chem@cam

Chemistry at Cambridge Newsletter

Autumn 2009

New materials for **better batteries**

Electron correlation: a solution

Novel catalysts in the car industry

Using fragments to **probe biology**

Martyn Twigg started life in academia, but has spent most of his career in the chemical industry. He tells Sarah Houlton how he ended up there, and the importance of catalysts in the motor industry

How did you come to work in industry?

After a junior faculty position at the University of Toronto, I came to Cambridge to work with Jack Lewis and Brian Johnson – the only kineticist working in a preparative group! It was one of the most exciting times of my life – working almost every day until midnight, and it was a very stimulating environment with eminent visitors from all over the world, many of whom I am still in contact with.

One of my colleagues was an ICI employee, visiting the lab for six months, and he invited me to visit ICI's corporate laboratory in Runcorn to see what they did there. When I first arrived, I was introduced to one of their senior people who told me there were 'no jobs'. I reassured him I was not after a job – to which his response was that there were no short-term contracts either! I went on to meet several of scientists, including one senior researcher whom I interrogated about what they actually made. He pulled a jar of little polythene beads out of his desk drawer, and I must have asked some good questions as later on I was intercepted and offered a job. So I ended up in industry very much by accident!

So what did you do at ICI?

I started off, bizarrely, managing the accounts of a research group of more than 100 people who were spending huge amounts of money developing an organometallic catalysed ethylene polymerisation process for low-density polythene. But I still had time to work on several of my chemical hobbies such as phthalocyanines and low-spin iron(II) complexes. I also got involved with the development of phosphate non-misting glasses.

After a couple of years I moved to the agricultural division in Billingham, where I first became involved with heterogeneous catalysis, with responsibility for developing and manufacturing catalysts for producing hydrogen, ammonia, methanol and so on. It was very exciting as it was a completely new field for me, and there were several significant successes. After 12 years, I moved to the US to manage a research group investigating new polymerisation routes to PVC with facilities in America, England and Italy, and an office in Brussels. I did an enormous amount of travelling!

In 1992, I was headhunted by Johnson Matthey as technology director in the automotive catalyst business, a very important area for the company that was being severely pressed by the competition who, basically, had better technology. The challenge was to improve the commercial situation by enhancing the technical performance of our catalysts.

Why are catalysts used in the car industry?

Catalysts have been fitted in cars sold in the US since 1975 to control tailpipe exhaust emissions of hydrocarbons, carbon monoxide and nitrogen oxides (NOx), but it was not until the early 1990s that it became mandatory to fit them in Europe. I came into the industry just as the European market started, and we focused on the development of fundamental chemistry required to make better catalysts. One of the key features is durability – these hi-tech products must meet minimum performance criteria and effectively last the life of the car. The better the catalyst technology the less amount of costly platinum, palladium or rhodium that is required, so making it overall more cost-effective. We pushed the scientific boundaries very hard, and did many things we were not supposed to do, we just got on with it and developed new advanced world beating products!

What do the autocatalysts do?

In a petrol engine, partially oxidised hydrocarbons such as aldehydes and carbon monoxide are produced, as well as the expected combustion products water, carbon dioxide, and nitrogen. Because the temperature is so high at the flame front, oxygen and nitrogen combine through a complex series of free radical reactions to form nitric oxide. This is a fascinating molecule – at room temperature it is thermodynamically unstable, it is a free radical, and it should fall apart, but it does not! Instead, its only facile reaction is oxidation to nitrogen dioxide and because this is a third order process (second order in NO) at low nitric oxide concentrations the homogeneous oxidation in air is extremely slow.

However, in combination with hydrocarbons and sunlight, NO_2 is more readily formed, and photolytically this can form oxygen atoms that react with oxygen to form ozone. This is a lachrymator – and in particularly sunny locations like Los Angeles, Tokyo and even Rome, other photochemical reactions can lead to very potent lachrymators like peroxyacetylnitrate . This can make you cry at levels of parts per trillion. These secondary pollutants are only formed if the primary pollutants are present, and as legislation has brought these levels down, catalyst technology has developed to meet the increasingly stringent demands. Today, tailpipe emissions have been lowered to levels that can be below those present in the natural environment, so this is really a tremendous success story of what can be achieved at the chemistry/engineering interface.

What about diesel engines?

One of our big success stories at Johnson Matthey involves particulates – soot from diesel engines – and while modifications to engines have reduced the levels that are produced, the particulate matter remains very worrying in terms of health effects. Initially, very expensive multicomponent filter systems were used, comprising one or more usually two oxidation catalysts, a large ceramic soot filter and a small tank of fuel additive that mediated the periodic combustion of retained soot in the filter. They were heavy and both material and energy intensive to produce, and they also consumed a considerable amount of energy in use.

Recently we introduced a new filter design that can remove the particulates from diesel exhaust, as well as control gaseous tailpipe emissions. The new single units are only six-inch long so they can be mounted directly in the engine compartment, preventing heat loss and thus adding to overall efficiency. Periodically, perhaps every 1000 km depending on driving conditions, the temperature in the filter is increased to above 600°C to initiate combustion of the retained particulate in the filter.

This is done by putting additional fuel through the engine, which is oxidised over catalyst at the front of the filter. The particulate oxidation is a very exothermic process that is carefully controlled to prevent a meltdown! The car does this computer-controlled process automatically, and the emissions generated during this process are controlled as well. This design has won several awards, most notably two Queen's Awards this summer – one for innovation and one for international trade. The uptake has been very rapid, and already more than four million of them have been made and exported to mainland Europe, and the quantity of particulates that have already been prevented from going into the atmosphere is astonishing. It is rewarding that chemists together with engineers are able to produce things like this that have such a major benefit to society.

What's the next challenge for catalysts in the car industry?

This is already being addressed. The composition of diesel exhaust is very different from petrol engines that operate around the stiochiometric point with no excess oxygen. Diesel engines also contain CO, hydrocarbons and NOx, but because of the higher thermodynamic efficiency of the diesel engine, its exhaust temperature is considerably lower. As if this was not a significant challenge itself, diesel engines run lean, so excess oxygen is present, making it impossible to reduce the NOx. We have developed two solutions. One is to trap and store NOx as nitrate so it does not enter the environment through the tailpipe, and then periodically enrich the exhaust gas to reduce the stored nitrate to nitrogen. While this is effective, there is an alternative strategy – selective catalytic reduction using ammonia as the reductant. Since it is not practical to store the necessary ammonia on the vehicle, an aqueous solution of urea is used, that readily decomposes to give the desired ammonia. The urea tank needs to be refilled at service intervals, but this is straightforward, and we are well on the way to making a success of this approach – already there are several tens of thousands of cars on the roads in Europe using this new technology!

CV Martyn Twigg

Born: Wolverhampton

Status: He and his wife Sarah have a six-year-old daughter, Isabella

Education: Studied 'special chemistry' at Hull. His PhD was in kinetics and reaction mechanisms of inorganic complexes at the University of Kent at Canterbury.

Career: He spent two years at the University of Toronto as an NRC Fellow, before returning to the UK and Cambridge on a personal 'Bring-Back Fellowship' with Jack Lewis and Brian Johnson. After two years he moved to ICI, and then to Johnson Matthey, where he is now chief scientist.

Interests: Applications of chemistry, including pyrotechnics. He is a Class A licensed radio amateur, and in the past was a member of the British Rocketry Association

Did you know? He did not study any science at school, and owes his chemical career to his mother's decision to arrange for him to sit entrance exams at a college of further education to do science O-levels. His chemical interest was ignited by an exceptional chemistry teacher called Ivan Nutter who, Martyn says, lived up to his name. In the evenings he and several other students stayed in the laboratory to do all sorts of fascinating experiments – he remembers preparing a series of mixed salts, while other experiments involved materials such as mercury and benzene. As this was taking place, Nutter carefully crafted crossbows, which he fired down the central isle of the lab to targets that appeared after the end of the normal working day!

Pictorial delight

Dear Editor,
I have for some time been meaning to write and say how much I enjoy *Chem@Cam* – not least the pictures on the back. I have one request, though; might we be told (perhaps on an inside page somewhere) the picture's original subject? I guess that the latest one shows Don Quixote, but do not know the occasion – or what would happen if he held his pose a few seconds longer!.

I did my PhD in Organic Chemistry from 1954 to 57, working under Dr Kenner (as he then was) but never getting as far as being involved in his main field of interest. I remember little of that time, but can say that I moved to Lensfield Road about half way through it, being placed in a small basement laboratory quite near the front entrance. Another occupant was an Australian named Brian Milligan (generally called 'Spike' for some reason); his habit was to come into the lab of a morning, look at the results of his latest chromatographic run or whatever, and declaim 'It's a cruel, cruel, world!'

Of myself, it was once said that I was always to be seen in the lab, but never actually doing anything – which sounds about right. Somewhere there is a group photo with Professor Todd in the centre, in which I may be identified as the one grinning inanely while everyone else looks properly serious!

Yours sincerely,
Chris Tylor
3 Meadow Close, St Austell, Cornwall
PL25 3UD

The pictures on the back page are all taken from Cassell's Dore Gallery, an ageing collection of tomes containing a 250 engravings by French illustrator Gustav Doré. Many – like the last issue's – are indeed scenes from Don Quixote. Dante's Inferno also provides the source for many of the images, as does Paradise Lost and the Bible. This issue's is Don Quixote again, with an image of the Don in his library.

Corrosive atmosphere

Dear Editor,
Seeing the article about fire extinguishing reminded me that one of the regular housekeeping jobs in 287 (1967-70) was to go around making sure the pins could be removed from the extinguishers – when I first arrived there, all of them (being brass) were firmly corroded in place and required superhuman strength or a pair of pliers to loosen them. I hope the atmosphere is less corrosive now.
Yours faithfully
Peter B Baker
9 Kenilworth Road, London, W5 5PB

Welsh confusion

Dear Editor,
I was interested to see the picture of the physical chemistry department of 1960 in the summer *Chem@Cam*. As an undergraduate doing practicals I was often observed – and chatted to in Welsh – by someone I assumed was the lab technician with long sideburns and usually dressed in a blue pin striped suit.

Imagine my surprise when I was introduced to him after the Sunday Welsh service in Wesley Chapel to find out he was Professor Moelwyn Hughes, the son of an eminent bard and preacher John Gruffydd Moelwyn Hughes, who wrote the famous Welsh hymn 'Pwy a'm dwg i'r ddinas gadarn'.

His brother, a lawyer, Rowy Moelwyn Hughes was Labour MP for Carmarthen and headed the inquiry into the Burnden Park disaster in 1946 when 33 football supporters were killed and hundreds injured in a cup match between Bolton and Stoke City.
Huw Idris Jones (1965-1968)
hijones@btinternet.com

Footy correction

Dear Editor,
I noticed that two names got omitted in the list of footballers in the last *Chem@Cam*.

The names omitted were John ('Bones') Connors and David Rand.
Best wishes
Ian Smith

chem@cam
Chemistry at Cambridge Newsletter

Contents

Cover

Anthoulla Papageorgiou from Richard Lambert's group operating a scanning tunnelling microscope, which is used to study surfaces

Photograph:
Nathan Pitt and Caroline Hancox

This newsletter is published three times a year by the University of Cambridge Chemistry Department. Opinions are not necessarily those of the editor, the department, or the university.

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A trio of tomes hit the shelves

Photo: Mary Bernard

Ian, Tony and Stuart: still writing away in the department. 'Visitors interested in discussing their chemistry are always welcome to visit us!' Tony says

The three retired(ish) professors who inhabit M21 have been busy. Ian Fleming, Tony Kirby and Stuart have been occupied with writing for years, and in the past few weeks all three have had books published.

The fruit of Ian's labours is the long-awaited second, completely revised, edition of his famous book on frontier orbitals, in the shape of 'Molecular orbitals and organic chemical reactions'. The original came out in 1976 and survived in print for more than 30 years.

'There was always a problem – computations showed the frontier orbitals do not make a significantly larger contribution than the sum of all the other orbital interactions,' he says. 'The difficulty is that it often works as an explanation where nothing else is immediately compelling.' He hasn't ditched them completely in the new book, but there's a greater emphasis on the molecular orbital basis for understanding organic chemistry.

Tony Kirby's 'From enzyme models to model enzymes', written with Florian Hollfelder from biochemistry, is about catalytic efficiency – how to measure, understand and create it using the tools and thinking of organic chemistry and molecular biology. 'By a happy coincidence, the cover picture of the ribosome is a gift from Ada Yonath, whose Nobel prize was announced the day the book was published,' Tony says.

Stuart's latest book is a new edition of the Workbook that accompanies 'Organic synthesis: the disconnection approach'. These have been completely rewritten, in collaboration with former Cambridge student Paul Wyatt, who's now director of undergraduate teaching at Bristol. This workbook completes a mammoth four-volume set of organic chemistry teaching books that have appeared since 2007.

'The first edition of these books were published in 1982,' Stuart says. 'They were typed, and the structures done with stencils. The results looked more like an underground publication in Soviet Russia than a modern chemistry book. The new editions look very different.' He's now working on the second edition of the big textbook 'Organic chemistry' with Jonathan Clayden, and aims to finish this in 2010.

Photos: Nathan Pitt

The Unilever Centre for Molecular Science Informatics held a workshop to start off the new £3.2m funding from Unilever. 'This is our core funding for the next five years,' says centre director Bobby Glen, pictured right at the workshop. 'It includes funding for three lecturers, computer officer and secretarial support, and £1.5m is reserved for projects with Unilever.'

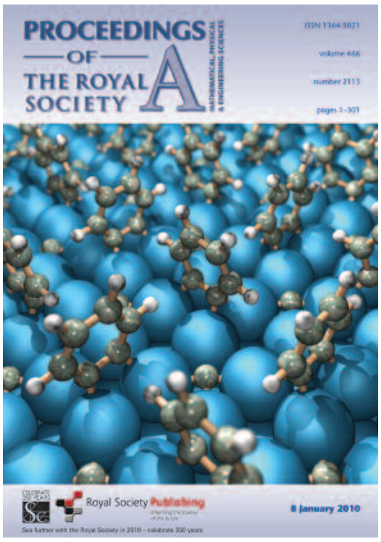
Eric the honorary RSC fellow

Eric (left) receiving his certificate from RSC president Dave Garner

Congratulations to Eric Walters, who was made an Honorary Fellow by the Royal Society of Chemistry earlier this year in recognition of his support for chemistry. Eric is also a long-time supporter of the department through the Walters Kundert Trust, with donations to our Science Day activities, as well as funding Next Generation Fellowships for promising young lecturers – he's currently supporting Jonathan Nitschke and Oren Scherman.

With their ANU hosts, from the left: Vance Lawrence, Mark, Pete, Mark Ellison, Geoff Salem and Paul Gugger

Pete Wothers and Mark Hudson took this year's Science Festival schools' lecture, 'Just add water', all the way down under in August. As part of Australian National Science Week, Canberran schoolkids were treated to the action-packed chemistry show at the Australian National University. It was so popular they had to perform four times! 'Some reactions didn't behave the same way as they do over here,' Pete says. 'We couldn't make cyclohexane ice cubes, and the silver nitrate and magnesium powders were more reactive. I spent several days with lots of black spots on my face from a rather frisky reaction!' They're now TV stars in Australia, too, as it was shown on the ABC channel. It went down so well they're returning to Oz next year, also visiting Sydney, Melbourne and Tasmania



Congratulations to Steve Jenkins, who's been appointed to a university lectureship. Steve works in surface science, and one of his hobbies is creating computer-generated images of chemical subjects. They make great journal covers, and here's his latest offering. It accompanies an invited review in *Proceedings of the Royal Society A* about aromatic adsorption on metals via first-principles density functional theory

The university's 800th anniversary celebrations are drawing to a close, and one of the recent events was a celebration for alumni and donors in New York. The Empire State Building was even lit up in Cambridge blue for the occasion. Guests included such luminaries as Stephen Fry, Sir David Frost… and Jeremy Sanders (above)!

Prizes for Steve, Ian and Oren

Steve Ley has added three more medals to his collection. The Tetrahedron Prize for Creativity in Organic Chemistry was presented at the ACS meeting in Boston in August, and the citation mentioned the wide range of chemistry he's been involved in over the years, including synthetic organic methodology, chemical technology and complex natural product synthesis.

He also received the Heinrich Wieland prize for his 'extraordinary scientific achievements in the fields of synthesis, structural analysis and biological characterization of natural products'. The prize is endowed by Boehringer Ingelheim, and was presented at a ceremony in Munich in October. 'I've had a very good year, and am very proud that our work is being supported and recognised in this way,' Steve says.

The third prize, the RSC's Perkin Prize for Organic Chemistry, was given at the RSC's awards ceremony in November. Two other Cambridge chemists were also given awards at the event – Ian Paterson and Oren Scherman.

Ian was one of three winners of the Tilden Prize for advances in chemistry. He won for his 'outstanding achievements in the total synthesis of complex natural products'. Over the years, Ian has introduced general methods for stereocontrolled synthesis, which have enabled the total synthesis of a large number of biologically important polyketides within his group. These include several which are promising anticancer agents that are in short supply from their natural sources, especially those of marine origin.

Oren was one of the three Harrison-Meldola Memorial Prize winners. These are given for the 'most meritorious and promising original investigations in chemistry and published results of those investigations,' and Oren won for his work on supramolecular polymers, in particular in aqueous environments. 'I was delighted to win the prize,' Oren says. 'The work wouldn't have been possible without the hard work of my talented group, and it was really nice to be in such good company with the other prize winners.'

On the funding front, Oren has been awarded a prestigious starting grant from the European Research Council. There were 10 times as many applicants as grants, so this is something of an achievement! The grants are designed to support scientists who are in the early stages of their independent research careers, and Oren has been given a grant of €1.7m to support his work on aqueous supramolecular polymers and peptide conjugates in reversible systems.

■ Congratulations also go to Dave King, who's been appointed Chancellor of Liverpool University. Dave was professor of physical chemistry in Liverpool in the 1970s and 1980s, before he came to Cambridge chemistry in 1988.

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Thanks to the generosity of the department's Corporate Associates, we have been able to benefit the education and environment for students and staff. For example, the Associates pay for university-wide access to SciFinder Scholar and ChemOffice. They also make significant contributions to the library for journal subscriptions. Moreover, they provide exam prizes, faculty teaching awards and summer studentships, and have recently funded the refurbishment of a state-of-the-art meeting room with teleconferencing and display facilities.

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The lab book enters the 21st century

The traditional lab notebook is great for recording results, but not very good for searching them. The electronic version changes all that

Photo: Caroline Hancox

Bhavinita Patel from Bill Jones' group is one of the pioneering souls taking part in the ELN pilot project

The department is in the throes of a pioneering project that will make it the first UK chemistry department to implement an electronic lab notebook system, or ELN. Based on a commercial system from IDBS, it will enable chemists to manage their data more effectively. The first 20 or so chemists are already using it, and their feedback will be crucial in designing the final shape of the notebook.

DATA MINING

The amount of data that experiments generate these days can be huge, yet there is currently no efficient way for our chemists to archive their spectra in a searchable way that also captures information about the experiment itself. 'Today, NMR spectra, for example, are filed away under date and scientist, but there's no chemical information there,' explains Tim Dickens, the department's IT manager.

'If you want to find a spectrum run by someone who has left, you have to dig out notebooks, papers or the thesis of the person who did the research from around when you think the experiment might have been done. If that person did a lot of reactions, that means a lot of files to wade through. Being able to link the spectra to the experimental results is something of a sea change.'

The system is really straightforward to use. For a synthetic reaction, the chemist draws the reaction scheme using ChemDraw, and the lab notebook will automatically calculate quantities of reagents given the stoichiometry. The ELN collects the health and safety data, displays the risk factors, and records the emergency procedures.

ELNs have been used in the pharmaceutical industry for some time. However, it's much more of a challenge developing a system for an academic chemistry department as the science is so much more diverse. It also has to work seamlessly on Macs, PCs, and even Linux machines. This is being addressed by using a terminal server – the data are kept on a central server, and the 'front end' which interfaces with that server can be on any type of computer.

'It's a neat way of doing things,' explains Brian Brooks, who implemented the lab notebook system at GlaxoSmithKline, and is helping the implementation process here in chemistry. 'You can log into your lab notebook area on any linked machine – whether in the lab, a write-up area or even the library. It also logs straight into the same session, so you don't have to start again. We're really pleased with the way it works.'

There's also the issue of who has access to the data. The ELN has three 'audience' areas; one which is restricted, one which allows their own research group to see the experiments, and one which the whole department can see. The scientist decides who they wish to be able to see their experiment, and then creates their experiment in the appropriate area. 'At some point in the future, we foresee this might be extended to the whole world,' Tim says.

This isn't as insane as it might sound – there's a big drive in the US to make all experimental data publicly available, particularly when the research was paid for by a public body like the NIH, and that's bound to spread.

It will certainly make producing papers and theses more straightforward as all the data are in one place. The ELN will make it easy to pull out all the data on the experiments and compounds from the database and drop them into a publishable format. Brian says many researchers currently store their data in Excel spreadsheets and write-up their experiments in Word documents; this raises the question of what advantage the ELN has over this approach.

'It's a good question,' he says. 'But ELNs have so much more functionality, quite apart from the searchability of the database. The ELN holds the whole context of an experiment in one location. And the ELN has capabilities to make the content more active; the viewer software, for example, allows you to rotate chemical structures on screen, and with an NMR spectrum you can take a small subsection and expand it to get a clearer view of the peaks.' All this is done within the same software environment, without having to jump between different packages, making life much simpler and easier for the chemist.

In the future, Tim envisages hi-tech gadgets being used in the lab to input and view data, such as devices that project virtual keyboards onto surfaces, and even data projectors within a fume hood. 'The technology is moving very fast,' he says. 'Devices like these only take up a very small amount of space, and so they can be activated wherever they are needed.'

CHEMICAL INVENTORY

It also offers the potential for further improvements in the future – such as an end to those 'has anybody got this chemical' email that clutter up inboxes on a regular basis. 'Implementing a chemical inventory would make us much more efficient,' Tim says. 'It would require cooperation from a lot of different groups, and also data such has how old chemicals with a finite shelf-life are would have to be included.

'I think we will look back in a few years' time and wonder how we ever managed to do science without the ELN,' Tim says. 'I also think it will become increasingly important as we form larger groups and partnerships, and people work in a more collaborative fashion in different locations. Being able to share data electronically in a seamless fashion like this is the way forward.'

Small is beautiful

It's important to know how drugs bind to their active sites if better ones are to be designed. Alessio Ciulli's using fragments to explore them

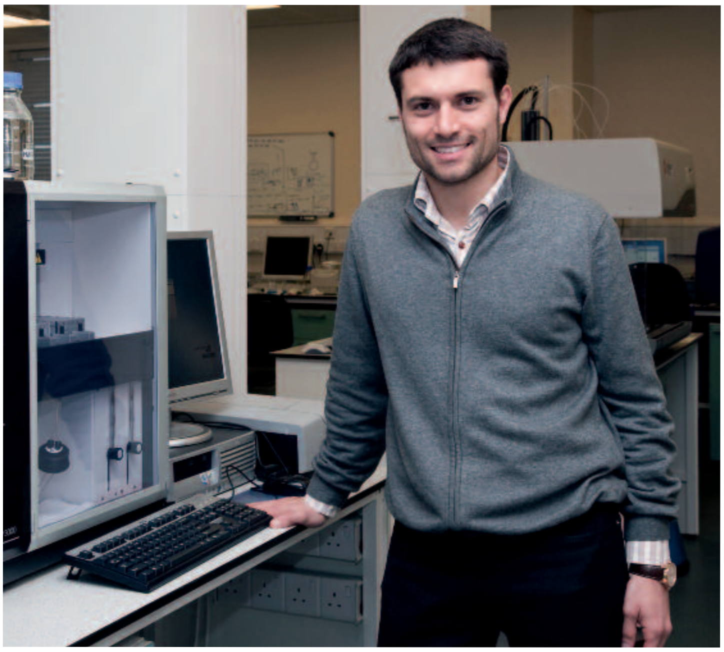


Photo: Caroline Hancox

Drug molecules work by binding to active sites within the body, often at some form of protein such as an enzyme. In recent years, huge advances in chemical techniques such as X-ray crystallography and NMR spectroscopy have made it possible to determine the structures of many of these proteins.

While this is a great starting point for finding a new drug, it's not always immediately obvious exactly where the drug needs to bind to the protein to work, or at how many points. One method that can help probe these active sites uses fragments – small molecules that interact weakly with the protein. While these in themselves won't make good drugs, they can provide optimal starting points for finding a molecule that binds more effectively to the protein and has the desired therapeutic effect.

Alessio Ciulli is using fragments like this to try and gain new insights into biology. 'During my PhD, I started working on enzymes from *Mycobacterium tuberculosis*, the bug which causes TB, with the hope of finding new compounds that might be useful in treating the disease, or at least find a starting point for a medicinal chemistry programme,' he says. 'TB is a tremendous health burden, especially in the developing world, and the newest drug that's currently used was discovered 50 years ago! So there's a great need for new targets and new drugs.'

Many people have been looking for potential targets within *M. tuberculosis* using genetics, but while genetics can tell you if that target is essential in its lifecycle, it can't tell you whether inhibiting it will prove lethal to the bacterium, so you need to try it and see.

'TB is a particularly nasty infection as the bacterium becomes latent, and completely changes its metabolism,' Alessio says. 'What's really needed is a chemical validation of new targets. Fragments are potentially fantastic tools to probe the druggability of targets, and to show whether inhibiting it will actually have a physiological effect in living cells.'

INTELLECTUAL CHALLENGE

During his JRF, he was involved in various collaborative projects with scientists in other fields, and has carried these on into his independent research career. 'This brings many different expertises together, such as protein chemistry, molecular biology, structural biology, biophysical screening and, ultimately, medicinal chemistry,' he explains. 'It would be impossible for a single person to work on all these different disciplines, so working together is essential.'

Because these fragments are such small molecules and bind so weakly, the real intellectual challenge lies in telling the difference between a specific, weak interaction between the molecule and the protein and a non-specific one. ' Why does a fragment bind, what are the key interactions, and what can we learn from it?' he says. 'We want to find out what the hotspots for binding are, and then how to go about designing a molecule that works effectively there, or taking them forward into new chemical tools.'

In collaboration with Chris Abell and graduate student Alvin Hung, he has recently published a direct comparison between two different ways of doing this – starting with a small fragment and making it larger by adding further functionality so it fills the binding site better, and taking two fragments that bind weakly to different parts of the protein and linking them together. 'We came up with two very similar molecules in this way, which differ very slightly at the ends, but while one binds like the two initial fragments, as you would expect, the other binds differently. Yet the core structure is very similar!'

A new collaboration is taking the idea into another area – sugars. 'Barbara Imperiali at MIT has a long standing interest in the biosynthesis of highly modified sugars in Gram negative bacteria, which are crucial to both their pathogenesis and their virulence,' he says. 'Most of the enzymes responsible for the biosynthesis of these modified sugars are unique to these bacteria, and we hope my fragment screening expertise will enable us to discover how we can target sugar binding sites.

'There have been very few drugs that target sugar sites, the exception being the neuraminidase inhibitors like Tamiflu. The general consensus is that the binding site has to be flat and polar in nature. This makes them difficult to target, and this excites me as my ultimate goal is to see if fragments can teach us how to design molecules that work against binding sites traditionally considered undruggable.'

CV

Alessio Ciulli

Born: Florence, Italy

Status: His girlfriend, Stefania Lanni, was brave enough to follow him to Cambridge when he started his PhD, despite speaking no English. She is now office manager at the acute neonatal transport service unit at Addenbrookes.

Education: He studied chemistry at the University of Florence, and his first experience of Cambridge was as an undergraduate Erasmus exchange student a decade ago. He returned to Cambridge in 2002 for a PhD with Chris Abell on a Gates scholarship.

Career: After three years as a JRF at Homerton and mastering protein X-ray crystallography with Tom Blundell, he spent five months as an HFSP fellow with Craig Crews at Yale. He returned to Cambridge and chemistry this summer as a BBSRC David Phillips fellow.

Interests: Skiing, road cycling, tennis, playing the guitar, and he's learning to play bridge.

Did you know? Alessio first came to Britain as a 16 year-old English language student. On a day trip to London, he and a friend headed to Wimbledon with the dream of watching the ladies' final, despite not having a ticket for Centre Court. They were foiled by a security guard, but he relented at the end of the match and they took photos of Jana Novotna crying on the Duchess of Kent's shoulder after throwing away a win. 'Since then, I've had a day out of the lab at Wimbledon every summer!' he says.

Designing new materials for energ

Clare Grey's chemistry is focused on helping identify novel materials for making better and more effective batteries to store energy

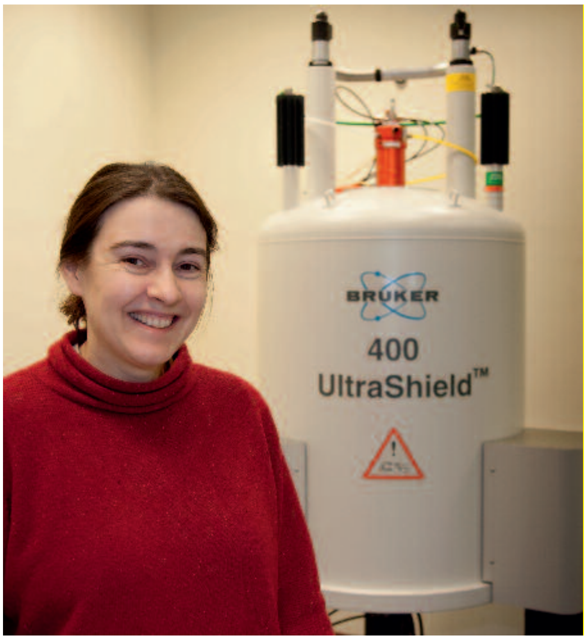
A sustainable energy supply for the future will require reliable renewable sources of power – and a mixture of sources. Yet wind turbines only produce energy when it's windy, and solar panels when the sun is shining. Neither is it easy to store the electricity that's produced for the times when none is being generated. Transporting it is another issue – it's all very well building huge wind farms in isolated areas or installing miles and miles of solar panels in the Sahara desert, but if the energy can't be distributed to where it's needed then it's a fairly pointless exercise.

It can't simply be stored on the grid as that's merely a series of interconnected wires. Too much of the electricity is lost on transmission down those wires to make very long-distance distribution viable, and it's expensive and logistically difficult to run the cables. Electricity distribution can be made more efficient by increasing the voltage and using superconductors, but even this has practical problems. The bottom line is a wholesale move away from fossil fuels to renewable energy sources will require the ability to store electricity, and transport it from where it's produced to where it's needed.

New and better materials will provide the key to solving some of these problems, and Clare Grey's chemistry is aimed at helping to find them. 'I'm an inorganic chemist, but my work bridges inorganic and physical chemistry, materials science and chemical engineering,' she says. 'I'm very interested in how local structure of the materials used in batteries and fuel cells – devices required to store and convert energy efficiently – affect their performance in specific applications.'

ELECTRIC VEHICLES

Electric cars are one example where better batteries are critical. Current technology is limited to hybrid electric vehicles such as the Toyota Prius, where the combustion engine is supplemented by a battery system that stores the kinetic energy lost on braking. New batteries are required to power the next generation of electric vehicles, which are plugged into the mains to recharge them. 'This doesn't solve the problem of where the energy comes from as a battery merely stores it,' Clare says. 'But combustion engines are massively inefficient, whereas electric motors can, in principle, be almost 100% efficient.'



It's not just the big picture of energy generation and transportation that is an issue – at a smaller scale, the batteries that are used in mobile phones and laptops are far from ideal. The standard laptop and mobile phone battery was developed by Sony in 1990 using chemistry from John Goodenough's lab at Oxford, Clare says.

'He came up with the chemistry for the cathode, a material containing layers of metal, oxide and lithium ions. When it's charged, the metal ions are oxidized, for example from Co^{3+} to Co^{4+}. At the same time, the lithium ions are pulled out of the structure, and then travel through a non-aqueous electrolyte to the anode, where they are then inserted in between the carbon layers of the graphite anode. The opposite process occurs as the battery is discharged.'

The ideal battery material will use reversible chemistry that can go back and forth thousands of times without degrading, will have large differences in the electrochemical couples between the two materials to give high voltages and thus high energy, and also be light and thus give a high capacity on a weight basis. Current materials fall short of these ideals.

'It takes a long time to charge a laptop, and for a car, consumers want to be able to charge it in 20 minutes,' she explains. 'But that's not even a problem with the battery – it would probably require cables half a foot thick and would probably short-circuit the power to the whole street when it was plugged into the mains! Fuel is a very efficient way of transporting power. The strategy is to design cars that would allow people to drive short distances regularly before charging up overnight, but that would combine a back-up source of power generation to allow occasional long trips – the plug-in hybrid.'

The main issues, she says, are cost, materials, resources, capacity, power and safety. 'I would argue that if you want to make progress in this field, you have to understand how some of these processes work, and then use this knowledge to design and improve the materials we have now, and come up with better ones.'

One of the main focuses of Clare's research is using NMR to understand what's happening to the lithium ions as a battery is charged and discharged. 'Lithium is a good nucleus for NMR, and it's intimately involved in the whole process,' she explains. 'We've been doing experiments *ex situ* by taking the battery apart, and also *in situ*, which means we can watch what is happening to the lithium ions in a working battery in real time.'

There is a number of reasons why this is useful. 'Even a simple material like lithium cobalt oxide is a layered material, and when all the lithium ions are pulled out the layers shear, making it very difficult for the lithiums to get back in again,' she says. 'So in practice, only about half of the lithiums are removed as the battery is charged to ensure it retains its structure, resulting in 50% dead-weight. If the layers could

Clare Grey CV

Born: Born: Middlesbrough, where her dad worked for ICI. She moved to the Netherlands at the age of 2, Belgium at the age of 7, and then at 14 went to school in St Albans.

Education: a chemistry degree at Oxford led to a DPhil there on the solid state chemistry and NMR spectroscopy of paramagnetic materials with Tony Cheetham, who's now Goldsmiths' Professor of Materials in Cambridge

Career: After a brief stint as a junior research fellow at Balliol, she moved to the University of Nijmegen in the Netherlands as a Royal Society research fellow, before heading to Du Pont's central research labs in the US. Two years later she moved to Stony Brook University in New York as an assistant professor, being made a full professor in 2001. She moved to Cambridge in July as Geoffrey Moorhouse-Gibson professor of chemistry.

Status: Husband Daniel Raleigh is an academic biophysicist, working on protein folding and amyloid formation

Interests: Cross country skiing, hiking, playing the cello

DId you know? Clare plays an18th century Czech cello that she found abandoned in an antique shop and rescued. It cost her the princely sum of £50!

y storage

How to run an NMR of a functioning battery

It may seem unlikely, but it is indeed possible to run an NMR spectrum of a battery in real time as it charges and discharges. In a solid state NMR machine, the sample is put inside a chamber about 1cm by 0.5cm in size. Normally, a battery would be encased in metal, but this makes it difficult for the radio waves to pass through. Instead, it is sealed inside a plastic bag with an aluminium coating that prevents oxygen and moisture from entering the system. These bags are exactly the same material as those ground coffee is sold in to prevent the coffee from deteriorating in quality.

The battery is inserted in the bags, with leads protruding from the edges, the air sucked out, and then it is heat sealed shut using a crimper, over the wires. The leads are then connected to the power source and placed in the NMR machine, and the battery can be charged and discharged while a lithium spectrum is being run. 'You can watch the whole battery, with the lithium ions going in and out, and the NMR peaks grow and diminish as it cycles,' Clare says. 'It's also possible to see what's happening to the electrolyte, for example in a silicon-based battery, it slowly forms a coating which ultimately stops the battery from working.'

It also shows the formation of lithium dendrites very clearly. 'That's why you can't use pure lithium metal as the anode – as you cycle backwards an forwards, instead of lithium plating on the surface it grows fibrous lithium dendrite structures,' she says. 'These grow and grow as the battery is cycled backwards and forwards, and they are incredibly strong. Even though lithium is quite a soft metal, they can force their way through strong polymer membrane separators.'

be stabilised somehow, the operating power of the battery could be doubled.'

One project she's carrying out, in association with GM, involves looking at the problems involved with inserting lithium ions into the graphite anode. 'In principle, carbon has a large capacity, but if the battery is charged too fast, the kinetics of the lithiums entering between its layers become challenging. Instead of going inside the layers, lithium plates and forms lithium dendrites, which eventually cause short-circuits,' she says. 'We're using *in situ* NMR to watch the dendrites forming to try and work out what conditions they form under, and then find a way to get rid of them. That would be impractical to do if you had to take the battery apart.'

She believes understanding what is happening is essential if new and better materials are going to be discovered. 'Although some discoveries appear to be a result of trial and error, most inventions are underpinned by an understanding of what's going on,' she says. 'Few inventions happen in a vacuum, and most require an enabling technology to inspire them. For example, lithium iron phosphate is a promising new cathode material, again invented by Goodenough, but it was a very poor electronic conductor, meaning that although the lithium ions could be extracted, the electrons could not be extracted, and you need to be able to do both at the same time.

INCREMENTAL ADVANCES

'Someone else thought that coating the material with a fine layer of carbon would decrease the distance the electrons would have to tunnel from the carbon coating through to the material to the iron ions inside. Then someone else showed that using nanoparticles could also reduce tunnelling lengths and showed that this resulted in very high charging and discharging rates. This material has challenged conventional wisdom, as insulators did not make good cathode materials! But now there is a strategy that might make them work, through incremental advances.'

She's just had a grant funded with Peter Bruce at St Andrews as part of the Supergen consortium for batteries, looking at iron silicate batteries. 'Silicon is the most abundant element after oxygen in the earth's crust, and iron silicate batteries could be very cheap,' she says.

'The material itself doesn't work well, but now we know we can try putting on a carbon coating. It then turns out that when the battery is cycled, the structure changes, so now we have to work out what changes. Can we stabilise this new structure? If we don't know the structure, we can't even begin to think about how to improve its performance.'

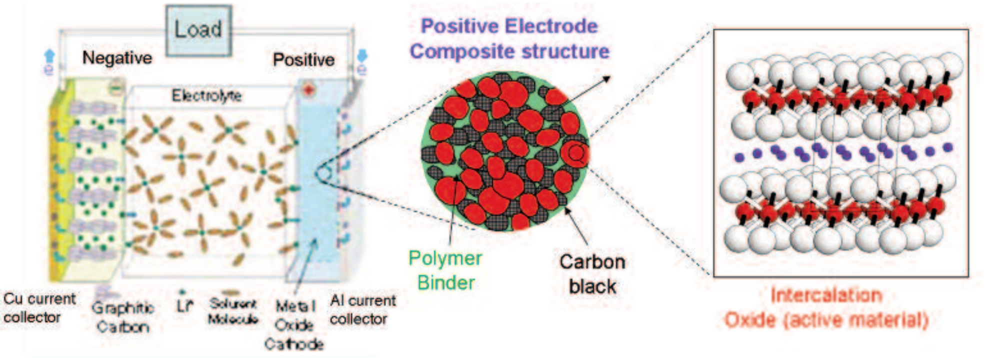
Part of the problem is that it's disordered, so techniques that look at long-range order such as diffraction are less useful. 'We can study the lithium and silicon NMR spectra, and use this to help us solve the structure, and with diffraction experiments we should be able to determine a complete picture of the material. When we know what the material changes to, then maybe we will be able to synthesise that structure from the beginning, or perhaps keep the original structure by doping it appropriately to add stabilising ions.'

Then there are different metals. While lithium iron phosphate works very well, if the iron is replaced by manganese, it doesn't work well at all. 'Manganese would be good as it operates at a higher voltage, and would give extra energy density and increase the battery's power,' Clare says. 'But why doesn't it work? Is it the crystal structure, or is a completely different reaction going on? We want to understand how things like this work to give us the basis for designing different systems that might be more effective.'

Another issue is the lithium itself – there's only a finite resource of lithium, so why not use something that's more abundant? 'As the ions have to move through the solid, that is very limiting,' she explains. 'An alternative for a tiny ions is magnesium, whose ions are 2+, and people are working on magnesium batteries, but while only a little is lost in voltage, a lot is lost on rate performance, because of the need to pull the the doubly charged magnesium ions out of the structure. Sodium is also a possibility, but it's pretty reactive! Some buses use a high temperature sodium battery based on ionic liquid electrolytes, which operate at 300°C but there are safety concerns.'

CHEAP MATERIALS

She's now collaborating with a group in Spain on an EU-funded project on sodium batteries. 'While they may well not be viable for widespread transportation uses as yet, they could have applications in the home – though probably not in laptops that could be taken on aeroplanes!' she says. 'But a combination of sodium with other cheap materials like iron silicates and phosphates might offer alternative batteries. I'm interested in how their structure impacts performance – we explore how to improve performance by systematically varying structure.'



Quantum complication

The electron correlation problem has confounded theoreticians for decades. A new method devised by Ali Alavi may provide a solution

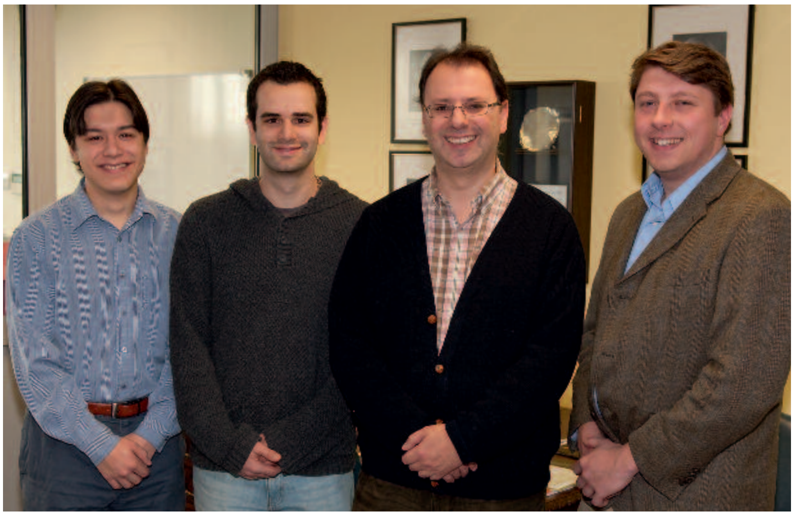


Photo: Nathan Pitt

Ali with some of his group: James Shepherd, George Booth, Ali Alavi and Alex Thom

Anyone who's studied for a degree in chemistry will be familiar with the Schrödinger equation. Dating back to the 1920s, it is central to quantum mechanics, but for a molecule it contains terms that arise from the fact that electrons repel each other, and this greatly complicates solving the equation. In practice, headway can be made only by making approximations known as self-consistent fields, which simplify matters by assuming each electron 'sees' an average field of all other electrons, rather than each one individually.

The electrons are assumed to move in an uncorrelated fashion, and the wavefunction solved in this way is said to be uncorrelated. In some simple systems this works well, but in more complex ones such as bond-breaking transition states and transition metal molecules, this simplification is just not good enough. However, computers are not powerful enough to cope if sufficient correlation between the electrons is included – in essence, the correlation is built up from a vast array of uncorrelated wavefuntions.

Ali Alavi is working on a method that will allow accurate solutions to the electron correlation problem to be achieved without massive computing power. 'The problem goes back to the very early days of quantum mechanics, and despite the vast increases in computer power over the years, it essentially remains unsolved as it's exponentially hard. It might be possible to solve individual cases, but the general solution looks impossibly out of reach,' he says. 'It doesn't help that the problem is not really understood at a fundamental level, either.'

The root of the problem is that the number of uncorrelated wavefunctions needed to account for electron correlation grows at an exponential rate. 'Each extra electron adds a factor of 10 to the number of terms, so by the time you reach about 20 electrons even a huge supercomputer cannot cope,' he says. 'The biggest system that people seem to be able to solve using this brute force approach appears to involve 10 electrons, such as the nitrogen molecule (with a frozen core). But if you want to look at, say, a magnetic cluster of iron atoms, even if Moore's Law [that computing power doubles every two years] holds, that will still be out of reach in 100 years.'

He has been working on the problem for the past 20 years, but last year achieved a breakthrough, with the inspiration to look at the problem in a different way. 'In the 1970s, the Cambridge mathematician John Horton Conway came up with something called the game of life,' he explains. 'This is a set of simple rules for entities that live on a lattice, and how they live or die or prosper.' Basically, every cell at the corner of a square lattice is adjacent to eight others. Conway's rules are that any live cell with fewer than two or more than three live neighbours will die because of under- or overpopulation. If it's next to two or three, it lives on to the next generation, and if a dead cell has exactly three live neighbours, it becomes live.

Ali realised that these simple-sounding rules, which lead to staggering levels of complexity, could be applied to the electron correlation problem, if the array of uncorrelated wavefunctions used to construct the correlated wavefunction are viewed as an enormous abstract lattice. He wondered whether it could be possible to devise simple rules to a game of life that, as it evolves, spontaneously leads to the ground state electronic wave function.

And it turned out that it could. 'There's an incredibly simple set of rules that enable you to do this – and which are very easy to programme,' he said. 'Once I'd worked the idea out, I had it programmed within three hours. The rules, essentially, are that there are two types of what we call "walkers" on the lattice, positive and negative. They can do one of three things at each step. They can spawn progeny, which can be either positive or negative depending on the sign of the parent and the sign of the connection to it; they die in a random fashion, with a probability that is proportional to their energy; and if two walkers of the opposite sign find themselves next to each other, they will annihilate each other.'

That simple computer simulation has allowed the solution to many electron problems to be calculated. 'We can use it to solve the 10 electron system very quickly and remarkably accurately on a desktop PC,' he says. 'It's also about an order of magnitude more accurate than the simplified system. My group has been having an incredible amount of fun with this, and I've been amazed at the amount of interest it's generated in the quantum mechanics community. It's pretty abstract as you can't really think of the points in a straightforward lattice, and it took me a very long time to piece together these abstract notions into a form that allowed game of life algorithms to be set out. But once the basic simplicity became clear, the rest followed quite quickly. It's still early days, but I believe the technique is incredibly promising.'

CV

Ali Alavi

Born: Iran

Education: He was sent to school in the UK at the age of 13, and came to Cambridge as an undergraduate, staying on for a PhD with Ruth Lynden Bell.

Career: After a two-year postdoc in Amsterdam, he returned to Cambridge as a JRF at Trinity in 1993. He took up a lectureship at Queen's University in Belfast in 1995, and five years later returned to Cambridge as a lecturer. He's now a reader.

Status: He's married to Sanam, a former high-flyer at Vodafone who's currently a full-time mum to their two-and-a-half year old son, Cyrus

Interests: Rowing in the fellows' boat at Trinity, skiing and being bossed around by Cyrus

Did you know? He first met Sanam when he was 14 and she was about 8 or 9, as their fathers were both Iranian diplomats based in India. They stayed friends ever since. In 2005 Ali was invited to speak at a conference in Sicily and fancied staying on for a holiday, but thought it would be more fun with a friend. On a whim, he asked Sanam if she fancied going with him. 'That whim gained me a wife – we married a year later!' he says. 'Sometimes whimsical decisions can alter the course of your life.'

Further memories of the 1960s

Norman Sheppard adds his own reminiscences to our collection of 50th anniversary memories

I was very interested in the reminiscences in connection with the opening of the Lensfield laboratories. Here are some of mine. I joined the University Chemical Laboratory as an ADR in spectroscopy, at the same time as the start of the move. I had previously held research fellowships in the department of colloid science, and had for several years obtained and interpreted infrared spectra for the organic chemists.

My teaching duties in the laboratory were to give the research students lectures on the spectroscopic methods of determining molecular structures, to supervise and develop the spectroscopic instrumentation, and to run a 'clinic' to help students interpret the spectra of their own samples.

When I was appointed ADR, I told Professor Todd that in my judgment the next spectroscopy for structure determination, after IR, was likely to be nuclear magnetic resonance. Commercial equipment from Varian Associates was just coming on the market, and Professor Todd applied for, and obtained, what in those days was a very large grant for the purchase of a 40MHz spectrometer. Ralph Elsey, a senior technician, and I got it to work and saw it through many technical updates. With a recently acquired very good group of NMR research students, we made contributions to the molecular structure database, and I developed appropriate lectures.

NMR turned out to be a very useful technique when applied to many structural problems, but it was very embarrassing that I was not able successfully to interpret the spectra from the erythroaphins, Professor Todd's main research interest, in terms of the structure proposed. I made this clear several times, but was told firmly that the chemical arguments for the structure were very secure.

This story, of course, relates to the incident in a research seminar described by Ian Fleming in his reminiscences in the Spring 2009 *Chem@Cam*. I learned that Yusuf Hamied was going to describe the chemistry and announce the preferred structure at a research seminar. The night before this I returned to the embarrassing NMR interpretation problem. There were complexities to the spectra because there was possible overlapping of spectra from the different conformations of aliphatic groups that occur on either side of the aromatic core of the molecule, and small chemical shifts led to distorted splitting patterns, but even so…!

It suddenly came to me (a Gestalt switch) that the assumption of an alternative isomeric structure would allow me to fully understand the spectra. It involved a change from aliphatic cyclic groups based on CH_3-CH< units compared with the preferred $-CH_2-CH_2-$ groups. What was I to do? If I told Yusuf straight away, I would completely upset his, doubtless already carefully prepared, research talk. So I decided to give my additional evidence – for what it was worth (though I was convinced) – at the end of his presentation. I did so as Ian described, and there was a pregnant silence. Then Professor Todd said, 'Well now, we thought that we had eliminated that structure *three years* ago. Perhaps we had better repeat that experiment!

I was never told the result of that repeated experiment, but the revised structure was rapidly published. After that episode, I did not have to make so many of my occasional 'five bob bets' during my structure/spectrum clinics when there seemed to be a serious clash of chemical and spectroscopic evidence! I never lost any of those bets.

ARMY VOICE TRAINING

My first personal experience of the new building was when I gave my first lecture in what I think was designed as a seminar room in the front of the building. The only problem was that a very noisy bulldozer was operating just outside – luckily I had been trained to use my voice by a regimental sergeant-major during the war, and I survived.

With respect to the building itself, Ralph Gilson should be remembered as the laboratory superintendent who came from Manchester with Professor Todd. He was a vital figure in equipping the laboratory, and he also checked every detail of the building under construction.

The staff members who came with Todd (they were inevitably christened the Toddlers!) were, if I remember correctly, Dennis Marrian (who went on to radiotherapy), George Kenner, Alan Johnson, Basil Lythgoe and later Malcolm Clark. John Harley-Mason was already in Cambridge at that time – as an undergraduate in 1940 I remember him demonstrating, in military uniform, in the first year organic practical laboratory in Pembroke Street – and so was Peter Maitland as well as the others mentioned in the earlier reminiscences, some of whom returned after 1945.

Christoper Longuet-Higgins succeeded John Lennard-Jones as professor of theoretical chemistry after the latter left to become first vice chancellor of the new Keele University.

Lennard-Jones was, I believe, the pioneer of molecular orbital theory in the 1930s and he developed it after the war, with his research students John Pople and George Hall, to show that it and Linus Pauling's hybridised orbitals were equivalent approximate treatments based on different starting assumptions.

It was the long-term effect of the 'weird' quantum theory, developed by the physicists in the 1920s, that led to the bringing together of physics and chemistry and the revolutionary, generation separating, transition from the 'preparation and properties' teaching of chemistry in the 1950s to the mechanistic or 'curly arrow' approach at the hands of Peter Sykes and Alan Sharpe.

One of the best chemistry lectures that I heard as an undergraduate was from Dr Emeléus (as he then was) who visited from Imperial College during the war to help with inorganic teaching. It was a revelation to learn of the electronic structures of the elements based on the Paul exclusion principle in relation to the periodic table. After the war, Todd persuaded Emeléus to come to Cambridge as inorganic professor.

They were exciting days with Crick and Watson doing work on DNA at the same time in the Cavendish Laboratory – and the new Cavendish professor, Neville Mott, looking for alternative accommodation for them as he considered this not to be real physics!

The original 40MHz NMR machine, being operated by Eric Liddell. How things have changed!

Back to the 60s

Dear Editor

Ian Smith's piece on Physical Chemistry in the Summer 2009 issue of *Chem@Cam* evoked many memories. Along with Ian and many others I moved to Lensfield Road as an undergraduate. In 1960 as a research student with Morris Sugden I worked in the basement of the Physical Chemistry wing (Room B68).

Ian's photographs reminded me of the great bond of friendship between the research students and the 'lab assistants' without whose skills we would have been lost. I was so pleased to see their recent photos.

Fred Webber, Cyril Smith and Brian Challis worked in the glass blowing room on the second floor and handmade most of the glassware used in the research labs. Cyril was an expert in making very delicate glass Bourdon gauges that involved collapsing one side of a microscopically thin glass bubble to create the 'spoon'. Cyril was also very adept at creating a viable cigarette from three or four shreds of Cut Golden Bar and a Rizla.

Eric Smith also worked on the second floor overlooking the main entrance. I suspect that many theses relied on his ability to (creatively) develop and read the plates from a spectrograph.

In the basement Donald Oliver was in charge of the instrument and equipment store with help from George (?). Next door was Ernie Cox and his store. He is beautifully recalled in the photo. While being every bit as spiky as Ian remembers, he nevertheless had one soft spot – he was a avid fan of the theatre organ and made occasional pilgrimages to the Tower Ballroom in Blackpool to hear Reginald Dixon (was it?). The magic word 'Wurlitzer' would effect a transformation in him. It wouldn't save you, though, from caustic derision if you lost a few grams of mercury from a broken vapour pump.

Across from Ernie was the main machine shop – the territory of Bill Symonds and Charlie Oates and occasional apprentices.

This pair of wizards of the lathe came, I think, from the great Cambridge Instrument Company. If one's apparatus were more metal than glass they would make sure it worked.

The necessary levels of precision machining required a separate language of measurement. One thousandth of an inch (usually a 'thou') was a 'fagpaper'. But this was regarded as verging on the crude and a proper finish (to less than a thou) was described as 'within a gnat's doodle'.

Mike Springett in B67 completed the basement team. He is the lad behind Princess Margaret in the photo. He was a trainee – very tall and deeply innocent. He would turn his hand to anything. He was asked by the staff of the undergraduate lab to help them re-label some reagent bottles. As a result, they acquired about 50 bottles of 'Ethly Alocohol'.

I was deeply saddened when you reported a few years ago that he had died at an air show in the US.

And to 'Norrish' himself as he was always known – I was never told what the "R" stood for. I received one serious reprimand from him.

I was joined in B68 by a Russian exchange student Igor Larin (a notable first in Anglo-Soviet relations). I was told by Norrish's secretary to take care of Igor and to see that he didn't get into any mischief.

At the same time an ebullient Greek-American called Peter Rentzepis joined the lab via Brooklyn. He was fascinated by Igor and was very keen to introduce him to the American Way of Life. One small aspect of this was the use of the phrase 'Keep tight!' as a substitute for 'Goodbye' when taking leave of a friend. Igor's good but not excellent command of English reduced this to 'Kiptie'.

One day to my great dismay I received a call to the prof's office – the only time I ever went there. Norrish was stern. 'Larin constantly says "Kiptie" to me whenever I see him. I know it's not Russian. What does it mean?' he said.

Cold terror hit me. 'I believe it means "Goodbye", Sir – "Keep tight!" It's American,' I replied.

'Keep tight! Keep tight what?' he growled back.

There was no way out. 'Keep a tight arse,' I said, 'It's American…'.

'Don't let it happen again, Green' he said with menace, and dismissed me back to B68.

Fortunately, when he had stopped laughing, Igor saved the day for me.

John Green
j.a.green@talk21.com

An expert in Pa and EtOH

Dear Editor,

I was saddened to hear of Alfie Maddock's death. He was always so cheerful and enthusiastic. He was my tutor at St. Catharine's from 1962 to 1965, though I am ashamed to say I did not keep in touch. Even at lowly undergraduate level we became aware that he was probably the world authority on protactinium.

One evening at dinner at his house, he gave us slivovitz, which we had never previously encountered, and he had to explain that it was plum brandy. So, an expert on ethanolic drinks also. On another occasion, a group of children charged through the house, and we asked if they were his, to which he replied that he thought some of them were!

He summed me up accurately in references for chemistry teaching jobs as not being of the highest academic standard (I got a third) but perfectly capable of becoming a competent teacher (I eventually made head of chemistry). A very good and caring man.

Yours sincerely,
Ian C Potts.
boo2ipc@hotmail.com

Oh mighty Chromic

Dear Editor

Although I welcomed the contribution from Peter Baker in the Spring 2009 issue to put my name in the limelight regarding the Chromic Frog made from Kleenex, sadly I must put the record straight. It was the invention of David Baird (two benches from me towards the door), using Delsey paper tissues. I have included the evidence in the form of a rendering of some of the occupants at that time (circa 1968) on the blackboard at the end of room 287.

David Baird, for some unexplained reason, had a habit of kneeling in front of his chromic acid bowl. He is apparently saying 'Oh mighty Chromic, deliver to me this day my Delsey frog.' I, on the other hand, am being quizzed by my supervisor, John Harley-Mason, who used to tell me what I was doing, and then I would confirm this: 'You're just running an alumina column, are you, Quarrie?' to which the characteristic reply was 'Yes Sir [those were the days!], I'm just running an alumina column.' The unfortunate soul between the squeeze bottles is Peter Cann.

Having never previously returned to the labs after completing my PhD in 1970, I was fortunate enough to revisit room 287 in its final year before reconstruction, and to my amazement my bench looked just the same as in the illustration! I shan't mention the stories about the lethal and the fire hose, or the solvent cupboard…

Happy memories.

Steve Quarrie
Kraljice Natalije 39, Belgrade, Serbia.

Head of photography John Holman retired in the summer after more than 20 years in the department. So the photography team could enjoy his party properly, junior assistant substitute photographer Sarah Houlton was handed the camera... Pictured from the left: Caroline Hancox, John, Vicky Spring and Nathan Pitt

A German wedding

This issue's wedding congratulations go to Matt Gaunt and Nadine Bremeyer. The happy couple met in Cambridge when they were both working in Steve Ley's group, and got engaged in Paris last December, their six-year anniversary.

The September wedding was planned for Nadine's native Germany, and as Matt speaks no German, Nadine reports that he managed to get out of most of the organising for the event. 'In fact, as he speaks no German, we also had to have a civil wedding in Cambridge,' she says. 'We'd have needed an official translator if we were going to be legally married in Germany!'

The wedding weekend began with a 'Polterabend' party in a rooftop rerrace bar overlooking Bremen on the Friday night. About 80 guests attended from five countries, and about half of them had a Cambridge connection from their times as PhD students, postdocs and working life here.

The wedding/blessing ceremony itself took place in the St Petri Dom, or cathedral, in Bremen on 19 September. The wedding cake was served at an afternoon reception in the garden of the theatre next door. Nadine claims this satisfied the German tradition of eating large quantities of cake at teatime!

'The afternoon was full of surprises planned by the guests,' she says. 'It started with the release of white doves, then Matt carried me through a heart after cutting it out from a sheet with blunt scissors, and red balloons – almost 99! – flying up to the sky.'

The evening reception was in Germany's oldest wine cellar, which is part of the town hall. 'We managed to survive the speeches, games and first dance without too much embarrassment – and the dancing lasted until 4am,' she says. 'The weather was wonderful all weekend, giving us and the guests plenty of time to visit several beer gardens!'

They had a short honeymoon in Sardinia and Venice, and are now busy planning a big celebration holiday.

Photo: Caroline Hancox

Melville Lab secretary Catherine Jordan turned 60 recently, and her desk was invaded by celebratory balloons and streamers. We suspect they might have made typing a touch difficult!

A trio of future chemists

Julius (right) and Tilly and Jasper (below). One, two, three, aaaaaaah!

We've got triple baby joy to report this issue. First up is young Julius Noam Scherman, son of Oren and his architect partner Sandra Leythaeuser. Julius was born on 10 September and weighed in at 2.8kg (that's 6lb 2oz in UK baby-units). Oren reports that he's very impatient – just like his father. 'I now sleep even less than I did before!' he says. 'But it's worth it – he's lovely, smiley and giggly, and never fails to let us know when he wants something!'

Meanwhile, it was two for the price of one for Keith McLuckie from Shankar Balasubramanian's group and his wife Rebecca, in the shape of twins Matilda Grace and Jasper Gabriel. Tilly and Jasper made their appearance six weeks early on 24 August, weighing 5lb 4oz and 5lb 15oz respectively.

'They're now smiling on demand – and also starting to demand quite a lot, too!' Keith says. Tilly is older by a whole minute, and already knows she's big sister – mum Rebecca reports that she likes to stamp her authority over her brother by leaning over and pulling Jasper's dummy out when he isn't looking.

Comings & goings

New staff
Sara Collins
Trevor Groves

Leavers
Christina Akosile
Chris Amey
Noah Maheya
Ernesto Prist

Retired
John Bullman
Alan Parsons
Barry Wilson

Playing in the rain

The weather wasn't kind to this year's sports day, but that didn't stop the fun and games – or the barbecue! Nathan Pitt wielded the camera

Left: Bill Jones shelters from the rain

Chris Chalk (left) and Matt Bushen (above) get some exercise; Caroline Hancox, Catherine Jordan and Jane Snaith contemplate the barbecue (below right)

Last issue's winners

ChemDoku

Last issue's ChemDoku garnered its usual excellent response. Correct solutions came from Alison Griffin, Danny Levin (who says he's now in California, where he's the president of contract pharma development company Noracpharma, still using the skills learned at Lensfield Road, albeit now having to forfeit the letters U and S to comply with US spelling), Ian Potts, Godfrey Chinchen, Annette Quartly, Robin Cork (who says he's from the completely unknown 1949 class), Mike Barlow, Tim O'Donoghue, David Wilson, Helen Stokes, A.J. Wilkinson, John Turnbull, Jim Dunn, John Billingsley, Diana Sandford, R.N. Lewis, Jennifer Trusted and Rachel Holland. And the lucky winner is... Godfrey Chinchen. Congratulations!

M	S	T	Y	E	H	C	I	R
Y	C	I	T	M	R	H	S	E
R	E	H	I	S	C	Y	T	M
I	M	C	E	H	T	R	Y	S
E	R	S	C	Y	I	M	H	T
H	T	Y	S	R	M	I	E	C
S	I	M	R	T	Y	E	C	H
T	Y	R	H	C	E	S	M	I
C	H	E	M	I	S	T	R	Y

Naphthalene resistance

Unsurprisingly, David Wilson's naphthalene resistance problem garnered far fewer entries. However, several brave souls got their heads around it, and entries were received from Richard Moss, Annette Quartly, Paul Stickland, Ian Potts and Richard Brown. The prize for the first randomly chosen correct answer goes to Paul Stickland. And the solutions?

a) 1→3, 2→4 and 2→9 have the same resistance as each other. Each pair is linked by a shorter path of one single and one double bond, and by a longer path of two single bonds and one double bond and the combined resistance between nodes 9 and 10. Similarly, 1→9 and 2→3 have the same resistance as each other. In this case the short path is one single bond, and the long path is 2 single bonds, 2 double bonds and the path from 9→10.

2→4, 2→9 and 2→3 drop out as duplicates, leaving fifteen unique values from the original list of eighteen.

b) By symmetry, the cases where there is no current are 1→8 and 2→7.

c) If there is just one case where the current flows 10→9, then it must arise from a connection involving the node nearest to 9, as 9 will then be at the lowest potential. 1→8 is already accounted for in (b) so the answer must be 2→8.

If anyone wants a copy of David's complete calculations and explanations, drop us an email and we'll forward it on to you!

£20 prizes are on offer for each puzzle. Send entries by email to jsh49@cam.ac.uk or by snail mail to Chem@Cam, Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW

Elementary recognition

This puzzle comes from regular contributor Graham Quartly, who professes himself 'really pleased' with it. As well as chemistry, he says, it involves logic (chess), English and general knowledge about scientists. By tracing out a path of knight moves visiting all 25 squares once only, spell out the name of a well-known scientist and a brief (albeit slightly cryptic) description of why they are famous. Spaces between the words have been suppressed! We'd also like you to tell us why this scientist has been in the news recently.

N	La	Re	Ni	Er
V	Er	O	U	S
Co	Ar	Cu	K	Ti
P	O	Th	N	S
Y	I	Co	Lu	In

Scrappage selections

Here's a logic-type puzzle from Keith Parsons. Motivated by the car scrappage scheme, Alan and his sister Dorothy persuaded three of their friends that all five should trade in their old cars for new models. Each chose a different combination of manufacturer, model, colour and engine type. From the information provided, list the combination each chose.

1. One of the men bought a red Flier model, manufactured by Jagro.
2. Edward bought a grey diesel engine car made by Vaumaz, which was not the Cheetah model.
3. The all-electric green car manufactured by Toylex was bought by one of the ladies.
4. Colin's black Sprint model was manufactured by Nissaud, who do not make hydrogen-powered engines.
5. Brenda bought a white Gazelle model, which does not have a hybrid engine.
6. Morsko manufacture only petrol engine cars, and their range does not include the Racer model.

And a bonus ChemDoku...

Because it's nearly Christmas (though it's probably been and gone by the time this magazine emerges from the postal system), here's an extra puzzle in the shape of another ChemDoku. Well, lots of readers seem to like them! This time, we've gone green, in honour of the Copenhagen summit. We've got green chlorine, seven metals which have at least one green chloride, plus a further one that's white but makes green fireworks. Solutions in green ink very acceptable!

Fe			U				Mo	
	V			Cu			Ni	Ba
					Mo			
U			Fe			Pt		
	Mo			Pt			U	
		Ba			Ni			Cl
			Cl					
Ba	Ni			Mo			Fe	
	U				Fe			Pt

Once I've got an electronic lab notebook, I won't have all this trouble finding my data!

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