis of molecular receptors for the biologically important pyrophosphate and sulfate anions. Her synthetic peptide-like receptor is capable of binding sulfate with better selectivity over competing anions than the sulfate-binding protein (doi: 10.1039/c6sc01011c).

In her tenure as Professor of Chemistry at the University of Sydney since 2009, Kate has been deeply committed to mentoring other researchers, whose successes give her a great deal of joy. As Fellow of the RACI and the Royal Society of Chemistry (UK), and as member of the American Chemical Society, she is also widely involved in the international chemistry community. Since joining the RACI in 1992, she has helped found the NSW Women in Chemistry group and chaired the Organic Chemistry Division.

Although like many other organic chemists she idly dreams of a reaction named after her, what Kate really wants is to see one of her molecular constructions used in the real world.

#### Le Fèvre Medal

Awarded by the Australian Academy of Science together with the RACI, the Le Févre Medal commemorates the work of physical organic chemist Raymond James Wood Le Févre. The purpose of the award is to recognise outstanding research in chemistry by scientists under 40 years of age at the closing date, except in the case of significant interruptions to a research career.



Associate Professor Amir Karton applies quantum chemical methods to tackling challenging problems in disciplines ranging from biochemistry to nanochemistry. Due to major advances in theory and high-performance supercomputer technology, computational quantum chemistry has become one of the most powerful means of understanding and even predicting chemical processes. Amir has played a leading role in the development of quantum chemistry methods that are capable of accurately calculating the energetic and spectroscopic properties of molecules.

Amir is a keen advocate for collaborations between theory and experiment. Combining the two approaches, he says, allows scientists to progress much further in the study of chemical problems than by using experiments or theory alone.

As a scientist, Amir's greatest driving force is the thrill of discovering something new about nature, and, as a research group leader at the University of Western Australia, inspiring students is his ultimate goal. Amir serves on the committee of the RACI Carbon Division and shares his expertise as Associate Editor of the Australian Journal of Chemistry.

#### Leighton Memorial Medal

The Leighton Memorial Medal is awarded in recognition of eminent services to chemistry in Australia in the broadest sense, including service to the RACI, research, technology, public service and national leadership. The Medal commemorates the distinguished career of Arthur Edgar Leighton, who carried out an enormous amount of work to secure the RACI's Royal Charter, and who, as a chemical engineer, served Australia's interests in both war and peace.



Emeritus Professor

Curt Wentrup works to
capture and study
reactive and unusual
molecules. The
isolation of such
challenging molecules
requires creative
methods: the marriage

of rapid intense heating under vacuum (flash vacuum pyrolysis) with capture of reactive molecules in an unreactive matrix (matrix isolation) at very low (cryogenic) temperatures is one of Curt's solutions. Combined with photochemistry and computational chemistry, this method gives a robust collection of tools for the fundamental study of chemical and physical properties, including bonding, reactivity, isomerism and the geometrical and electronic structure of molecules. A selection of these tools recently allowed Curt's team to directly observe for the first time an imidoylnitrene - previously only a hypothesised reactive intermediate (doi: 10.1002/anie.201712689).

Curt has been a Professor and Chair of Organic Chemistry at the University of Queensland since 1985. As Editor of the Australian Journal of Chemistry and Fellow of the RACI, he has worked to foster a closer relationship between the journal and the RACI. Notably, Curt founded and still coordinates a cornerstone of the Australian organic chemistry community: the Heron (Island) Conferences on Reactive Intermediates and Unusual Molecules, a highly acclaimed conference series, which regularly lures high profile international chemists to Australia.

#### Margaret Sheil Leadership Award

The Margaret Sheil Leadership Award was established in 2017 to honour the trail-blazing contributions of Margaret Sheil, the first Australian female Professor of Chemistry. The Award aims to recognise an outstanding female leader working in an area of a chemistry-related field who has helped to inspire and mentor junior female chemists and/or help to provide a more equitable work place.



By programming strands of DNA, Professor **Amanda Ellis** can induce them to assemble as tubes, boxes, sheets and crystals. Arising from this ability are endless possibilities for applications, from medical diagnostics to nanorobotics. To realise this potential, Amanda works to counter, or take advantage of, a high rate of error in DNA self-assembly by striving to attain a deeper understanding of the mechanism of this process.

Aside from her 145 publications, the chief mark Amanda envisions leaving on the chemistry profession is through her students: the research students she has supervised and the undergraduates she has taught, each of whom she believes has, or will, make their own impact on the world. The science itself is important, but she loves the translation of science and the training and mentoring of young scientists best. As the Margaret Sheil Lecturer, Amanda would also like to see equity and equality in science be recognised as a norm rather than a metric to be achieved.

Having eluded breast cancer in 2014, every day offers new potential for Amanda. She currently works at the University of Melbourne, serves on the RACI Board and the Australian Research Council College of Experts, and advises for several international scientific bodies, including for Qatar, Canada, Kazakhstan and Chile.

#### Masson Memorial Award

Established as a memorial to the late Sir David Orme Masson, founder of the RACI, the aim of the Award is to assist a young chemist to proceed in further studies in chemistry.



From volunteering as a glassware cleaner to the preparation of stock solutions, **Angus Olding** has pursued any chance to take residence in the University of Tasmania chemistry laboratories. In his third and final year of undergraduate study in 2018, Angus' research experience already spans chemistry disciplines as well as continents.

After dabbling in microchip electrophoresis, Angus discovered his true calling in chemical synthesis. Under the guidance and mentorship of Dr Alex Bissember, he has pursued several projects, including a mechanistic investigation of the Suzuki-Miyaura cross-coupling reaction. Examining why aryl iodides react slower than corresponding bromides at low temperatures, they discovered the culprit: an inefficient step of the catalytic cycle (doi:

10.1021/acs.organomet.8b00189).

Angus receives the Masson Memorial Award to continue on his path in chemistry research, which he hopes one day will result in the development of a new chemical reaction – that he promises future students he shall not name after himself.

#### Rennie Memorial Medal

The Rennie Memorial Medal is awarded to a member of the RACI with less than eight years of professional experience since completing their most recent relevant qualification, who has contributed most towards the development of a branch of chemical science. The Medal commemorates the achievements of Edward Henry Rennie, the third President of the Institute.



At the juncture of solid-state chemistry and electrochemistry, Dr Neeraj Sharma designs new materials for improved electrochemical devices. To analyse the performance of devices, such as batteries, at the atomic scale, Neeraj applies synchrotron or neutron diffraction. The most useful information is captured while the devices are in operation (doi: 10.1002/cssc.201500152) – a method of analysis that Neeraj has helped place at the forefront of Australian and international research communities.

Although he is passionate about leading the charge in the uptake of new batteries, Neeraj believes that training and the development of new minds in chemistry is even more important. Helping produce high-achieving but well-rounded chemists to revolutionise materials research and development in Australia is among his foremost goals.

Neeraj is a senior lecturer at the University of New South Wales. Among a list of professional organisations, he is a member of the International Society of Electrochemistry, The Electrochemical Society (US) and the Royal Society of Chemistry (UK). He is current Chair of the Materials Chemistry Division of the RACI and a member of the Australian Academy of Science National Committee for Crystallography.

#### Rita Cornforth Lectureship

The Lectureship was established in 2017 to provide an outstanding female early career chemist with the opportunity to achieve broader recognition of her career achievements to date. The award celebrates the pioneering contributions of Lady Rita Cornforth, the collaborator and wife of Nobel Laureate Sir John Cornforth.



Dr Yuning Hong develops chemical probes to detect dysfunctional cells. Proteins are essential for the maintenance of many cell functions. When the biological quality control process that ensures proteins fold into correct shapes fails, the ensuing proteins can damage cells – at worst leading to conditions such as Alzheimer's, Parkinson's and Huntington's diseases. Yuning studies how these proteins are generated and how they damage healthy cells. Her goal is the development of tests for the early diagnosis of and treatments for dementia and other neurodegenerative diseases.

Working at the intersection of the traditional boundaries of chemistry and biology, Yuning hopes to promote communications between chemists and life scientists. Such knowledge interchange, she believes, could facilitate biological research and promote clinical applications with the advance of chemistry technologies. As a member of the RACI and the Chinese Chemical Society, as well as the Australian Society for Biochemistry and Molecular Biology and the Biophysical Society, she is well placed to cultivate this relationship.

Yuning is a senior lecturer at La Trobe University. Her academic work recently surpassed 10 000 citations, an achievement only eclipsed by her success in helping her overweight ginger cat lose 2.5 kg in only one year.

#### Weickhardt Medal for Distinguished Contribution to Economic Advancement

The Weickhardt Medal is awarded to a member of the RACI who has contributed significantly towards the economic advancement in Australia through work in a chemistry discipline. The Medal commemorates the life and work of chemist and business executive Leonard William Weickhardt.

Tania Notaras is founder and Managing Director of Envirolab –laboratories that test for environmental contamination, workplace exposure and veterinary medical and agrichemicals. With 185 people employed in Sydney, Melbourne, Perth, Adelaide, Brisbane, Darwin and even Auckland,



Envirolab is now the largest privately Australian-owned environmental laboratory group in the country.

Tania is responsible for the overall strategy and direction of the company. Under Tania's leadership, the laboratory group has grown from conducting routine testing to include research and development. For example, the Sydney laboratory recently began offering blood testing for per- and poly-fluoroalkyl substances (PFAS), meeting a current demand. Recent expansions also include the newly opened world class laboratory facility in Melbourne.

Tania hopes to reinvigorate the field of sciences as a fulfilling career choice. Her dedication to mentoring and the development of young scientific minds is shown by her commitment to frequently host students – ranging from year 9 to the final year of university – in work experience placements at the Envirolab Group of laboratories.

Tania is also an active member in the Australian chemistry community, having recently served on the RACI Board and as the President of the NSW Branch.

Anna Ahveninen

#### **Centenary fellows**

RACI's centenary ended on 30 June 2018, and as part of that special year the RACI Board, Branches and Divisions suggested names for consideration for fellowship status. Congratulations to the following people on becoming Centenary fellows during the centenary year.

The first group of Centenary fellows was announced on pp. 26–28 of the April 2018 issue.



Associate Professor Rose Amal University of New South Wales



**Dr Sarah Cresswell**Griffith University



Associate Professor Guillaume Lessene WEHI



Miss Michelle Neil Forensic Toxicology, Forensic and Scientific Services





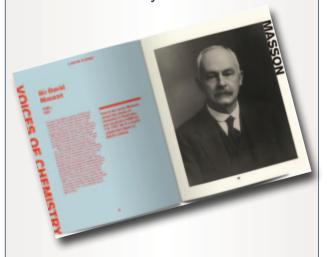
**Professor Huijun Zhao**Griffith University – Gold Coast

# Secure a piece of chemical history



Remember the RACI now and in years to come with this limited edition publication celebrating the Institute's centenary year.

160 pages of perspectives, profiles, facts and photos tell the story of RACI from 1917 to today.

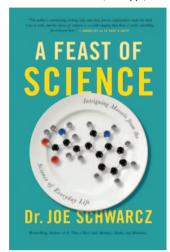


To order your copy of this hardback book, email robyn.taylor@raci.org.au. \$50 plus \$10 postage (in Australia).



#### A feast of science: intriguing morsels from the science of everyday life

Schwarcz J., ECW Press, 2018, paperback, ISBN 9781770411920, 240 pp., \$22.99



Dr Joe Schwarcz is the director of the Office for Science and Society at McGill University in Montreal, Canada. He hosts a popular radio show, appears on television, is a long-time columnist for the *Montreal Gazette* and is the author of 16 popular science books, so far. His most recent, *A feast of science*, is aimed at an adult audience.

I declare an interest. I love what my mate does.

A major thrust of Joe's efforts is to tackle scientific false news as it appears in the North American media. Mostly he does this in a cool, calm and collected manner, but sometimes he simply can't help himself, and rightly so. For this we can thank the US Constitution's first amendment concerning free speech. Joe also reinforces much of the good science that features in the news.

A feast of science is a selection of material Joe has previously disseminated locally and is thus particularly useful for us not living in North America.

The key to his success is the winning combination of academic organic chemist and great storyteller, together with a keen ear for the language that a wider than usual section of the general public will understand. So, while chemical

names do feature in the text, there are no formulas, equations or reactions. All this is reinforced by a good index.

The book consists of around 90 vignettes, each averaging around three to four pages, most triggered by an 'annoying' (North American) media 'event'. There is also some overlap where an online piece led to further discussion.

Where to start? Perhaps with Joe's rebuttal of attacks on Monsanto's glyphosate (Zero™, Roundup™) by a US researcher in computer science. That resonates, because the same issue was raised here in Australia recently by the ABC's 4 Corners program on 8 October 2108.

Joe systematically dismantles the arguments of the panic merchant blow-in from the high-tech world by explaining how glyphosate's safety parameters are set.

He also points out (as we all must continue to do) the difference between the inherent hazard of a material and its actual risk that depends on exposure.

But Joe adds further value by delving into the history of glyphosate's discovery. Back in 1970, Monsanto, then a chemical company, was searching for novel watersoftening substances. New compounds were also put through a battery of tests, revealing a couple of compounds with weak herbicidal properties. Some molecular manipulation then yielded the very active 'glycine phosphonate', quickly shortened to glyphosate. This resourceful scientist was awarded the very prestigious Perkin Medal in 1990.

Other brief accounts include: Are there fish genes in tomatoes? Can snail slime cream and bone broth really make your wrinkles disappear? What's the problem with sugar, resistant starch, hops in beer, microbeads and the 'secret' cancer cures? Plastic packaging, pros and cons. Some beefs with beef. Preserving preservatives. Then add in another 80 or so.

While you can find much of the book's material online, why would you bother when this book provides a neat package of bite-sized stories perfect to illustrate and enliven even those dull (organic) chemistry classes!

Why is Joe's style so entertaining?
Well, it has been my own personal
experience with a talkback radio segment
'Dial-a-Scientist' on ABC (ACT and
regional) that went for some years that
the negative, instant feedback regarding
a less-than-adequate answer can be
highly educational!

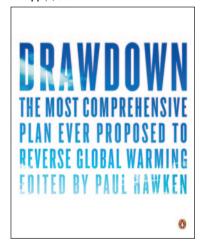
I also learned that the word 'chemistry' in a title is the kiss of popular sales death. Yet ... we all feel some sort of obligation.

I highly recommend you watch and listen to the author describe how he came to write this book (www.youtube.com/watch?v=6owcDRQjnOo). Then you can decide.

Ben Selinger FRACI CChem

# Drawdown: the most comprehensive plan ever proposed to reverse global warming

Hawken P. (Ed.), Penguin Random House, 2018, paperback, ISBN 9780141988436, 240 pp., \$35



Drawdown: the most comprehensive plan ever proposed to reverse global warming is an optimistic book. It reflects an ethos that says that we should not only be working to stabilise global warming, we ought to be striving to reverse it. To this end, the 'Drawdown project' has assembled a substantial group of experts to look at 80 potential ameliorating technologies, assessing their costs and

potential greenhouse gas 'savings' projected forwards to 2050, and giving them a rank ordering.

Essentially, the book provides a twopage overview of each of the proposed solutions, which fall into one or other of the broad areas associated with Energy, Food, Women and Girls, Buildings and Cities, Land Use, Transport, and Materials, as well as describing numerous emergent technologies ('Coming Attractions'). This is all well written and splendidly illustrated, which adds to a pleasant experience. However, at 240 pages or so, the coverage is, de facto, reasonably superficial. Inspirational essays from a number of prominent environmental thinkers also appear throughout. There is an accompanying open website (www.drawdown.org), which is more expansive.

The book pulls together a broad group of disciplines and areas. That is good. There are a few features, however, that are not so good. For example, everything is at the macro scale, so it is hard to see how anything one could do at a personal level (e.g. installing solar hot-water or photovoltaic arrays, using public transport more, forgoing hugely environmentally expensive international air travel for trivial reasons) would fit into the scheme of things. If, as the book does, one wants to project forward

to 2050, it is very important to firmly establish your starting point and clearly delineate, and defend, your projection model. Otherwise, you may as well just pluck figures supporting your 'desired answers' from the ether. While I am certainly not suggesting this is the case here, I did not find convincing evidence in either book or website of such a disciplined approach. Results need authenticating by external auditing, by either external experts or appropriate publication.

Editor Paul Hawken is an author who writes about environmental topics. He is also an entrepreneur whose work includes starting 'ecological' businesses as well as the Drawdown project described in this book. In brief, the aim of the Drawdown project is to generate and foster a groundswell social movement to tackle global warming. Hawken is reframing climate debate away from the notion that solving problems leads to sacrifice towards a scenario where solving greenhouse problems will result in better health and well-being, greater prosperity, and better and more secure employment.

I said at the start this is a hopeful book. If, like me, you often feel a sense of doom and gloom about the future of our wonderful and wondrous planet (Heck! I've even had to install a polycarbonate protective screen in front of my television, just in case I so forget myself as to throw *Drawdown: the most comprehensive plan ever proposed to reverse global warming* at climate sceptics paraded on screen!), then this book flawed as it may be, is cheery reading at a modest price. In effect, it says we have the solutions already. All we need to do is get a move on implementing them (before it is too late!)

R.J. Casey FRACI CChem

# Our 2018–19 media kit is now available at chemaust.raci.org.au.

For further information, contact Mary Pappa: mary.pappa@raci.org.au, (03) 9328 2033



# Post-filing data: a valuable tool for gaining patent protection

Brittany Howard, Patent Attorney, FB Rice



In the November–December 2018 edition of *Chemistry in Australia*, we discussed the necessity of experimental data to underpin a patent application to an invention, and, in particular, to demonstrate that the invention works across the scope of the patent claims.

There is often a difficult line to tread in deciding whether and when to file a

patent application. On the one hand there needs to be enough data/experimental results to adequately support the scope of the claims in the patent application, while on the other hand there may be a need to file the patent application as quickly as possible to obtain the earliest priority date, before research is published.

During prosecution of the patent application, along with examining the novelty and inventive step of the claims, the Examiner will consider whether the patent application meets a series of internal requirements (Section 40 requirements as discussed in the November–December edition). This assessment is based on a review of the patent specification, particularly the description and included working examples.

Should the Examiner initially consider that the claims lack patentability, the Applicant has the opportunity to try and convince the Examiner to change their mind by providing arguments in support of the invention. The arguments are strengthened by drawing upon the included working examples. For example, should the Examiner consider the claims to lack an inventive step, the Applicant may be able to refer to the data to demonstrate an unexpected technical effect that could not have been predicted from the prior art.

However, as discussed above, in order to beat publication of the research, in some cases it may have been necessary to file the patent application containing only limited experimental results. In such cases, the Applicant may want to draw upon data that was not included in the filed application, to provide additional evidence that the claimed materials or methods are inventive. This may be, for example, experimental results from additional studies carried out following the filing of the patent application. Such data is referred to as 'post-filing data'.

Whether an Applicant is able to provide post-filing data to support the patentability of the claims, and whether the Examiner is required to consider such data, is heavily dependent on the relevant jurisdiction in which patent protection is sought. In Australia, consideration of post-filing data is permitted and generally viewed favourably by an Examiner. In my own experience, an Examiner will welcome further evidence that allows them to clarify their understanding of the patentability of the claims. However, in some jurisdictions, such as China, there is no guarantee that post-filing data will be considered.

Post-filing data is of particular importance in the pharmaceutical and biotechnology fields, where such inventions have long development times. Oftentimes, experimental data pertaining to the invention, such as in vivo or clinical results, is not obtained until long after the initial patent application has been filed.

It should be noted that the post-filing data does not formally become included in the patent application, rather it is provided separately to the Examiner. As a further point, it may be difficult to rely solely on post-filing data to underpin arguments for patentability. Rather, post-filing data should be considered primarily as a means to further support and clarify the patentability of the claims, by expanding on experimental results already present in the patent specification as originally filed.

Ultimately, if the Examiner does not consider it plausible that the claims being pursued are patentable across their entire breadth, the Applicant may be forced to narrow the scope of the patent claims, and therefore forego patent protection to particular aspects of the invention. In the worst case, an Applicant may be required to narrow the scope of the patent claims to such an extent that pursuing patent protection for the invention is no longer of strategic and/or commercial value.

Accordingly, the submission of post-filing data, in permitted jurisdictions, can be a useful way to provide additional evidence as to the patentability of broad claims, and thus can be a valuable tool to obtain commercially relevant patent protection.

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

FB RICE



#### Wine, SO<sub>2</sub> and a mobile phone

Wine, electrochemistry and song' was the title of an article I wrote for the December 1996 issue of this magazine. This was all part of the repositioning of my research on wine chemistry after dabbling in environmental chemistry for several years: wine was a much more attractive medium for study. I was 'converted' to electrochemistry, perhaps more specifically electroanalytical chemistry, during a period of study leave at the University of Mainz in 1981. As many past members of my research group will testify, it was almost impossible to get through a thesis without some involvement in the joys of electrochemistry. The song part came about as a recently purchased voltammetric system would play 'I'm forever blowing bubbles' during the degassing step.

The challenge in determining  $SO_2$  in wine from a winemaking perspective is to obtain an accurate measure of the free  $SO_2$  concentration. This measure represents the pH balance between molecular  $SO_2$  and  $HSO_3^-$ , the former being the critical value for the antimicrobial action.  $SO_2$  may be bound to various wine components and this bound concentration plus the free concentration gives the total, a value often regulated in many countries. Just to complicate matters, some  $SO_2$  in red wine is weakly bound to pigments. This is often released in the measurement of free  $SO_2$ , leading to a clear over-estimate of the actual, or 'true' in wine industry jargon, concentration.

When seeking approaches to developing an electrochemical method for  $SO_2$ , the problem that we faced was the prior removal of dissolved oxygen in the wine. Degassing was not an option because the degassing step would remove some or all of the free  $SO_2$ . While working on this problem, I was fortunate to be invited to join the PhD advisory team for Guo Nan Chen in the Department of Chemistry at La Trobe University. Chen took up the  $SO_2$  challenge with great gusto, completing the PhD requirements in April 1991.

After establishing two flow injection/electrochemical methods, the measurement of the true SO<sub>2</sub> concentration in red wine still remained a challenge. This is when Chen came up with the idea of using AC voltammetry. The electrochemical reduction of oxygen is a slow electron transfer and, when using the second harmonic AC mode in particular, there was sufficient discrimination between the peaks for SO<sub>2</sub> and dissolved oxygen. Similarly, any interference from anthocyanin pigments is minimised in the second harmonic AC voltammetric approach. A comparison of the results between the AC method and a spectrophotometric method (the only check method available at the time) was sufficient to validate the AC voltammetric approach in measuring the true free SO, in red wine (Analyst, 1991, vol. 116, pp. 253-6). Despite my best endeavours at the time, I was unable to convince the wine industry or instrument manufacturers to develop a commercial instrument based on Chen's work.

There have been rapid advances in electrochemical equipment in the 20 years since Chen did his thesis work. Disposable screenprinted electrodes are now readily available, which are much easier to use than the dropping mercury electrode when I started in this field. There have also been significant advances in simplifying the size and cost of potentiostats.

This is where
Associate Professor
Conor Hogan FRSC,
FRACI CChem, and
Darrell Elton from
La Trobe University
enter the story. After
demonstrating the capacity
of utilising a mobile phone

for electrochemiluminescence (ECL) detection, the researchers then turned their attention to adapting a mobile phone for 'good old-fashioned electrochemistry' (to use their term). It turns out that

within the mobile phone electronics, there is sufficient diversity that it can be used as an analytical instrument. In the ECL procedure, the audio output can generate an applied voltage to the sample and the resulting luminescence can be collected by the phone's built-in camera.

For an electrochemical measurement, the audio output applies the voltage that Conor tells me consists of 'an AC perturbation superimposed on a triangular waveform'. The resulting oxidation or reduction current can then by monitored utilising the microphone connection of the phone. The current/potential output is mathematically treated to generate what ones expects for a second harmonic AC voltammogram with peak area related to concentration. This simple and elegant approach is now under patent (WO 2017/156584 A1).

The image gives an indication of what the system looks like – all that is missing are the electrodes. Having seen the system in operation for assessing  $\mathrm{SO}_2$  in wine, I was amazed at the simplicity of its operation, and while the technology is still at the proof-of-concept stage, there is every possibility of its success in measuring the true free  $\mathrm{SO}_2$  in red wines in a rapid and easy-to-use way.

The 'ElecTrobe' project, as it is known, has received considerable funding from La Trobe University's Strategic Innovation Fund as well as Wine Australia. Collaboration with the National Wine and Grape Industry Centre at Charles Sturt University will provide the necessary wine expertise to ensure that the ElecTrobe measures what is of vital importance in wine production quality control.



Geoffrey R. Scollary FRACI CChem (scollary@unimelb.edu.au) has been associated with the wine industry in production, teaching and research for the last 40 years. He now continues his wine research and writing at the University of Melbourne and the National Wine and Grape Industry Centre at Charles Sturt University.

#### **Guts and grunts**

The Australian Open is on again this month, so we can expect to hear the ping of racquets and the grunts of tennis players in Melbourne. As with other mass-public events such as football, quasi-religious festivals and horse racing (the sort of event where not all of the participants survive), we can expect to see media coverage that runs along familiar lines. But no doubt bored by the sameness of each year's event, journalists will be striving to find novelties to write about or to present. Here I'm following up on one that caught my eye a couple of summers ago. It seems there's more to stringing a racquet than you might imagine. Players might favour 'natural' or synthetic (mostly polyester) strings, adjusted to their preferred tension, and in some cases strung by only their chosen specialist.

'Gut' is the natural material, and it's made here in the Melbourne suburb of Braybrook by a firm whose origins go back to the 1920s. There is a small area, just a few streets in the western suburbs, where companies turn the by-products from local abattoirs into useful products. It started with the production of glues and sausage skins, and moved on to surgical sutures. We used to call it catgut ... but it was never made from cats! In fact, the company started with mutton but moved on to beef because the fibres were stronger. The starting point for preparing fibre was the serous membranes, such as those enclosing intestines, the raw material being known as serosa and consisting of collagen. Newspapers of the

period report the concerns of the local council about the odours associated with such noxious trades (as they were known), as several businesses set up in the area.

The business that survives today (lower photo) was founded by the Baker family, but the earliest entry in the directory I could find, and the name on the Tennis String Factory (upper photo), was Ficken, Halliday & McClelland. In the 1930s, the business became Klipspringer, named after a particularly springy antelope, and that's the present name on the building. Contracts were secured with the makers of tennis racquets, Dunlop/Slazenger and Spalding. The string was made in pieces, rather like the old way of producing rope on a rope-walk, and as tennis racquets grew larger and larger, string was made in 36-foot (11-metre) lengths, and then 40-foot (12-metre) lengths.

Klipspringer are still making natural (gut) tennis strings at the Braybrook factory, but in the 1980s they began to import synthetic strings from Japan, and then began to market stringing machines. In both natural and synthetic strings, several component strings are twisted together, and the natural strings may be coated with a polyurethane to minimise the





effects of absorption of moisture by the collagen.

Historically, natural fibres were used in stringed musical instruments that are plucked, like harps, or bowed, as with violins and the like. Some musicians eager for a baroque sound still prefer gut, but most of today's strings are synthetic. Even with polyester, however, some of the magic of natural products survives in the form of the rosin (from pine trees) that is used to accentuate the vibrations from a bowed string. The rosin comes in several grades, to be chosen by the musician, and a range is available from music shops. It's mostly applied before the musicians come on stage, so you are unlikely to spot it being used. You see it at another type of public event, one that most of us only watch at Olympic Games times. When gymnasts need a good grip, say on the parallel bars, they dust their hands with powdered rosin that they shake out of a cotton bag.



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

#### cryptic chemistry

#### Safety in Laboratories and Laboratory Design and Construction Standards Explained

4-6 February 2019, Parkville, Vic labsafety.com.au

#### 4th Future of Surfactants Summit

6-7 February 2019, Madrid, Spain wplgroup.com/aci/event/surfactants-summit

#### PhysChem 2019

11-14 February, Perth, WA physchemperth2019.com.au

#### Industry Meets Academia – Be More Ready for Industry – Collaboration

13 February and 10 April 2019, Melbourne, Vic ivvy.com.au/event/VCB829 ivvy.com.au/event/VCB830

#### ISE Student Symposium on Electrochemistry

29 April 2019, QUT, Brisbane, Qld ivvy.com.au/event/ELD822

#### 21st Australia and New Zealand Electrochemistry Symposium

30 April 2019, QUT, Brisbane, Qld ivvy.com.au/event/ELD822

#### Asian Federation for Medicinal Chemistry International Medicinal Chemistry Symposium

8–11 September 2019, Istanbul, Turkey aimecs 2019.org



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#### Across

- **1** Sounds absurd, trick to make an element. (7)
- **5** Sarcastic man trod erratically. (7)
- 9 None cuter! Mess up face. (9)
- 10 Sing time stream. (5)
- **11** Bird germane to concentration. (5)
- **12** Our home has one opening which lets in UVB. (5,4)
- Four or five elements with two amine groups attached to the same carbon atom. (7)
- **15** Tie in boron/sulfur reaction to yield a pnictogen hydride. (7)
- **17** Pressures of 91211316. (7)
- **19** Love arm wrestling elimination. (7)
- **21** Our side of mess. Something smells! (9)
- 23 Earliest beginnings to film integrated rapid storage technology. (5)
- 24 See 4 Down.
- 25 Picky with sulfur option. (9)
- 26 Not as long: rots her socks. (7)
- 27 Structural analogs of ketones relocated one less. (7)

#### Down

- 1 Magic carpet's lines. (7)
- 2 Cut thin slice of mixtures of glycerophospholipids. (9)
- **3** Generate calcium application. (5)
- **4 & 24 Across** Tried noxious unstable gas. (7,5)
- 5 Typifies specula. (7)
- 6 Rare transition metal makes him untrue. (9)
- **7 & 8 Down** Emulate ion on forming ethylaniline. (12)
- 8 See 7 Down.
- **14** Lessening bet at mean deviation. (9)
- 16 Transposition in account. (9)
- 17 They're positive! No sport being played! (7)
- **18** Back! No time! No sports being played! (7)
- 19 Outcomes from lustres. (7)
- 20 Tenants' old messages. (7)
- 22 I'm making ion with a carbon/nitrogen double bond. (5)
- 23 Describes the centre of attention emanating from a floc. (5)

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

#### Historic vote for four SI units

A convocation of delegates representing 60 countries voted on 16 November in Versailles to implement the most significant change to the International System of Units (SI) in more than 130 years. For the first time, all measurement units will be defined by natural phenomena rather than by physical artefacts. The event was the 26th General Conference of Weights and Measures and was hosted by the International Bureau of Weights and Measures.

While consumers and most industries will not notice immediate impacts, scientists expect the change ultimately to inspire new technologies and to reduce the cost of calibrating industrial processes and scientific instruments.

After decades of scientific work by national measurement institutes (NMIs) from around the world, the delegates have voted to redefine the kilogram and three additional basic SI units: electric current (ampere), temperature (kelvin) and amount of substance (mole). The new definitions will be effective on 20 May 2019, World Metrology Day, which celebrates the establishment of the SI, or metric system, in 1875.

Currently, there is only one true kilogram, Le Grand K, which is secured in a vault outside Paris and used to calibrate all measures of mass throughout the world.

Made of platinum-iridium, Le Grand K, like any alloy, may change over time by absorbing molecules from the air or losing them through cleaning. However, these incredibly tiny changes mean that the artefact is no longer accurate enough for anticipated future advanced research and technological applications.

Over the last 40 years, with the advancement of quantum science, scientists have measured natural constants such as the speed of light and the Planck constant with exceptional accuracy. Using combinations of these constants and the equations of quantum mechanics, scientists created revised SI units for measuring mass, electric current, temperature and the mole that are at least one million times more stable than artefacts such as Le Grand K.

Since the 1700s, scientists have dreamed of having an accurate and precise measurement system that could be realised anytime, anywhere. Scientific advances in quantum science, many of which have occurred at NIST and other NMIs around

the world, have finally made this possible.

Quantum phenomena that are identical everywhere are already used to define the second, which is the SI unit for time, and the metre, the SI unit for distance. The second is defined as 9 192 631 770 natural oscillations of microwave radiation released by the element caesium, and the metre is defined as the distance travelled by light in a vacuum in 1/299 792 458th of a second. These revised definitions, implemented in 1967 and 1983, respectively, were necessary for the invention of GPS and many other modern technologies.

In May 2019, when the revised definition of the kilogram is implemented, it will be based on three fundamental constants: the Planck constant, the speed of light and the caesium atom's natural microwave radiation. The Planck constant describes the size of the packets of energy or quanta that atoms and other particles use to absorb and emit energy.

The current kilogram mass exerts a specific amount of force in Earth's gravity. The revised definition replaces this determination of mechanical force with an electromagnetic measurement tied to the Planck constant and based on electrical current and voltage. Using an instrument called a Kibble balance, after its inventor Bryan Kibble, an electric current is generated in a coil to produce a magnetic field strong enough to balance a mass of one kilogram. The method requires a precision measurement of local gravity, which varies depending on elevation and several other factors. It also requires moving the coil through a magnetic field of known strength and at a known speed;



The US delegation at the 26th General Conference of Weights and Measures where more than 55 countries voted to redefine four of the seven base units for the International System of Units (SI).

G. Porter/NIS

hence the tie as well to constants used to determine time and frequency.

In a similar way, the SI unit for the ampere will now be based on the constant for the charge of the electron. The kelvin will be based on quantum-level measures of atomic motion and will be tied to the Boltzmann constant that relates an object's energy to its temperature, as well as on the Planck and caesium frequency constants; while the mole will be based on an improved value for Avogadro's constant.

According to Jon Pratt, a long-time researcher and supervisor for the NIST group, the two industry sectors most likely to benefit fastest from the redefinitions are electronics and pharmaceuticals. The current SI unit for the ampere is impractical to realise, and as a result, precision electrical measurements have been based for 30 years on quantum measures such as the quantum Hall effect and Josephson junctions that generate quantum voltages. The change puts electrical measurements back into the SI where all other measures are made.

This capability to more accurately scale measurements from the quantum level to the massive sizes of galaxies is a key advantage as well for the other newly revised SI units based on natural constants

For further information, visit nist.gov/si-redefinition.

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..the small business sector accounted for close to 44 percent of total employment in selected private sector industries, it accounted for 35 percent of total Industry Valued Added (IVA) of those industries..."

Source: ABS, Australian Industry, cat. no. 8155.0, June 2017



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