

Synthetic polymers with DNA properties
Wood preservation on the **Mary Rose**

Automated synthesis: joining the dots
The impact of **atmospheric chemistry**

How did your education lead to your job as a journalist?

I really enjoyed chemistry at school, and after my A-levels I spent a year in industry at GlaxoWellcome (as it then was) in Ware. I was doing analytical chemistry, testing how new valve designs for asthma inhalers affect how the drug inside is delivered. During my degree I was geared up to work in pharma – I went back to the same lab the summer after my first year, then had a synthetic placement at GSK in Harlow after my second, and another summer doing synthesis with AstraZeneca at Alderley Park after my third year.

I stayed on in Cambridge for a total synthesis PhD with Jon Burton – he was fantastic to work with and was doing interesting chemistry. I moved to Oxford with him at the beginning of 2007, so I actually have a DPhil from Oxford rather than a PhD from Cambridge! But I slowly realised that while I enjoyed mixing chemicals in the lab, I didn't have a particularly strong interest in strategic planning and working out what molecules to make next. I was much more interested in what other chemists were doing – I'd be the one bringing wacky papers to literature meetings, while everyone else brought hardcore total synthesis.

I entered the *Daily Telegraph's* science writing competition, and somehow managed to win. This led to me going to conferences with BASF and Bayer, and I wrote a piece for *Chem@Cam* on sustainability after meeting you there. I also wrote a few more things for the *Telegraph*. This made me think I should seriously consider writing as a career.

I finished my PhD in 2008 and I returned to Cambridge as my fiancée (now wife) Jess was still there as a post-doc in materials science, having already finished her PhD in biomedical materials. She's more efficient than me! I applied for the Royal Society of Chemistry's graduate scheme, and was given a place. I spent four months in the international development team looking at opportunities for RSC involvement in advancing the chemical sciences in India and the Middle and Far East. It was fascinating.

But my aim was a job on *Chemistry World* and, luckily, one came up four months after I joined. I've now been on the magazine just over six years.

What roles have you had on the magazine?

I started out as a science correspondent, and I think it's the best non-lab-based job any chemist could want to have. I was reading a lot more papers than I ever would as a student, on much more varied topics. I would be speaking to the people doing the most cutting edge chemistry in the world on a daily basis – Nobel prize winners, chemists work-

Cambridge chemistry (and *Chem@Cam*) alumnus Phillip Broadwith is now business editor at *Chemistry World*. He explains to Sarah Houlton how he got there, and what makes his job so exciting



ing at the atomic scale, on interstellar chemistry, or even synthetic biology. It was an amazing way to broaden my horizons. I then spent a year covering the features editor position, which is very different – the articles are longer, and the role was much more editorial, dealing with other people's writing. It also helped me develop my own style.

Then, two years ago, I became business editor. This means I've moved slightly away from the science, but I have a strong desire to bring the science done in industry into the magazine's business section. There's a lot of really interesting chemistry going on in the commercial sector, and I want people to see that. It can be difficult to get people to tell you about it, but if you get hold of someone who knows what they are allowed to talk about and exactly how far they can go into the chemistry before it becomes sensitive, you can find out some really interesting things.

The internet has made a huge difference to the way many magazines work, hasn't it?

Yes, it means we're constantly putting news items up on the website, and once a month many of them are packaged up and put into the print magazine. The printed version isn't an afterthought, though – it does a very different job. We're lucky to get the time and resources to pursue some longer term, more investigational work, as well as having a pool of talented freelancers to call on.

The role of the editor, in some ways, is to be mindful of the wider trends, and see the bigger picture. I think that because we talk to so many people and see so many papers, we're some of the best informed people in the general

chemistry community, at least at a superficial level. Sometimes we spot connections between scientific fields that seem disparate, and it's the same on the business side – you get a view of what's going on in the tumultuously changing landscape, and can pick out trends. Being in the middle gives us the opportunity to see things as they are happening, and draw them together.

Our new editor is keen that we should become more involved in the chemical sciences community, and use that top-level view of what's going on across the chemical sciences, how industry integrates with academia, and what's happening on the political side.

How has your Cambridge chemistry experience assisted you in your career?

Natural sciences was an absolute boon. I took chemistry, materials science and biology of cells in the first year, so that was quite broad. Physics was a bit too hard! I followed that with chemistry and pharmacology in Part Ib, gaining a good grounding in general chemistry and how it feeds into other subjects. My experiences in pharma helped, too, as I've seen what an industrial lab is like from the inside. I still supervise Part IA chemistry students at Robinson, which helps me keep in touch with basic chemistry knowledge. Chemistry gave me the critical and analytical eye that allows me stand back and ask the important questions.

You must always be on the lookout for stories!

Absolutely! We have a staff of seven or eight journalists, but there's no way we can cover every journal, every company, and know everything significant that's going on. We do try, but some of our best stories come from people who've got in touch with us. I would encourage anyone with an interesting story to tell, whether it's academic or from industry, to tell us about it.

It's not always clear from the information in an academic paper or a company press release what the most interesting parts really are. We want to know the human angle. How long did it take? Where did the idea come from? These things bring a story to life, and allow people to relate to it, but they're systematically removed from papers!

It's usually best to go to a named person, and people can email ideas to me at BroadwithP@rsc.org. Of course not everything we're sent will go in, but if we don't hear about it, we can't write about it.

A thank you

Sarah Houlton, who has been the writer, editor, designer and producer of *Chem@Cam* since the Spring 2003 issue, has told us that she will be stepping down after the current issue.

For more than a decade she has brought us a lively mixture of stories, from heavy-duty science and personal profiles of staff to news of weddings, births, parties, prizes and deaths.

She refreshed the design some years ago, and took over all the production steps herself except the printing and posting.

Her articles have helped inform past and present members of the department with clarity, humanity and humour.

We'll greatly miss her, and wish her well in her future career. Meanwhile, the search for a worthy successor has begun.

Jeremy Sanders

From Eagle to Arms

Dear Editor

Although it is more than 50 years ago and memories fade just a bit, I think I can substantiate the substance of Tom Banfield's letter, (*Chem@Cam*, Summer 2014).

The taxi ride back from the Spread Eagle to the department certainly happened in around 1961, and I think it was when Professor Norrish was entertaining some Russian visitors.

Earlier in the day I had been in the library when the Professor brought in the visitors, and pointed out the Leys School through the window explaining that it was an English public school, which meant that parents paid for their sons to attend the school. This seemed to horrify the visitors but Norrish responded, 'You have the same thing in Russia, you know!'

Of course, we all have our weaknesses but not all of us have a Nobel Prize!

Tony Kallend (1956-1962)

eChem@Cam

Chem@Cam is now being sent out by email to those who have asked for a pdf version rather than a hard copy in the mail.

If you would like to swap your paper magazine for an e-version, send an email with the subject line 'eChem@Cam' to news@ch.cam.ac.uk, and we'll send it to you electronically from the next issue. Don't forget to tell us your postal address so we can check that the correct person is removed from the mailing list for the paper magazine.

You can check out e-back issues at www.ch.cam.ac.uk



Letter from the editor

Regular readers may have spotted that the Autumn 2014 issue did not happen. There's a good reason for this – as I was putting the pages together in December, I had a subarachnoid haemorrhage. Thanks to an exceptionally talented vascular neurosurgeon and his team, I am still here, and in remarkably good shape, albeit with rather more titanium in my brain and skull than is normal. I have been incredibly lucky.

However, it's rather difficult to craft stories and wield Quark XPress page layout software when one's in an ICU bed, and the magazine was somewhat delayed. But here, finally, is another issue of *Chem@Cam* for your delectation.

It will also be my last. I had already decided before that recent brain surgery escapade that it was time to move on. Eagle-eyed readers of the puzzle page will have already worked out that I now live in the US – just outside the 'other' Cambridge, in fact – having moved here with my husband's job at Pfizer four years ago.

The modern electronic world made it possible to put the magazine together remotely, with the odd trip to the original Cambridge to keep in touch with the department and the people there. But it was getting increasingly challenging to keep up with all the comings-and-goings from 3000 miles away.

I am sad to be leaving – it has been an honour and a privilege to be part of the department for the past dozen years. Thank you to everyone who has helped make the magazine what it is, particularly photographers Nathan Pitt and Caroline Hancox (not forgetting John Holman and Paul Larham from past days), Brian Crysell for his encyclopaedic knowledge of the department past and present, Dave Pratt for computer support, Sheila Bateman for knowing everyone's name (invaluable when captioning pictures!), Steve Ley for all his support (and for introducing me to Cambridge chemistry all those years ago), and Jeremy Sanders for his unwavering support, advice, and proof-reading skills. Plus all those who have contributed the stories and ideas that make the magazine what it is. And, of course, you, the readers, letter-writers, reminiscence-senders and puzzlers, without whom the magazine would not exist.

I remain a freelance science journalist, and shall continue to take a keen interest in the exciting chemistry that's done in Cambridge in the future!

Sarah Houlton (sarah@owlmedia.co.uk)

chem@cam

Chemistry at Cambridge Newsletter

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Cover



Giulia Iadevaia, a postdoc in Chris Hunter's group, operating a microplate reader in the new Dudley Williams lab

Photograph:

Nathan Pitt

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A welcome family visit!

The department had a surprise visit recently from Katie Franks, who's the daughter of Sir Harry Melville, after whom the Melville Lab is named. She had called Melville secretary Glenda Harden on the off-chance that she could pop in to take a look at the lab her father founded. Glenda assured her that she would be most welcome, and Silvia Vignolini had the happy task of showing her around the lab.

Harry Melville died in 2000 at the age of 92. His polymer chemistry research played a vital part in the development of industry in the fields of plastics, synthetic rubber and man-made fibres. He studied in Cambridge in the 1930s, and in 1938 became Eric Rideal's assistant research director in the Colloid Science laboratory, with a focus on polymers. Following his war work as scientific adviser to the chief superintendent of chemical defence, he moved to an academic role in Aberdeen in 1945 and, later, on to Birmingham.

As a physical chemist, his research included the bonding mechanisms that occur in the formation large polymer molecules, and the development of methods for measuring the rates of chemical reactions in the unstable environment immediately before an explosion. These were important in develop-



Katie and Silvia with Sir Harry's portrait

ing new polymerisation reactions.

Katie found the visit both exciting and memorable. 'I know my father would be very proud and pleased about all the research that is going on,' Katie says. 'It was very special seeing his portrait hanging up on the lab wall, and amazing to have photos taken beside it.'

Photo: Caroline Hancock

A lifetime's achievement

The 2014 Economic Times Lifetime Achievement award has been made to Yusuf Hamied. Yusuf studied here as an undergraduate in the 1950s, and then gained a PhD in organic chemistry in 1960, working with Lord Todd.

The award recognises people whose corporate achievements set an example for the current generation of leaders, at home in India and around the world.

His company, Cipla, was a pioneer in the development of generic medicines. A particular achievement is its provision of affordable antiretroviral medicines to treat HIV infections in developing countries. He is now the company's chairman, after half a century as its managing director.

In his acceptance speech, he highlighted the importance of producing affordable drugs to address the health issues facing the world today.

Chris Abell is to be the university's next pro-vice-chancellor for research. He will be one of five PVCs, who support the vice-chancellor in providing academic leadership to the university, and help drive strategy and policy development.

'I think it is a very important role and a very exciting opportunity,' Chris says. His three-year appointment starts in January next year.

Cambridge chemistry's REF excellence

The eagerly awaited results of the UK's Research Excellence Framework, or REF, were released in January, and Cambridge chemistry performed extremely well.

The highest rating, 4*, was given to 57% of our submissions. This rating is defined as 'world leading'.

This proportion of 4* gradings makes us the department with the largest percentage of world-leading papers. We also topped the grade point average, with a score of 3.54 out of 4. And we were second in impact performance, too.

The results demonstrate the department's strength as a leader, both in the UK and internationally, says head of department Daan Frenkel.

'Our competition is international,' he says. 'In that competition, scientific excellence is crucial.'

He also thanked all members of the department for the time spent on the submission. 'This result would never have been possible without these efforts in carrying out top research,' Daan says.



As part of last September's university alumni festival, we invited former members of the chemistry department to visit us to find out what we're up to. The event was hosted by Alan Battersby. Come and visit next time – we'd love to see you!



Photos: Nathan Pitt

Remembering Lord Lewis

A symposium was held at the end of February to honour the late Lord Lewis, who died last year.

The symposium, which took place at Robinson College, showcased Jack's contribution to both science and the wider world.

It included talks and reflections on Jack's life and work by several scientists who worked with Jack at key points in their careers, including our own Melinda Duer and Clare Grey, plus Brian Johnson, who was the event's host.

Other speakers included Nobel laureate Richard Schrock of MIT, Lutz Gade of the University of Heidelberg, Edwin Constable of the University of Basel, Robin Clark of UCL, Sir Ronald Mason, who is a former chief scientific adviser to the Ministry of Defence, and Nicola Nicholls, chair of the Woodland Trust.

For donations in memory of Jack, the department and Robinson College have set up a three-year graduate studentship in chemistry in his name. This fund will allow a talented individual to study at Cambridge, and will be a fitting tribute to Jack's legacy.

You can find out more about the studentship by visiting the the Robinson website, at <http://bit.ly/1EqmFsW>, where there is also a link for donations.

Maximum impact at NERC

This year, for the first time, UK funding body the Natural Environment Research Council, or NERC, made impact awards to recognise and reward the contribution of NERC science to the UK's economy, society, well-being and international reputation.

Awards were made in four different categories – economic impact, societal impact, early career impact and international impact.

John Pyle, Neil Harris and colleagues in Cambridge and the National Centre for Atmospheric Science won the international impact prize – and were also adjudged the overall winners. The awards were presented at a ceremony

held in London in January, which also marked the start of NERC's 50th anniversary year.

The award citation explained that the team's atmospheric research has played a leading role in demonstrating the effect of man-made gases on the ozone layer, and the consequences for human health. Their contributions played a key part in the strengthening of the Montreal Protocol, widely regarded as one of the most successful international agreements ever enacted. The protocol, along with other pieces of related legislation, has ensured the rapid phase-out of ozone depleting substances. As a result, the hole in the ozone now



John and Neil receiving their awards from Jim Al-Khalili and Lord Selborne (left), and celebrating their win (above)

appears to be slowly closing, preventing a number of UV-related health problems worldwide, including skin cancer, sunburn and cataracts.

'I am sure that you will all join me in congratulating Neil, John and their collaborators present and past with these exceptional marks of recognition,' says head of department Daan Frenkel.

John also appeared on the Australian news programme AM, discussing a report that revealed the ozone layer is on track to recovery in the light of concerted international action against ozone-depleting substances.

The 2014 report, 'The scientific assessment of ozone depletion', attracted widespread media coverage for its positive message on the success of the 1987 Montreal Protocol, which relies on international cooperation to reduce the production and consumption of ozone-depleting chemicals. John was a co-chair of the assessment, and Neil a lead author. The report is published every four years by the United Nations Environment Programme and the World Meteorological Organization.



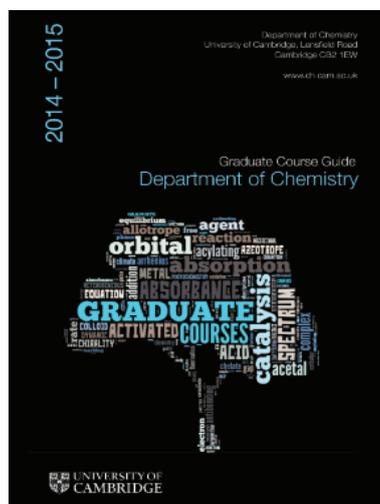
A new deputy head for the department

The department has a new deputy head responsible for staff-related matters – Nick Bamos. He takes over from Jane Clarke, who has fulfilled this challenging role since 2011.

Jane was the driving force behind our successful application for the Athena Swan bronze award. In addition to the deputy head role, Nick will also chair the Athena Swan task force that is preparing our forthcoming submission for a silver award.

'I am extremely grateful to Jane for all the things she has done for the department,' says Daan Frenkel.

'All the changes in the department that Jane has instigated have made everyone of us aware of the continuing need to make it an even better place in which to work.'



Following two years of trial lectures and workshops, the department now has a training programme open to all graduate students, whether MPhil or PhD. Postdocs are also welcome to participate, as are students from other departments

Your department needs you!

Please come back and talk to our current graduate students and postdocs about how your PhD, MPhil or postdoctoral work led to the career you now have!

We currently have several confirmed sessions, on patent law, teaching in schools and in higher education, going on to postdoctoral research, chemical science publishing, entrepreneurship & innovation, science policy & government, the energy industry and analytical chemistry. But we'd also love to have input from those who have taken other career paths that might be of interest to our current cohort of students. Sessions will be scheduled around May 2016, so there is plenty of time to prepare...

If you think you might be able to contribute, please contact Deborah Longbottom at dal28@cam.ac.uk – she would be delighted to tell you more.

A prize for JMT



Sir John Meurig Thomas has been awarded the Ahmed Zewail prize in molecular sciences. It was awarded to John for his outstanding contributions to the fundamental understanding of the structures of solids, and the development and application of the concept of single-site heterogeneous catalysis.

As well as a gold medal and a cash prize, John presented a lecture at this year's American Chemical Society's spring meeting, held in Denver.

This is the fifth time the prize has been awarded – and the second time it's been won by a Cambridge chemist. David Buckingham was the first recipient, back in 2007.

The library's all of a Twitter

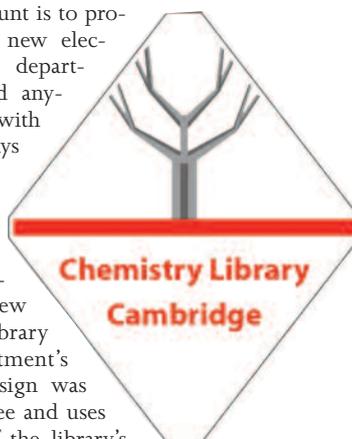
The chemistry library has entered the social media age, with its own Twitter account, at @chemlibcam.

'The aim of the account is to promote library services, new electronic resources, new department publications, and anything that will help with research and study,' says librarian Clair Castle.

'You can also use it to communicate with us.'

The Twitter avatar features the library's new logo, designed by library staff and the department's photographers. The design was inspired by the steel tree and uses colours reminiscent of the library's décor. The steel tree symbolises Yggdrasil, the huge ash tree from Norse mythology whose roots are in the underworld, and branches reaching up towards the light in the heavens.

The library's Twitter feed is also embedded in its blog, which is full of other useful information for library users. It can be found by going to cambridgechemlib.wordpress.com.



Transferring knowledge

It's a warm welcome to the department to Yolande Cordeaux, who joins us as our new knowledge transfer facilitator, or KTF. This represents a refocusing of the previous research facilitator role, which was held by Isabelle de Wouters.

Yolande was previously with the university's academic division, where she was the NERC impact coordinator, having previously been involved in supporting the university's REF submission.

The role, facilitated by EPSRC impact acceleration funding, has a strong focus on developing impact activities and relationships with corporate partners. She will support the academic staff in their applications for research funding, and help to promote wider and more effective engagement across the department with the 'impact' agenda. The aim is to enhance our efforts to translate basic research into applications.

Her activities will cover the whole of research in the field of chemical sciences, including activities at the interfaces with life, medical and environmental sciences.

Meanwhile, Isabelle has taken up the post of director of scientific development for the energy@cambridge strategic initiative. This is funded by the vice chancellor's endowment fund, and reports to the pro-vice-chancellor for research. She remains a member of staff here in chemistry, but her role will focus on university-wide activities under the initiative.

A bilateral Polish meeting

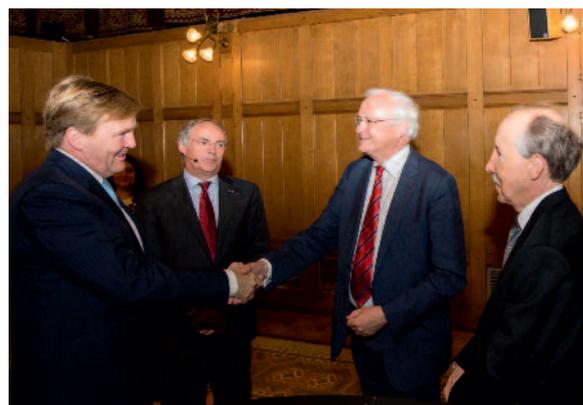
In September, Cambridge played host to the second Cambridge–Warsaw Young Scientists meeting, under the auspices of the EU's 7th Framework Programme.

The annual bilateral meeting aims to bring together young investigators from Cambridge and the Institute of Physical Chemistry at Warsaw's Polish Academy of Science. It is part of the Noblesse project, designed to establish the Polish institute within the European nanoscience community.

During the intensive two-day event, lectures from leading scientists in the broad field of materials chemistry were presented, including Clare Grey, Erwin

Reisner, Silvia Vignolini and Andrew Wheatley. There were also about 20 short presentations by young Polish and UK-based chemists, plus a large number of posters.

It also provided a platform for PhD students and postdocs to present their research, take part in scientific discussions, and build informal networks. Lectures were held in the BMS theatre here in chemistry – as you can see from the photo, it was a pretty big event, with 120 delegates, half of them from Poland. The Polish visitors were hosted in Jesus College, and social events organised throughout the university.



We reported in the last issue that Chris Dobson had been chosen as one of the recipients of the Netherlands Academy of Sciences' prestigious Heineken Prize, in the prizes' 50th anniversary year. These prizes are given every other year to five internationally renowned scientists, and Chris won the award for biochemistry and biophysics. The prize was presented at a ceremony in October, which was held in Amsterdam. Dutch King Willem-Alexander was in attendance to meet the awardees – the picture shows Chris meeting the king.



With 120 delegates, there were plenty of opportunities for dialogue and network-building

Climate model training

At the beginning of January, the department welcomed a group of scientists for a training course on the UK chemistry and aerosols (UKCA) composition-climate model, developed in John Pyle's group in collaboration with groups at Leeds, Oxford, and the Met Office.

'It allows chemistry and aerosol processes in the atmosphere to be simulated in the Met Office Unified Model,' explains Luke Abraham, who ran the course. 'This means that it can be used for air quality forecasts, for example Defra's air quality forecasts are provided by UKCA. It's also been used in international assessments, such as Met Office simulations that contributed to the IPCC 5th Assessment Report. UKCA results have also fed into the WMO Scientific Assessment of Ozone Depletion.'

Luke contributes to the model's development and provides national support for users. In the past, he has been funded to write online tutorials and run several two-day face-to-face sessions. The January course, funded by NERC, expanded on this.

The week-long course featured a series of lectures in the mornings which focused in detail on the different processes simulated by UKCA. These were given by a number of people from Oxford, Edinburgh, Lancaster, Leeds, Reading, and the Met Office. In the afternoon, the attendees took part in practical sessions that allowed them to learn how to configure and run UKCA, add new chemical reactions, and output new diagnostics.

'We had 22 attendees, plus a dozen lecturers,' Luke says. 'As well as Cambridge, they came from UEA, Exeter, Reading, Leeds, Birmingham, Edinburgh, and one came all the way



from Melbourne in Australia.'

Luke has already applied for funding to repeat the course next year, and hopes it will become a regular event. 'The participants got a great deal out of the course, and the number who came was encouraging,' he says. 'It was hard work, with all that information condensed into a short time, but the feedback I've had has been positive. It was very worthwhile.'

Practical sessions and lectures made for a busy week!



Prizewinning trio

The 2014 Bob Hay lectureship was awarded to Oren Scherman. The lecture, awarded by the Royal Society of Chemistry's macrocycles and supramolecular chemistry group, is given in memory of Bob Hay, one of the pioneers of macrocyclic chemistry in the UK.

Each year's winner is a younger chemist, who can work anywhere within the field of macrocyclic or supramolecular chemistry. Oren gave his lecture at the group's annual conference in Norwich in December.

Andreas Bender won the Hansch Award. This prize goes to someone under 40 who has made a significant contribution to the field of quantitative structure-activity relationships.

He won for his 'outstanding contributions in the field of molecular similarity,

and integrating biological and chemical descriptors for *in silico* pharmacology'.

The awards are presented at the European QSAR symposia, and the Gordon research conferences on computer-aided drug design.

It's been a good few months for Gonçalo Bernardes, whose chemistry has brought him two prestigious prizes.

First, he was awarded the European Young Chemist Awards' Silver Medal. He received this after presenting his group's research at the European Chemistry Congress in Istanbul.

He also received the 2014 European Prize of the Royal Chemistry Society of Spain's chemical biology division. This award recognises outstanding young research leaders in the field of chemical biology. The prize also includes presenting a lecture at the society's biennial meeting in La Coruña this coming July.

Stork lecturer

Ian Paterson recently visited the University of Wisconsin in Madison, where he had the honour of being the inaugural Gilbert Stork lecturer.

'Gilbert has generously endowed a lectureship series in organic synthesis at Madison where he did his PhD, and I was invited to be their first speaker,' Ian says. 'My postdoc, in 1979-80, was with Gilbert Stork at Columbia University, New York.'

Gilbert is world renowned in the organic chemistry community as a giant in the field of synthesis, and was the Todd visiting professor in Cambridge back in 1979.

'He still goes to work at the age of 92,' Ian says. 'Perhaps some of my colleagues would like to emulate this?'

NMR addition

The new 300 MHz NMR spectrometer recently installed in Clare Grey's lab offers a whole suite of new capabilities to apply this powerful, nondestructive, technique to the development of the next generation of electrochemical devices – from batteries to fuel cells and supercapacitors. Fitted with large gradient amplifiers, the system allows very low diffusion coefficients to be measured, and magnetic resonance imaging techniques can be applied.

Clare's group will primarily use this new equipment to investigate electrochemical devices for large scale grid storage applications. These include gaining insights into the behaviour of electrolytes confined within porous electrodes, redox flow batteries and supercapacitors. Monitoring the influence of device scale and geometry using MRI will help guide the design of next generation grid storage devices, while optimising the diffusion coefficient will lead to enhanced performance.



NMR installation in action!

Frank Allen

Frank Allen, former executive director of the Cambridge Crystallographic Data Centre, died in November.

Frank joined the university's chemical crystallography group in 1970, and played an important role in the establishment of the Cambridge Structural database. Following his retirement in 2008, he remained with the CCDC as an emeritus research fellow, which allowed him to continue indulging his passion for structural chemistry.

His research involved collaboration with many scientists around the world, resulting in more than 200 papers. He was also involved in the British Crystallographic Association, and was its vice-president from 1997 to 2001.



Photo: Nathan Pitt

The 2014 BP lecturer was Sharon Glotzer of the University of Michigan. She visited the department in November, and gave two lectures, one on soft matter quasicrystals and their complex cousins, and the other on digital discovery and design – the new age of materials on demand

Carl Djerassi

We are sad to report the death of Carl Djerassi. He died on 30 January in San Francisco at the age of 91.

Often described as the father of the contraceptive pill, he was a pioneer in various fields over the years.

These include steroid chemistry and optical rotatory dispersion in the 1950s, the application of mass spectrometry and NMR spectroscopy to organic chemistry in the 1960s, and computer-aided structure determination in the 1970s.

His new approach to structure determination came to Cambridge via the appointment of Dudley Williams as a postdoc in 1964 – a lineage continued today through Jeremy Sanders, who worked for Dudley, and Chris Hunter, who worked for Jeremy.

In later life, he switched from chemistry to art collecting and writing science-in-fiction plays and novels, and was a substantial donor to gender studies here in Cambridge. He was also a member of the Cambridge chemistry advisory board.

Carl had last visited Cambridge in November for a 'conversation' event at Sidney Sussex, where he was discussing his life and work with the Astronomer Royal, Martin Rees.

This coincided with the publication of a book of his reflections, 'In retrospect: from the pill to the pen'.

Open for admissions!



Photos: Nathan Pitt

Cambridge Chemistry held its first graduate admissions open day in October. More than 100 people interested in pursuing an MPhil or PhD here came to visit the department.

'The idea was to give potential students an insight into what Cambridge chemistry is like, and find out more about us and the research we do,' says Rebecca Myers, who was one of the organisers of the event. 'It was a very busy day!'

The event included a wide selection of talks from all areas of research that are going on in the department, both from senior PhD students and academic staff. Attendees were able to tour our labs and other facilities, engage in poster sessions, talk to current students and meet potential supervisors.

A second graduate admissions open day will be held in the autumn, probably in October, although no date has been finalised as yet. Watch this space!

Dudley Williams lab opened



Photo: Gaby Bocchetti

Pat Williams performs the official opening, watched by granddaughters Alexandra, Isabelle and Sophie

The new home of Chris Hunter's group, the Dudley Williams lab, had its official opening in November.

The ribbon-cutting was performed by Dudley's widow, Pat, and was followed by a champagne reception and a tour of the new facilities.

Chris's group moved from Sheffield to Cambridge in September into newly refurbished labs. Dudley and his chem-

istry have played an important role in Chris's career, ever since he was a student here in the department.

'Dudley was a great inspiration to me, and it seemed only right to name the lab after him,' Chris says.

'My group and I will be proud to work in a lab bearing Dudley's name, and look forward to doing exciting chemistry there.'



Wood preservation on the Mary Rose

Cambridge chemists have been helping preserve the Mary Rose, Henry VIII's shipwrecked wooden warship which was raised from the Solent in 1982. Exposure to air after so long in the water poses real degradation problems, and various techniques have been applied over the years to preserve the wood.

The Cambridge connection began following a chance conversation between Oren Scherman and the ship's director of conservation, and he thought his group's chemistry might be able to help preserve waterlogged wooden artefacts. Zarah Walsh was just about to start a postdoc in the group, following an analytical chemistry-based PhD at Dublin City University, and was keen to get involved. 'I have no specific background in conservation science, but I thought the project sounded fascinating,' she says.

AVOIDING SYNTHETICS

The brief from the conservators was that synthetic materials should be avoided where possible. They had been spraying the wood regularly with polyethylene glycol-containing biocides as a preservative, but that is fully synthetic. They were looking for something more natural that would not need repeat applications, and that would be able to treat all three causes of wood degradation – instability upon drying, the build up of iron in the wood acting catalytically to cause the formation of sulfuric and oxalic acids, and bacterial degradation.

After a lot of trial and error, the Cambridge team finally alighted on a two-tier system, with a cucurbituril handcuff to maintain the structure, and a strong iron binder that would cross-link the polymer to any iron that happened to be present. This made it more responsive to the environment, with the strength of the material changing relative to the level of iron present but always maintaining a basic level of support.

The idea behind this two-tier system

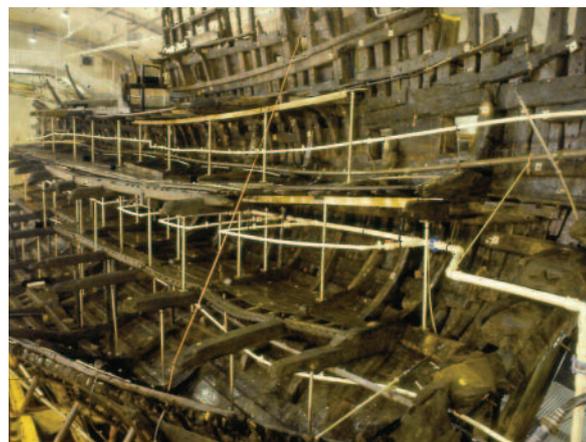
arose after Zarah and PhD student Emma-Rose Janeček were bemoaning the progress of their individual approaches. 'Emma-Rose had made an interesting guar-based material that was rather strong, and she was explaining that it could bind well to itself that it didn't need to bind to anything else,' Zarah says. 'But mine had no strength at all – once iron was present it went very liquid. We idly wondered what would happen if we mixed the two together – would we end up with something in the middle?'

And it turned out that they did. 'We still needed to remove a few kinks, but it was a major leap forward,' she says. 'It allowed us to bind iron, and create a polymer network to give it strength.'

They were then let loose on conservation. 'After two years working on the material, we took it down to Portsmouth, and – once they had explained what we could and couldn't do – they allowed us to apply the material ourselves to a wooden archeological artefact,' she says. 'That was really exciting – and it worked very well, even though at first it was not obvious that anything had happened.'

The conservators kept an eye on the wood over the coming days, and after about three weeks the polymer started to delaminate from the surface. Once the conservators removed it, they found pristine-looking wood underneath, with the iron salts having been removed from the surface without damaging the wood underneath – something they had not been able to achieve before.

Two years later, the iron deposits have not returned, which represents a significant improvement over the poultices they had applied previously, where the surface iron started to reappear after six weeks or so. 'It looks like our system creates an oxygen barrier at the surface, preventing the iron underneath it from being oxidised and moving through the wood,' she says. 'This is really important



for conservation! Long-term tests are now under way to see how it behaves as a structural stabiliser. But regardless of the outcome, we have managed to develop a material significantly better than poultices at cleaning iron deposits off wooden surfaces.

'It's very satisfying to have made such a positive contribution – and to be doing chemistry that non-scientists are interested in as they can relate to the idea of preserving the Mary Rose.'

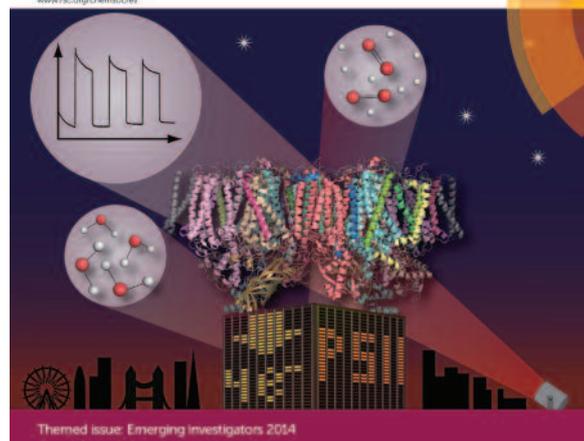
Z. Walsh et al. PNAS, 2014, 111, 17743

Preserving a wooden ship from the 16th century is a challenging task, especially one that sank in 1545 and spent centuries under the sea

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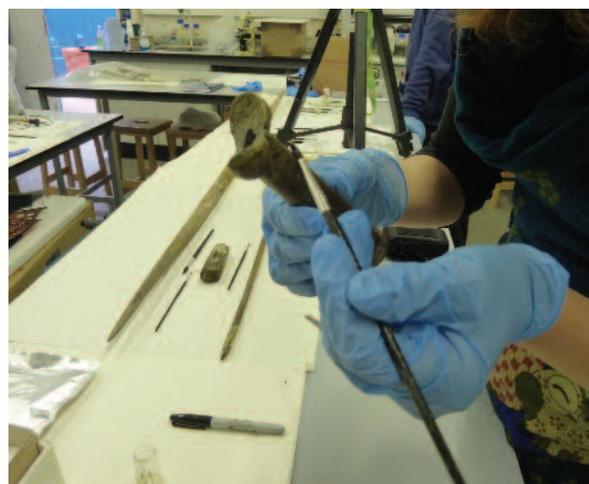


Themed issue: Emerging Investigators 2014

ISSN 0304-0327



TUTORIAL REVIEW
Erwin Reisner et al.
Protein film photoelectrochemistry of the water oxidation enzyme photosystem II



Carefully painting the polymer onto a wood sample

This striking image on the cover of Chem Soc Rev accompanies a tutorial review from Erwin Reisner, postdoc Jenny Zhang, PhD student Nicholas Paul and former group member Masaru Kato, who's now at Hokkaido University in Japan. The review looks at the protein film photoelectrochemistry of the water oxidation enzyme photosystem II, which is at the heart of the photosynthesis process. The technique enables the enzyme's light-dependent activity when adsorbed onto an electrode surface to be studied.

The power of structure predictions

Chris Hunter has returned to Cambridge after 25 years. His science includes the prediction of DNA packaging and complex stability

The new Herchel Smith professor of organic chemistry, Chris Hunter, is no stranger to the department, having completed his PhD in supramolecular chemistry with Jeremy Sanders in 1989. He moved back to Cambridge from Sheffield in October, and is now settling back into life in the flat Fens after nearly 25 years in the hills of South Yorkshire.

He cut his synthetic teeth with Jeremy making molecules designed for artificial photosynthesis. These large, complex molecules proved extremely difficult to make, and a change of approach was much more successful – applying non-covalent chemistry, so that coordination bonds were used to hold the assemblies together. ‘Almost by accident, we also found a theoretical model for the stacking of aromatic rings,’ Chris says. ‘It wasn’t anything we were looking for, but it came to us as a result of some of the experiments we’d done, and we created a computational model to explain it.’

On leaving Cambridge and starting his independent research career, he returned to this model for aromatic pi-stacking, applying it to interactions in proteins and DNA. ‘I’ve had a long-running research programme aimed at understanding how the stacking of the bases in DNA determines the relationship between sequence and three-dimensional structure,’ he says. ‘How does it bind to proteins, and how is it packaged in the nucleus of a cell?’

In a new project that’s just getting underway here in Cambridge, he is trying to make synthetic polymers that have all the properties of DNA. ‘If you’re looking for an interesting molecule to try and make or emulate, it doesn’t get much more exciting than DNA!’ he says. ‘It’s capable of evolving – or being forced to evolve – to generate functional properties without actually having to design the molecular structure. It essentially finds its own way.’

The secret to how it does this lies in the fact that it’s a linear polymer that can be copied, which means that in vitro selection experiments can be done. ‘We’re trying to make synthetic polymers that are more like conventional plastics such as polystyrene, but equipped with hydrogen bonding sites,’ Chris explains. ‘This would allow the polymer chain to template its own synthesis. We could therefore use it in forced evolution experiments, essentially allowing us to make evolvable plastics.’



His starting point is designing systems that will form a duplex structure, mimicking the double-stranded formation of DNA. If this is made up of oligomers of a defined sequence that have hydrogen bond donor or acceptor units, these could pair in a sequence-selective manner analogous to the way thymine pairs with adenine, and cytosine pairs with guanine, in DNA. ‘So, for example, if you make an oligomer with the sequence acceptor–acceptor–donor–acceptor, that would pair in a sequence-selective way with another molecule that has the sequence donor–donor–acceptor–donor,’ he explains.

SYNTHETIC CONTROL

And they’re now starting to get this idea to work. The next stage, Chris says, is to investigate whether the sequence can be used to control the synthesis of a complementary oligomer. ‘We hope to be able to show that DNA isn’t such a super-special molecule,’ he says. ‘I believe there are huge numbers of different kinds of chemical structures that have replicating properties similar to DNA, but which might function in a

different manner. We want to understand the basic chemistry of how that works – and whether it can be done!’

If it were possible to make something that could be forced to evolve, there are many potential applications. ‘It could, in theory, be used for anything, provided you can think up a way of forcing the molecules to evolve to that function,’ he says. ‘There are straightforward things people have done with nucleic acids in forced evolution, such as making new synthetic receptors, sensors and catalysts. Those are obvious examples, but there may be many more interesting applications in the materials field – imagine a self-replicating plastic!’

Returning to DNA itself, and starting with the model developed all those years ago for how aromatic molecules stack, they have created a piece of software that enables DNA sequence to be translated into a three-dimensional structure. They are now using it to try and understand the first level of packaging of DNA in the nucleus.

‘If you stretch out the DNA in a human cell nucleus out into a long string, it is about two metres long, yet it is packed into about 1µm of space,’ Chris says. ‘This is achieved by wrapping it around protein molecules, and the way in which it’s wrapped around those proteins depends on its sequence. Certain sequences get packaged very efficiently and are tightly wrapped, while other sequences are much less tightly wrapped and are therefore more accessible. These are the regions where transcription factors bind to initiate gene expression. So the way DNA is packaged in the nucleus is, somehow, organised or controlled by the sequence of the DNA itself. Our software has allowed us to take the first step towards understanding this process.’

BINDING PREDICTIONS

The first level of packaging in this process is called a nucleosome, and comprises 147 base pairs of DNA wrapped around a protein complex. ‘We searched the whole of DNA sequence space to predict which 147 base sequences would have the highest affinity to make those nucleosome complexes,’ he says. ‘We then experimentally tested the 12 sequences we predicted would be the best binders, and all had very high affinity. It was good to know that it worked – we were able to make quantitative predictions of binding affinity from just the DNA sequence.’

A large amount of effort in the group is taken up by running experiments to quantify non-covalent interactions like these, in various different systems. ‘We

synthesise molecules that are designed to allow us to make a quantitative measurement of the thermodynamic properties of aromatic stacking interactions, hydrogen bonding interactions and halogen bonding interactions,' he says.

An important technique for measuring these interactions is the double mutant cycle experiment, developed by his predecessor as Herchel Smith organic chemistry chair, Alan Fersht, in his work on side chain–side chain interactions in proteins. Basically, if there are two groups in a complex system that form a non-covalent contact, and you can quantify the stability of that complex, this technique can be used. First, the stability of the complex with that non-covalent interaction, such as a hydrogen bond, is measured. Then one of the two groups is removed and the stability measured again, and then the other removed before stability is measured once more. Finally, both groups are removed at the same time, and a fourth stability measurement is made. From these four measurements, a cycle can be constructed that enables a single interaction to be dissected out from a system in which there are very many different interactions.

SOLVENT EFFECTS

The idea that these non-covalent contacts can be quantified means it should be possible to start predicting the stability of the complexes, too. This has obvious applications in fields such as drug design, where predicting how a new molecule might bind could be used to decide whether it is worth making and testing.

Another model they've developed is designed to quantify how a solvent affects non-covalent interactions. Most experimental studies of weak non-covalent interactions are done in very non-polar solvents, with the assumption that the solvent has no impact as it is so overwhelmed by the much stronger non-covalent interaction that is being measured, such as a hydrogen bond. 'The idea is that if you have a solvent that cannot make hydrogen bonds, it will not affect the hydrogen bond that is being formed in the solvent,' Chris says.

Surprisingly, he explains, this assumption is not correct. 'From the data we collected, we could see very clearly that the solvent was actually playing quite a significant role – even an innocuous, very non-polar solvent such as carbon tetrachloride.' Indeed, it turns out that everything affects everything else, so while molecules like carbon tetrachloride are non-polar, they actually have little patches on their surface that are slightly positive or slightly negative – slightly positive in the case of carbon tetrachloride. This means they do actually form weak but significant interactions with the molecules that are dissolved in them, perturbing the

Front row, from the left: Mark Williamson, Geneva Peterson, Cristina Misuraca, Elena Sanna Martinez, Marina Blanco Lomas, Ana Belenguer and James McKenzie
Back row: Diego Nunez-Villanueva, Jeremy Sanders, Jon Swain, Elkin Lopez Fontal, Filip Szczypiński, Maria Ciaccia, Alex Stross, Maxime Guitet, Rafel Cabot Mesquida, Chris, Michael Aiden Jinks and Cristina Navarro Reguero



behaviour of the hydrogen bond that is being measured.

This has enabled them to tease out a quantitative way of predicting what happens in different solvents, as they are now able to account for how that solvent had affected all the measurements – something had been making predictions difficult as the system was not behaving as expected. And they have now managed to create a general treatment for how solvents affect non-covalent interactions.

'There's a hierarchy of interactions in a uniform gradation, from the truly non-polar like noble gases interacting with each other, up to completely polar like the hydrogen bonds between water molecules,' he says. 'It's not a case of non-polar things not interacting and hydrogen bonded things interacting strongly –

there is a continuous scale, with everything interacting with everything else to an appreciable degree. Almost everything is weakly polar, even alkanes. That tiny effect we found and could quantify actually turns out to correlate nicely to some quite big effects, and the measurements in these very non-polar solvents extrapolate well to water and the common polar organic solvents.'

While this initial approach was very empirical, they are now in the process of developing a predictive computational model and trying to generalise it to include interactions between any molecules in any solvent. 'One of the big challenges in computational chemistry is dealing with solvent as it is so difficult to do simulations on a practical level,' he says. 'Most of the chemistry we are interested in happens in the liquid state, and to simulate what happens in a solution all of the solvent molecules and the interactions between them must be included. This makes the process extremely demanding in terms of computer power and time.'

Chris's new approach simplifies the system greatly, while being rigorously benchmarked against the experimental data. This renders it pretty accurate – and practical to use. One way they've been putting it into use is to predict the formation of co-crystals. These have gained a lot of interest recently in the pharmaceutical industry as by forming a co-crystal between a drug molecule and a suitable partner molecule, the physical properties such as solubility and bioavailability can be changed and improved.

They have developed a software tool that enables thousands of compounds to be screened in a matter of minutes to work out which molecules might successfully make co-crystals with an active pharmaceutical ingredient. 'We have experimentally verified that it works pretty well,' Chris says. 'We're now applying it to practical problems – carrying out a full crystal structure prediction for every potential pair-wise combination would be completely unworkable. By predicting what might make a good co-crystal in a quick and simple way, it should greatly facilitate the development of better drug formulations.'

Born: Dunedin in New Zealand, to Irish parents. After a spell in Nigeria, they returned to Portstewart in Northern Ireland when he was four years old.

Education: After school in Northern Ireland, he came to Cambridge to study natural sciences, staying on for a PhD with Jeremy Sanders.

Career: On finishing his PhD, Chris returned to New Zealand and a lectureship at the University of Otago in Dunedin, the world's most southerly university. 'It was a little like the end of the earth, but it's a really great place, and I learned a lot,' he says. Two years later, in 1991, he moved to Sheffield, where he remained until his recent return to Cambridge.

Status: His wife Rosie McHugh is a director in the NHS Sheffield Care Trust, and will remain in Sheffield until next summer with their youngest son, Finn, who is doing his GCSEs. Son Conor is 25 and an accountant in Glasgow; 18-year-old daughter Ciara is studying architecture in Bath.

Interests: He loves surfing, although Cambridge is no better for that than Sheffield. 'I thought I was moving closer to the sea until I realised just how much the East Anglian coast bulges out to the east – it's actually the same distance from here to the closest decent surfing beach, Sandilands, as it is from Sheffield!' He also loves walking, cooking and cinema.

Did you know? Continuing in a fine tradition of student disco among Cambridge organic chemists (after Shankar Balasubramanian and Joe Spencer), he used to run the Pleasure Machine, Churchill College's undergraduate disco. 'Disco is clearly the secret of success in organic chemistry!' he claims.

Chris Hunter

CV

DNA interactions in action

Transcription factors are proteins that control the transcription of genetic information from DNA to messenger RNA by binding to very specific sequences within the DNA. A recent project in Robert Glen's group, in collaboration with Boris Adryan in the department of genetics and Sarah Bray at PDN, was designed to create a better understanding of how these transcription factors actually interact with the DNA. How do they recognise the right DNA sequence among all the possibilities, and how do these sequences of DNA result in either blocking or initiating transcription?

As Rubben Torella, who's just finished his PhD with Robert, explains, the original idea was to create a computer model that simulated all the common interactions of the transcription factor CSL with DNA. This factor is an important part of the Notch signalling pathway, involved in cell-cell communication that controls multiple cell differentiation processes.

'We created all the possible combinations of different strands of DNA bound to CSL,' Rubben explains. 'This took some time as we calculated the binding between CSL and each individual DNA sequence – all 65,536 of them!' This enabled them to rank the interactions in order of binding ability.

It's all very well making these sorts of calculations, but are they actually correct? To find out, they ran *in vitro* assays to test binding of DNA sequences with CSL, and also *in vivo* studies in a cell line where binding to the same sequences

could be measured in a more physiological context.

'It turned out our predictions were largely correct, and were able to predict which DNA sequence could be bound, and which wouldn't,' Rubben says. 'As a consequence we have shown that actually a much larger repertoire of DNA sequences can be bound. This is important in the context of the whole genome where these subtle differences in binding may help in distinguishing the functional DNA sites from the vast amounts of available DNA, where the factor might also bind but less strongly. There is therefore the interesting question of why binding at some sequences influences transcription, while binding at others does not.'

One hypothesis why particular sequences are so selective in cells is that the binding with the 'correct' sequence is stronger, so it will remain bound for longer so enhancing the effect. To better understand what might be happening at the molecular level, they applied molecular dynamics calculations to the system, which takes into account the way the proteins and DNA move in real time.

'By applying Newton's laws of motion, and allowing the system to dynamically evolve over time during the simulation, we can appreciate how the entire DNA/protein system explores different dynamics,' Rubben says. Calculating these dynamics for selected examples revealed some interesting features.

'We found that when the transcription factor is bound to the best-match DNA, there is a much stronger correlation in

the dynamics of the system, increasing the binding energy, and allowing the transmission of a "dynamic signal" through the protein,' he says.

'There is a better signal transmitted to the whole protein, whereas this does not happen with weaker binding. This is an exciting discovery, as regions of the protein that are not directly bound to DNA, but are at a large distance from the binding event, are also affected when the binding is strong. Since the next step in initiating transcription requires the signal to change the conformation of the protein at a distance from the DNA binding event, this can explain why some DNA-protein interactions promote this, and others don't.'

The hypothesis was tested by mutating some residues within the protein, which appeared critical for the dynamic internal signal, to see if this reduced the signal transduction *in vivo*. The effects *in vivo* from mutating three residues that, when altered, strongly reduced the signal transmission across the protein in computer simulations, were tested using fruit flies.

The CSL gene affects the development of the fruit fly wing veins and, sure enough, the mutated gene stopped the wing growing properly – highlighting the importance of the dynamic correlation between the protein and DNA sequence. This strongly supports a signal transduction step within the proteins that regulate transcription, potentially explaining their selective actions and demonstrating the fine level of control within this process.

R. Torella et al. *Nucl. Acids Res.* 2014, **42**, 10550

The importance of being reversible

A good battery material needs to have high capacity and high voltage, be cheap, and be reversible to enable the battery to be charged and recharged. A few years ago copper(II) fluoride was something of a hot topic among battery researchers, as it ticks the first three of these boxes – but making it reversible proved impossible, and no-one could work out why this was so.

CuF₂ has a high operating potential, thanks to the high electronegativity of the fluorine, but the high ionicity of the copper-fluorine bonds means there

is a large band gap, which makes it a poor conductor. And it's difficult to study – CuF₂ is a nanomaterial, and thus forms multiple different phases on charging, making it extremely difficult to characterise. 'High heterogeneity on a small scale is challenging!' says Xiao Hua, a PhD student with Clare Grey.

The answer, Xiao says, lies in a combination of NMR experiments and synchrotron X-ray techniques. The synchrotron experiments enable the battery to be studied in real time while it's charging and discharging, and NMR facilitates the measurement of light elements, in this case, lithium. 'When a battery finishes one discharge-charge cycle, ideally you expect to get the initial materials back,' he explains. 'But in the case of copper fluoride, you do not see copper fluoride form after the battery finishes the full cycle.'

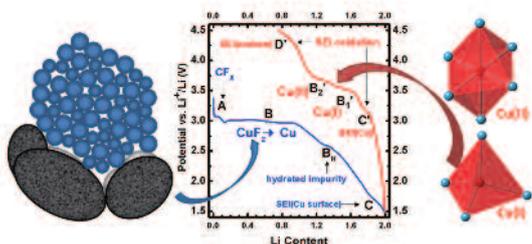
They found that what was happening was the copper dissolved in the electrolyte, combined with the lithium fluoride, and formed Cu¹⁺ during the first

charge cycle. The copper dissolution consumes the majority of the LiF, thereby stopping the CuF₂ from being re-formed on charging. This is why the capacity disappears in the second and subsequent cycles, and explains why CuF₂ will not make an effective battery material, despite its initial high capacity and voltage.

Although CuF₂ seems to be problematic as a successful battery material, explaining why it doesn't work is still important – and the paper was highlighted as a 'hot paper' by the American Chemical Society. 'We created a guideline for future researchers, giving an idea about where it is worthwhile spending their efforts,' Xiao says. 'It's not as if the material can be easily improved by doping or surface coating like what many researchers are focusing on – it's more about how to engineer this material or to change the electrolyte to make this material perform better.'

X. Hua et al. *J. Phys. Chem.* 2014, **118**, 15169

CuF₂ cannot match the performance of other systems



The next step towards automated synthesis

There are many advantages in carrying out reactions in a continuous flow process rather than a traditional stirred flask or batch reactor – not least that it is possible to connect multiple flow reactors together so more than one step of a synthesis can be performed, one after another, without any need for isolation between each step. However, the practicality of daisy-chaining reactors together is not as straightforward as one might think.

Claudio Battilocchio and his colleagues in Steve Ley's Innovative Technology Centre have been looking at ways this can be achieved more successfully. The idea was to create a holistic approach that could be applied to any general synthetic process.

'Chemists automatically think about the chemical transformations, but the intermediate steps that link them together are not as important,' Claudio explains. 'Our idea was to divide the design of a synthetic flow procedure based into three different layers. The top layer contains all the chemistry whereas the second layer is associated to the downstream processing operations to connect the chemistry steps together. The bottom layer handles information, which connects and controls the chemistry steps together.'

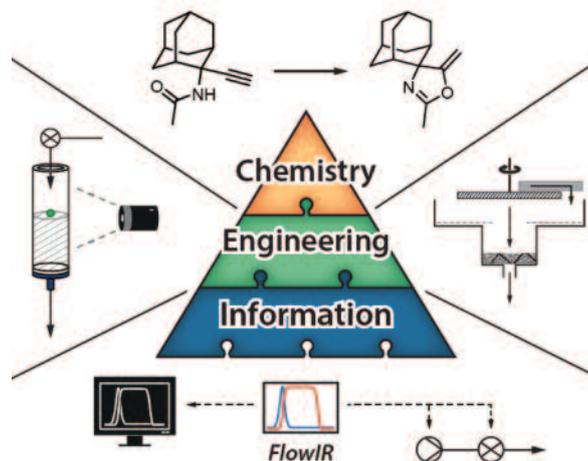
This information layer manages the flow chemistry data that is collected about the formation of intermediates between the different steps and gives the system the ability to respond to any changes, such as the amount of that

intermediate that has been formed. This allows each step to be self-regulated for the best results.

'The different machines in a flow sequence operate different steps, but without any information layer we would need several people to control them,' Claudio explains. 'One person can control one or two machines, but more than that is often impractical. However if the system looks after most of them, with each module responding to stimuli such as the formation of intermediates, we can be much more productive.'

As an example, they created a system that connected three chemistry steps and their associated work-ups, with the system designed at each step to automatically respond to changes, enabling self-regulation. 'We designed the system to self-regulate in order to reduce the amount of reagents used and waste produced, but it could also send alerts if there was a problem,' he says. 'This is very different from the current system – there is a paradox in continuous flow chemistry that, despite the promise of automation, the operator has to spend a lot of time in front of the machine to check it is working properly.'

The key to the remote controlled automated system that regulates the sequence of steps is that they are not treated individually, but each module of the system is regulated in order to interact with each other. 'If there is a problem with the first step, the second and third will continue to process material while they can, but that first part will shut



down to enable the operator to solve the issue and start it up again. On the other hand, if the operator is not there, each module will shut down safely once "their" starting materials are used up.'

Essentially, this modular configuration of the system enables remote control by a single operator. Now, Claudio says, they are looking to use specific sensors that detect intermediates, enabling the system to optimise itself as well. 'This would allow the single chemist operating the whole system to focus on the chemistry, and deciding what to do next, rather than running the synthesis,' he says. 'All the routine operations would be performed and controlled by the machines.'

R.J. Ingham et al. *Angew. Chem. Int. Ed.* 2015, 54, 144

Taking care of all the layers of the flow procedure allows better system control

Switch off and save energy

The aim of Switch Off Week is to raise the awareness of how our daily use of energy has an impact and how, by switching off electrical equipment, the university can become a more sustainable place. The week features a programme of events organised centrally by the environment and energy team, and more locally by environment & energy coordinators and Green Impact teams.

The first university-wide Switch Off Week was held in February 2013 during



a week that had an unusually cold snap of weather, so it was highly challenging and demanding requiring a determined effort to switch off especially heaters. It was therefore very encouraging that, during that period, there was an overall 2.1% saving (corrected to take into account the cold weather) on the university's energy bill compared to the previous week.

The 2014 Switch Off Week was held in November. On the Wednesday, the Switch Off Week Roadshow came to the CyberCafé, bringing with it the Energy Bike Challenge that allowed people to experience the effort required to power a 90W sound system and light show. Tim Hele spectacularly smashed the university's previous record by cycling for 1 hour, 1 minute and 1 second!

There were also opportunities to make energy-saving pledges, and sweep up the many freebies including water bottles, cycle seat covers and fortune cookies. At lunchtime, there were repeat showings of Green World Rising's series



Richard Turner and Sheila Bateman run the stand in reception (far left); Tony Gill from the Cybercafé makes his energy-saving pledge to turn off non-essential electrical items at the end of his shift

of short films on the state of climate and solutions to the climate crisis, narrated by Leonardo DiCaprio.

At the end of the week, the chemistry department decreased its electric use by 0.89%. Overall, during the whole week, the university used more than 3000kWh less electricity, a reduction of 0.36%.

Of course, the message of switching off to save energy continues all year. You can make a difference in making the university a greener place by switching off lights and equipment when it's not needed. Every little helps. Richard Turner

Last out of Free School Lane

I believe I was the last person out of Free School Lane Physical Chemistry, as it was closed down in 1958 for the move to Lensfield Road. Like many a 'brain-drainer' I was hot foot for America, having completed a PhD's research under Ronald Norrish, but had been offered another year for writing up and extending the work, staying on in the old building. I had also managed that year to get married.

My lab was on the top floor, up the steep staircase, and I painstakingly built a gas-kinetic flow system for reactions of chlorinated hydrocarbons. An old project left over from the 1940s, it was not my choice of research topic – I came to Cambridge from London eager to do flash photolysis and spectroscopy, but found myself drafted into this because there was some petrochemical money left over in Norrish's budget. The lab had an unforgettable feature, a cavity blasted into the plaster wall by a detonation in which Fred Dainton (later Sir Frederick, Baron Dainton) had once mangled his hand when treating an organic peroxide with insufficient respect.

My arrival coincided with the departure of George Porter, whose genius with flash photolysis helped propel Norrish to a Nobel Prize. After Porter left for Sheffield, Brian Thrush, to his great credit, kept the field alive in Cambridge in the 1950s, with great experimental talent, but limited resources.

Usually, on Norrish's visits to the third floor, he would simply ask what I had been doing, snort, and move on. What I had enthusiastically been doing actually elicited no more than mild curiosity and a certain suspicion on his part. This had been to make some of the earliest advances in gas chromatography prompted by the late, delightfully Welsh, Howard Purnell. Together we staked our claim to the earliest studies of temperature effects on elution-times, all this with makeshift columns and detectors feeding a mirror galvanometer, whose swinging light-spot we excitedly plotted on graph paper as each peak arrived. The luxury of a pen-recorder came much later.

Howard and gas chromatography were the rescue of my PhD. By using the latter to measure trace by-products of the pyrolysis and combustion of CH_2Cl_2 and CH_3Cl , I was able to concoct a plausible set of chain-reaction mechanisms, with the usual under-determined finesse of: 'the following mechanism is consistent with the experimental results...'

As my contemporaries will know, the tensions of the Norrish entourage were not reflected in the rest of the department. The waggish Morris Sugden, the courteous, stone-deaf Moelwin-Hughes and the shyly expert John Agar, kept their research and academic intelligence well clear of the department head, while, in my own case, college life at

King's, in a brilliant international post-grad community, was just the distraction I needed. I also remember with great affection Fred Webber, the top-floor technician whose kindness and support at difficult times I shall never forget, not to mention his prompt emergency licking of my eyeballs after an acid splash on one occasion. Not all technical staff were as easy-going, however. I particularly remember the store-keeper whose response to every request was an automatic: 'We're cutting down on that', followed by: 'Are you sure you really need it?'

Looking back, I think I owe my later cultural development to one incident more than any other – the enforced closing of the Free School Lane labs at 6.00pm. on safety grounds. (As well they should have been in view of the frequent explosions and lax attitudes to safety in those days.) This, along with the libraries and the marvellous Cambridge provision that one could turn up at any lectures whatever, was the beginning of my eventual long march through the academic world to become a linguist and literary historian. I confess that I snuck out to many a morning humanities lecture, knowing that Norrish was always a late starter on his rounds of inspection.

And so to America and the delight in being addressed by my Christian name. My connection with generous and free-thinking King's continues to this day, where periodic non-resident dinners make the perfect night out from London.

Michael Hoare

Cyril John Smith

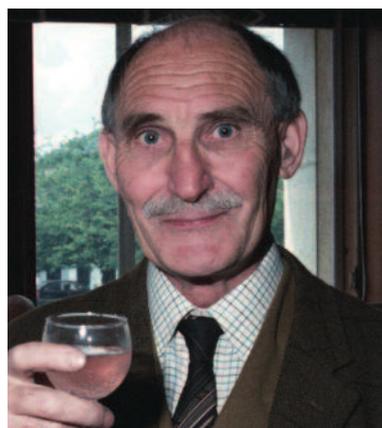
Former Physical Chemistry glassblower Cyril John Smith passed away on 25 August after a short illness.

Cyril was born in Cambridge in 1930, the second of four children. He attended Coleridge School until the age of 14, when he left to become a laboratory technician for students at Barts Hospital, who had been evacuated from London and temporarily housed in the chemistry department, then in Pembroke Street. After the war, when the Barts students returned home, Cyril obtained a job in chemistry, working with John Woodcock carrying out chemical preparations in the XL lab.

When chemistry and physical chemistry, then two separate departments, relocated to Lensfield Road, he joined physical chemistry as a research technician for the flash photolysis groups. The apparatus required for this work was not commercially available as it had to be created from quartz, so Cyril became an expert in designing and making such equipment. Much of his handiwork was

used by the 1967 Nobel laureates, Norrish and Porter.

During his long career with the University he worked alongside his brother Eric, who was the department's head of photography. Cyril was also a very keen member of the lab cricket team, and its secretary for some time. He took early retirement in 1990, and spent a lot of time enjoying his two main hobbies, gardening and fishing.



'Tiger' Coxall

Edgar 'Tiger' Coxall, who was chief technician in charge of the electrical workshop for many years, passed away in December 2014.

Tiger was born in Longmeadow in 1928, one of three children, and went to school in the village of Lode, just north-east of Cambridge.

He joined the chemistry department in November 1942 as a lecture room assistant when the labs in Pembroke Street were not only home to Cambridge students but also to evacuated students from London universities and the Ministry of Supply.

In 1946 he joined the Royal Navy for his two years' national service. On being demobbed, he returned as a technician on the inorganic floor, specialising in maintaining the fluorine generators both in the 'old lab' and then in Lensfield Road.

He gradually became involved in the repair of electrical apparatus and set up the electrical workshops, where he eventually designed and built a great deal of novel equipment that was not commercially available.

Tiger retired in 1992, having completed 50 years with us. He was a very active sportsman, playing cricket for the department, football for local clubs and an avid West Ham supporter. He was also a very keen motorcyclist, and rode regularly until a few months before he passed away.



Smile for the camera!



Without the talents of the department's photographers, Chem@Cam wouldn't have those wonderfully striking images on the front cover – or the lovely portraits of our chemists inside. But why does a chemistry department employ photographers? As Nathan Pitt says, when people ask him what he does for a living, they're often rather surprised when he tells them he does photography in a university chemistry department.

In reality, although taking photos is an important part of what they do, there's rather more to it than that – they're responsible for anything and everything involving graphics or imaging. 'On the photography side, we do portrait shots for publications, passports and visas, but we also do still life photography of science equipment and interesting experiments, either for papers and theses, for record-keeping, or even because they've managed to make something really pretty,' explains Caroline Hancox. 'Our colleague Gaby Bocchetti in reprographics also does a lot of graphic design, such as creating journal covers. She's something of a whiz in Illustrator!'

There's also a good deal of events photography, such as conferences and lectures, and corporate and other visitors to the department. 'We're well practised in the art of taking photos of Nobel prizewinners and other distinguished scientists waving their arms around during lectures!' Nathan says. 'We also cover outreach events such as the department open day, and other events involving Cambridge chemists outside the department itself. Science week is always fun – Peter Wothers' lecture is good for dramatic photos, and finding interesting shots of the kids doing science in the labs is never dull.'

Perhaps unsurprisingly, for such a var-

ied occupation, Nathan and Caroline cite different aspects as their favourite. As well as the more explosive parts of demonstration lectures, Nathan loves the variety – he could be photographing lectures one day, poster printing another and creating stretch canvases another.

Caroline, meanwhile, gets a huge amount of satisfaction out of taking portraits, particularly ones on location like those we use in Chem@Cam. 'Teasing a good photo out of someone who doesn't like having their picture taken can be a challenge!' she says. 'I start by chatting with them, and once they've relaxed I tell them it will soon be over!'

'If they're still looking really miserable, I'll tell them to smile as this is the last photo – they go "phew!" and relax into a good pose in their relief. It's all about showing them it's not scary, and that I'm not trying to make them look awful in the picture. It's good to break down their barriers and let them come through in the photo. Getting that good shot is incredibly satisfying.'

TECHNICAL CHALLENGES

Chem@Cam's cover shots can also pose interesting technical challenges. 'A lot of the time, working out how to get the best shot is a case of trial and error, and in future shots we can build on what we learnt before,' Nathan says. 'That's a lot of the fun of it – working out what we want a shot to look like, and how to achieve it.'

The flaming letters on our last cover are a great example. 'With shots like this, we have to work with people who know how to create the effect we're looking for,' Caroline says. 'Chris Brackstone really enjoyed working out how to make them, and without his technical help it the shot would not have been possible.'

Caroline, Gaby and Nathan, pictured with the assistance of a self-timer!

Photographing lasers is another fun one. Way back in Summer 2003, the cover featured a student in Dave Klenerman's lab who was working with a laser. But visualising a laser isn't simple. The answer lay in taking a shot using the flash with the lights off to visualise the student and the equipment, and then leaving the shutter open while wafting dry ice at the laser, giving it something to 'hit' so it could be seen. Having already worked out how to visualise lasers meant taking the laser-based cover shot for Autumn 2013 was just that little bit easier.

A decade ago, film was still routine, and part of their office was a darkroom. Not any more – everything is digital. 'We use programmes like Photoshop and Lightroom – a digital darkroom in a light room!' says Caroline.

Going digital also allowed them to lose the darkroom in 2009, giving them more space for the increasingly large equipment they need. 'With a very large printer and the laminators, it was a bit of a squeeze to trim posters and laminate things,' Nathan says. 'Looking back, it seems a little farcical – our now-retired colleague John Holman had to breathe in so we could squeeze past between him and the laminator when he was sitting at his desk.'

POSTERS AND VIDEOS

Printing is an important part of what they do. 'We do all the poster printing in the department,' Nathan says. While their input into the design is limited, they swap lo-res screen-grab logos and crests for hi-res vector graphics so they look sharp, and do occasionally offer design and technical advice.

'Poster printing comes in peaks and troughs, but generally we do about 250 a year, of different types,' he adds. 'We still make traditional paper and laminated posters, but increasingly we're making canvas and cloth posters. These have been really popular – you can fold the poster up in your bag, and not have the battle of trying to get away with a poster tube as hand-luggage on EasyJet!'

An activity that's in its infancy for them is taking videos. They don't get asked to do it very often, and their equipment remains limited, but occasionally they're asked if they can take a video. 'A good example is the replacement of one of Clare Grey's NMR machines a little while back, when the magnet was being purged,' Nathan says. 'Safety officer Martin Maunders thought it would be good to have footage of the clouds of gas coming off, so we took about five minutes of footage as a record. What we do is fairly infrequent and very simple at the moment, but we have half an eye on expanding in the future, if the demand is there.'



Photo: Nathan Pitt

Computer officer Chris Chalk retired in March after 23 years in the chemistry department, and more than 40 with the university. He's pictured with head of department Daan Frenkel at his leaving party in the Todd Hamied room. Despite the smiles, we're sad to see him go!



David Plumb retired in September, after almost a decade working in the department's electrical workshop. Department members will recall him going around the building testing all the electrical equipment to check it's safe. Colleagues past and present were on hand to give him a rousing send-off.



Photos: Gaby Bocchetti

A wedding full of chemistry

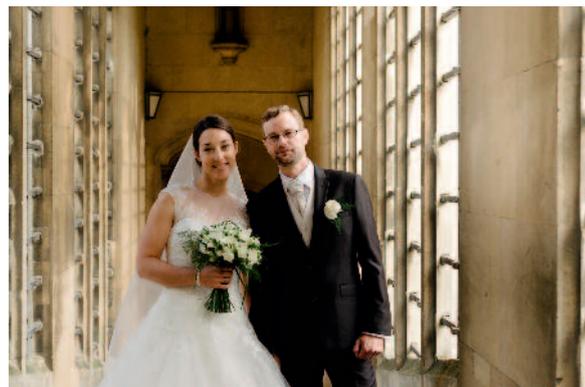


Photo: Caroline Hancox

As readers will be well aware, we love a nice wedding photo in Chem@Cam. And this one involves not one but three members of the department – the bride and groom and, as a bonus, the photographer.

Celine Galvagnion, a postdoc with Chris Dobson, and Alexander Buell, a research fellow in the Dobson and Knowles groups, got married on 6 September in Magdalene College – and the pictures were taken by our very own Caroline Hancox.

Celine is originally from Pontoise, near Paris, and Alexander hails from Stuttgart in Germany, and they first met in the lab on the day of Alexander's viva in June 2011. 'Jane Clarke had ordered everybody to vacate lab 290, as my viva

was to take place in an adjacent room,' Alexander says. 'Celine, who had started her postdoc a few weeks earlier, was the last person remaining in the lab, desperately trying to finish her work before she left. I was a bit early for my viva, so we got to talk...'

He proposed a couple of years later during a road trip in the US. The year after they were married. 'We went on honeymoon to the Galapagos Islands, which was a trip to remember – and the ideal destination for two scientists!' he says.

And they're greatly enjoying working together, too. They've published four papers together this year – and are rather hoping there will be many more to come.



Jeremy Sanders sent this pair of snaps along. He was recently in China, and was made an honorary professor at Nanjing University of Science and Technology. He and his wife Louise were rather taken aback to see his name up in lights outside! And he's also been hob-nobbing with royalty... with a visit to Buckingham Palace for the presentation of his CBE by Prince William.



Michael Pittas

We are sad to report that one of our cleaners, Michael Pittas, has died. He joined us in chemistry in 2010. Our thoughts are with his wife Cheryl, who is also a cleaner here in the department.

Three Peak challenge



Hiking Yorkshire's Three Peaks makes for a challenging expedition at the best of times, but in filthy weather that challenge increases somewhat. But that's what personnel administrator Emma Graham and glassblower Keith Parmenter did back in September.

The 25-mile trek takes the intrepid walker up 2277 ft Pen-y-Ghent, then Whernside, which tops out at 2415 ft, and finishes off with Ingleborough, at 2372 ft high – all within 12 hours.

'I'm pleased to say we managed to complete it as a team in 11 and a half hours,' Emma says. 'We set off at 7am and the weather was awful – it rained continuously for at least eight hours, but as we approached the third peak the sun broke through and saw us through to the end.'

Emma says the plan to do the walk originally started as something to do herself to mark her 40th birthday, but she then persuaded a friend, her cousin, and Keith to join her so she had some company on the hills.

'I'd also recently gone through a really tough time at home as my son, who is 17, had recently attempted to take his own life and proceeded to spend a number of months in hospital,' she says. 'So, as we were putting the effort in, I felt it was an excellent opportunity to raise money for the Young Minds charity.'

'Shockingly, suicide is the third leading cause of death in 15-24 year olds, and Young Minds is a charity that helps to prevent teenage suicide by working closely with children, young people and their families to improve the emotional well being and mental health of adolescents. They incredibly important work.'

With donations from family, friends and colleagues in the department, Emma raised just over £1000 for the charity. 'It was a fantastic experience, made all the more worthwhile from the money I raised,' she says. 'Keith and I hope to continue with mountain treks next year. Hopefully we'll get better weather next time!'

Every year, South Cambridge Rotary Club borrows the department's car park in the run up to Christmas. They then charge shoppers for parking, all in the aid of charity. This year, the chemistry car park raised £5828 – more than a fifth of the £35,827 total raised from all the club's Christmas parking activities. The good causes supported this year include East Anglia's children's hospice, Cambridge Dial-a-Ride, Romsey Mill, the Guildford Rotary Eye project, Wintercomfort, Campod, and the University of Cambridge Veterinary School Trust.



Four more future chemists!

Minkoo Ahn's wife Sookjin gave birth to their daughter Christine (right) on 31 October. It was just four days after Minkoo's PhD viva... 'What a week for me to receive two titles – dad and Dr!' he says.

Christine was born at the Rosie, and weighed in at 2.84 euro-baby-units (that's 6lb 4oz in a more Imperial way). Minkoo has stayed on for a year's post-doc in Chris Dobson's group, and says he's loving being a dad.

'It's demanded various responsibilities for Christine such as changing nappies!' he says. 'But it has also granted me the great privilege to be overjoyed by being with her, and seeing her adorable face every day.'



Slightly belatedly, here's Hugo David Ward (right), who was born on 1 March last year. He's the first child of Vanessa de Souza, a research fellow at Darwin who works in David Wales' group, and her husband Edmund Ward, who did a PhD in materials with Paul Midgley and now works for Ofgem.

Belatedness makes for a great picture though... 'Hugo likes messy play,' Vanessa tells us. 'In the picture, he's covered in chocolate Angel Delight, and is sitting in (and eating from) a tray of spaghetti.' The boy will go far!



On the left is Francisco Pinteus da Cruz Lopes Bernardes (pew!), son of Gonçalo Bernardes and his wife Filipa Pinteus da Cruz, who's also DPhil organic chemist.

Francisco was born on 23 September in Gonçalo's home town of Lisbon in Portugal, and weighed in at 3.6 euro-baby-units (that's almost 8lb in old UK baby-units).

'He is very relaxed,' Gonçalo says. 'Being a father is the best thing ever!'



Andrew Wheatley's wife Wendy gave birth to Joseph Henry (left) on 29 July, weighing in at 7lb 15oz (that's 3.6kg for the euro-baby-unit-lovers among you). His arrival in the middle of a heatwave contrasted somewhat with his big sister Abigail's arrival – a CD case had to be pressed into action to scrape the car free of snow then!

Andrew says he's now learning the joys of ironing miniature shirts, and preventing the adoring big sister from smothering her little brother with overzealous attempts at cuddles.

Christmas cheer

The usual mix of faces old and new attended the assistant staff Christmas party in the Cybercafé, including Nathan Pitt, who was wielding the camera



Clockwise from above right: Chris Chalk and Pat Chapman; Alex Archibald and Ray Freshwater, David Plumb and Chris Lowe; Tim Dickens and Finian Leeper; Chris Brackstone, Mark Hudson and Dave Pratt get stuck into the wine; John Offley, Chris Sporikou and Mike Sleep; Mike Todd-Jones, Sabina Cole and Patrick Donnelly



Last issue's solutions

ChemDoku

It had to happen. A dozen years of ChemDoku-setting, and finally I succeeded in rendering it insoluble thanks to a typing error. As numerous readers pointed out, there was insufficient room for all the gold (a grand problem to have, if you're not a ChemDoku!). Chris Cornish-Lawrence summed it up nicely – maybe the alchemists had been at work, and succeeded in converting another metal to gold during the printing process.

This didn't put a handful of intrepid readers off, however, and by the judicious act of turning silver into gold managed to come up with a solution. Gold stars to David Wilson, Godfrey Chinchin and Morgan Morgan. And a £20 reward also goes to Godfrey Chinchin, as chosen by Ginola the cat-shaped office assistant, who dragged herself off the heated floor in the bathroom briefly to pick catbiscuits.

Triads for the 21st century

The Triads puzzle didn't pose an impossible challenge, probably because it was set by David Wilson and not me. The alphabetically adjacent element symbols in the triad whose atomic numbers are less than 72 are Mo/Mn, Sb/Sc and Cs/Cr; those less than 82 are Tb/Tc, Ce/Cd and Ta/Tb; and the under 92 group are Th/Ti, Pa/P and Hg/Hf.

Correct solutions came from Godfrey Chinchin, Richard Moss, Richard Brown, Tom Banfield, Ian Fletcher and Keith Parsons. And the feline prize-picker's final furry fling sends the £20 prize in the direction of Tom Banfield.

Email puzzle entries to news@ch.cam.ac.uk, or by snail mail to Chem@Cam at the address on p3

This issue's puzzles

Elemental word chain

Graham Quartly sends along this puzzle, his latest variant on is theme of words made from atomic symbols... Using the symbols for atomic elements a word chain can be constructed changing just one element at a time e.g. Fe N S -> Fe At S -> B At S -> B At He What are the sequences of triatomic words specified by these clues? (Remember only one element may be transmuted at a time.)

- 1) Flavour / Objective / Water holder / Connection / Big ship / Organ / Put a top on / Be frightened
- 2) Provide food / Impact hole / Town Announcer / Maritime construction / Baked goods / Provides with drink / Friends / Plants providing a bitter purgative
- 3) Geographical feature / Small child / Pile of stones / Biblical murderer / Rubbish collector / Cereal / Organ / Wash bowl

Elementary, my dear chemist

And here's one from David Thompson. He says... There have been 169 Nobel laureates in chemistry, from the first recipient in 1901 to the latest in 2014. In many of these years, there was more than one recipient. Only one person has received the prize twice – Frederick Sanger. When I looked through the list of laureates I was surprised to see how many names were unfamiliar, but it is a few years since the last lecture I attended! Some of these people have surnames that can be built up from chemical elements – the first laureate was van't Hoff (surname can be made from fusing hydrogen with oxygen and

two atoms of fluorine), but perhaps the best known recipient is Marie Curie whose surname cannot be made up from atoms unless a new element has just been named... How many chemistry laureates can be synthesised from the elements in this way?

Chemical killer ChemDoku

And finally... another one from David Thompson, who spares my potential blushes by filling the ChemDoku slot. However, as a fiendish bonus, the inner 'cages' one might expect to see in a killer ChemDoku are absent. He adds that there are no single-value inner cages, and offers this hint – vanadium, if made from three separate elements, can only be synthesised by adding fluorine and oxygen to carbon. This will release a large number of neutrons but this is, fortunately not relevant, he says!

O		V		Mg		Ne		
Na			C		Si		S	
	N	F	Cl	Ne			Si	
N				Ti	F		Be	
	Sc		B			Ti	C	
Cl	Mg				Be			Ne
			O			Na		
O		Ne		Cl		Li		Ne
Na		O			V			

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So long, and thanks for all the fish...



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