

chem@cam

Chemistry at Cambridge Newsletter

Spring 2007



Informatics and chemistry
Predicting crystal structures

Dynamic assembly of materials
Carbon reduction technology

Sarah Houlton talks energy with BP's David Robertson, who describes his role as coordinating the company's efforts to create syngas from any raw material, and then converting the syngas into a variety of products its customers want to buy

What is BP doing to plan for changing global energy policies?

Several emerging themes are driving much of BP's forward planning. These include a growing energy demand, particularly in developing countries; increasing concern about energy security, driven by large consumers of energy; and a growing global awareness of climate change and the impact of our activities on the general environment. These three key factors are causing people, companies and governments, including BP, to think about their energy policy. We have recently announced an energy biology institute, for example: biology is routinely applied to medicine, but we really haven't applied it to energy yet. It could reveal many interesting ways to tackle the apparent dichotomy of needing more energy while needing to be more respectful of the environment.

What are you looking at in terms of biomass conversion?

We're at the start of a journey, and we're really open to ideas – we're not trying to be too specific. Bioethanol, for example, is largely produced today from the 'food' part of a crop, with the rest of the crop not being used. The next step would be to use that waste in a more productive way. Whatever we do, it's got to make sense from a commercial level; it's got to be something that's applicable around the world as we're not trying to solve any particular region's problems – we're a global company and we want solutions for a global problem. And that may, perhaps, mean using a variety of approaches; for example the requirements in Africa where more drought resistant crops may be more appropriate, which will be different from China where large amounts of rice are grown, and different again from the north American prairies.

Brazil's been so successful at producing bioethanol as the climate allows them to grow several crops a year, whereas most countries have just one crop a year, with the added complication of storage, which ties up lots of working capital. But in Brazil, with three or four crops a year because of the climate, there is a lot more potential for production and capital isn't tied up in quite the same way. A large proportion of their vehicles have been converted to run on fuel with a high ethanol content, and now they're exporting bioethanol as well. North America has been trying to do the same thing, but the climate isn't quite as suited as Brazil's so different tactics are required.

Does formulating fuels with ethanol pose a technical challenge?

In many parts of the US, Europe and India, it is not unusual for gasoline to contain 10% ethanol. However, once you increase the proportion, much more thought has to be put into the design of the engine. It's also possible to run vehicles on methanol, which can be made from syngas. China is certainly interested in adding methanol into gasoline. Butanol might be an even more

important alcohol additive, but it's slightly more difficult to handle. There's always a trade-off between some of the physical and chemical properties and the efficiency as a fuel. So much of this is driven by policy. Within the EU, if we're lucky we might emerge with a consistent policy!

What about more conventional approaches?

It's certainly worth investigating some of the more conventional, less futuristic ways. Vast amounts of natural resources exist, but how do we best access them? And how do we become skilled as a company at handling very large, complicated projects which involve large amounts of capital investment, with the added overall complexity in the delivery of products that may have less impact on the environment than many his-

ucts have? Much of this concerns our ability to capture and then responsibly sequester CO₂. It could either be reinjecting it into oil or gas fields to enhance recovery, or it could be simply sequestering it in something like a sealed aquifer or a coal seam, or just an underground cavern. There's a lot of work to be done to define what suitable conditions for those are. We certainly think there's a lot of opportunity in that space to do the right thing.

We're very interested in syngas, which can be made from any of the primary feedstocks. We have modest experience in the field, but we would like to build a much deeper capability, and we want to understand more about coal as a potential resource. The creation of syngas and its conversion into products while remaining mindful of the CO₂ produced, and being able to do appropriate things to minimise the amount of CO₂ released, is certainly part of my agenda.

How close are we to a practical method of carbon capture?

There are already a number of processes available for capturing CO₂ in post-combustion situations, but their applicability really depends on the value placed on the CO₂. If you can sell the CO₂ to oil companies, for instance, for enhanced oil recovery, that would generate a revenue stream as opposed to a disposal cost. And if there were a system of carbon credits that accounted for the fact that you were sequestering CO₂, that would help. I think the development of the technology will go hand-in-hand with the value that can be created. In China, for example, they are currently bringing on about a gigawatt of power a week (about enough to power half-a-million homes), with little attention being paid to CO₂ capture.

China has publicly said that they understand there is an impact on the environment, and at some point they will need to put in sequestration techniques, so there could be a fantastic business opportunity if you were able to retrofit carbon capture into all those power stations!

If there were some form of reward for doing the responsible thing, then that would help the economics. As the economics become more attractive so more attention will be placed on it, and better solutions, better ideas, new ideas will emerge, it's just a question of pushing the wheel over on that first part, getting the momentum going so it will start spinning more freely. But we've got to start somewhere, and we are already setting up a hydrogen power plant in California, converting syngas made from petroleum coke, a by-product from our local refinery, into a stream of hydrogen and CO₂, then burning the hydrogen in turbines to make green electricity, and capturing and using the CO₂ for enhanced oil recovery.

Last year was BP's most successful for some time in finding new reserves, but we still need to understand that things change, and if we're not looking at future energy needs now, we'll have problems later. We need to create the technology and capabilities now: if we don't start to build it until we do need it, it will be too late.



David Robertson

CV

Born: Tanzania, and grew up in Glasgow.

Education: Studied chemical engineering at Strathclyde University.

Family: He's married with three sons. He describes his Australian wife Kim as a saint for putting up with all the travelling he has to do! Their sons all have good Scottish names – Donald is 12, Angus 10 and Alasdair is 7.

Career: David has spent his entire career at BP, in both technical and commercial jobs. He started off on the technical side in Grangemouth, moved into marketing which led to a succession of commercial jobs, and then returned to the more technical side to do technology management in 2001. After an itinerant life in the UK, France, Switzerland and the US, with his longest stint in any place being six years, he's currently based in Houston, Texas but is due to return to the UK once more this summer.

Interests: Because of all the travelling, he greatly enjoys spending time with his family. He also loves music, reading, the cinema, cooking and watching sport. 'I'm addicted to baseball,' he says. 'We'll have to make sure we get the right TV channels when we come back!'

Did you know? David is a member of the Bonnetmakers and Dyers Guild in Glasgow, through his grandfather. He has a bonnet that was passed down through the family but, strangely enough, has never actually made a bonnet himself.



Remember the fun

Dear Editor

Well done! The Autumn edition of *Chem@Cam* arrived in Koenigstein-im-Taunus (near Frankfurt, Germany) at my new home address just in time for a good read over the Christmas holidays.

Good to see both the department and new blood within it continuing to thrive. However, every edition seems to announce the departure or retirement of a familiar face.... Dudley Williams, Brian Johnson, Andy Holmes (off home to Australia) and now Anthony Stone and Stuart Warren. Even Jeremy is relinquishing head of department. Very shortly, there will be no-one I recognise and I will have to admit that I, like them, am just getting older!

Therefore it was very nice to see the 'Spot the Difference' picture of aca-

dem staff members at the back of the magazine. I recognised every face with no trouble at all. In fact, I think I own the original!

My memories are of fun times despite the hard work. I still have my signed copy of 'Williams and Fleming' from 1st year Chemistry (when I thought my destiny was astronomy); second year inorganic lectures from BFGJ with a lesson in chiral centres that is still remembered – something about holding hands (with girl) rather than shaking hands (with boy) – I bet he does it every year; third year taking on a summer project with Andy post-finals which put me off synthetic chemistry for life (sorry Andy!), followed by a fantastic three year PhD with Dudley where I could run spectra in the morning and interpret them over a glass of wine and the test match or Wimbledon in the afternoon.

Best wishes to everyone! I just hope my daughters – now 14 and 10 – have manage to combine a good education with as much fun.

**Yours, Linda Summerton
(formerly Poulter)
Koenigstein-im-Taunus, Germany**

One of the team

Dear Editor

Tony Kallend's letter with the heading 'Formidable humility' reminded me of another incident concerning Lord Todd.

Lord Todd entered the large practical class in order to see F.G. Mann, who was in charge. However, Dr. Mann was talking to an undergraduate. There was no way that Lord Todd would interrupt an undergraduate, so he was waiting his turn standing at the end of my bench.

He sidled up to me and said, 'I may not be good at this sort of thing, but...' and he then tried to see if he could provide ideas to help me in my experiment.

At a later time, he was in my Christ's college 'choir' when I was conducting them in their first appearance in the rugby Cuppers final. The spirit in the college from the top down at that time ensured that we won.

**Yours sincerely, John Keenan
Whaley Bridge, High Peak**

Two more spotted

Dear Editor

In view of the recent Test match results in Australia, it seems timely to respond to your request for help with the names of the above 1955 event. In the back row there are two notable Australian cricketers: Emeritus Professor Tom O'Donnell (standing 4th from the left with bushy black hair) and Dr Bill Brett (standing 6th from the left with not much hair).

Tom assures me he was only picked for the team because, at the time, he had the largest car! He had a distinguished career as Professor of Inorganic Chemistry at the University of Melbourne and, although retired, he is still carrying out active research in chemical engineering.

Bill has had a successful career in industry but I have not seen him for several years.

Perhaps I should take this opportunity to let you know how much I enjoy receiving and reading *Chem@Cam*, which keeps me in touch with my alma mater.

**Yours, Emeritus Professor Ray Martin
Monash University, Australia**

chem@cam

Chemistry at Cambridge Newsletter

Contents

News	4
Research	7
Alumni	13
Chat lines	15
Puzzle corner	18

Cover



Andrew Robinson, a postdoc in John Pyle's group, performs a helium leak test on a gas chromatograph

Photograph:
Nathan Pitt and John Holman

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.

Editor-in-Chief: Steve Ley

Editor: Sarah Houlton

Photographers:

John Holman, Nathan Pitt,
Caroline Hancox

Editorial Board:

Brian Crysell, Jonathan Goodman,
Rosemary Ley, Jeremy Sanders

Address:

Chem@Cam, Department of Chemistry,
University of Cambridge, Lensfield Road
Cambridge CB2 1EW

Phone: 01223 763865

e-mail: news@ch.cam.ac.uk

website: www.ch.cam.ac.uk

This publication is supported by
Cambridge University Press

A portrait of Carol



Photo: Robert Taylor

Carol Robinson is one of six women scientists featured in the 2007 'Women of Outstanding Achievement in SET' photographic exhibition, having been nominated by the women in her group. 'The aim of the exhibition is to raise the profile of women scientists in the UK,' she explains.

It's the second year the exhibition has been run, and photographer Robert Taylor visited Carol in her office to take her picture. 'I was nervous, but he did a really good job of making me feel at ease,' she says.

The exhibition was launched at the Science Museum in March, at the start of National Science Week, and will be shown at various other places in coming months, including the British Museum and the Royal Society. 'The photos are about five feet high, which was a little alarming!' Carol says.

Money for surfaces

The surface science group has recently received a grant of £2.5m over the next four years from EPSRC. Jointly awarded to Dave King and Royal Society research fellow Stephen Jenkins, this time Steve is named as principal investigator on the grant.

'We're using the grant to look at the reactions of molecules on surfaces, focusing in particular on complex systems, such as arise when biologically important species adsorb on intrinsically chiral surfaces,' Steve says. 'We will do this using state-of-the-art techniques for the characterisation of surface systems, including the world's first fibre-optic low-energy electron diffraction instrument (for low beam-flux studies of weakly-bound adsorbates), coupled with sophisticated first-principles modelling within density functional theory.'

Dave's group focuses on experimental work, while Steve specialises in more theoretical aspects of the subject. As a result, a substantial portion of the grant is earmarked for paying for computer time on the university's high performance computer facility. Originally set up

as a collaboration spanning a number of departments now, under the full economic costing regime, the time must be paid for.

'They have just started running a new computer, Darwin, which currently ranks 20th in the official "Top 500 Supercomputer Sites" list,' Steve adds. 'The surface science group's contribution of £300,000 over the next four years will give access to about 10% of Darwin's total resource.'

Another grant received by the group recently is from BP, to study the catalysis of the reaction between carbon monoxide and water to give carbon dioxide and hydrogen – the reaction being used by BP in its hydrogen-based power generation programme.

The group's scanning tunnelling microscope will be used to provide atomically-resolved images of complex coadsorbate overlayer structures relevant to the reaction. On the back of the BP grant, Dave and Steve also gained further money from the Isaac Newton Trust to pay for a postdoc to work on the theoretical side of the project.

Chris to become Master

Chris Dobson has been pre-elected as the next Master of St John's College. He is due to take office in October.

'I think I'm the first chemist to become Master of this particular establishment, which reaches its 500th anniversary in 2011,' Chris says.

He also reports that he passed another 500th anniversary recently – the number of papers he has published. 'It's a sign of advancing age, I'm afraid!' he claims.

Chris is also keeping busy with a couple of visiting lectureships. This year, he's the Sammet Guest Professor at Johann Wolfgang Goethe University, Frankfurt, Germany, and Distinguished Visiting Professor at Rutgers University in the US.



Chris: soon to be Master at St John's

Alex appointed by Defra

Alex Orlov has been appointed to Defra's Advisory Committee on Hazardous Substances. The politically independent committee's role is to provide expert advice on the science behind hazardous chemicals, and is made up of 11 scientists from industry, academia and NGOs.

The scientists are experts in environmental and industrial chemistry, toxicology and ecotoxicology. Alex was

appointed to the committee because of his knowledge in areas such as environmental nanotechnology, water quality and environmental remediation.

'I'm delighted to have been asked to be a member of such an important committee,' Alex says. 'It's vital that decisions are informed by real science, not by scare-stories, and I look forward to helping make sure that government ministers are given sound advice.'

Reading matter

The department's library has received an unexpected boost in the form of about 150 books from the personal collection of Alan Carrington.

Alan, who was here in the 1960s (you can see a photo of him in his Cambridge days on p13), has recently retired from Southampton University.

He has fond memories of his time here in Lensfield Road so wanted the books to come here.

'There are some real classics in the collection!' says Jean-Pierre Hansen. 'It was a really nice gesture to donate them to us.'

Jean-Pierre's medal



Royal Society vice president Martin Taylor makes the presentation to Jean-Pierre

At the Royal Society's Anniversary Meeting Day in London at the end of November, Jean-Pierre Hansen was presented with the Society's Rumford Medal.

One of the Society's most prestigious awards – and the second oldest after the Copley medal, which was given to Stephen Hawking the same evening – the Rumford medal has been awarded every other year in recognition of an 'outstandingly important recent discovery in the field of thermal or optical properties of matter made by a scientist working in Europe'.

Jean-Pierre was honoured for his pioneering work on molten salts and dense plasmas that has led the way to a quantitative understanding of the structure

and dynamics of strongly correlated ionic liquids.

He's in good company, as some of the most famous names in science have won the medal over the years, including Michael Faraday, Louis Pasteur, Frank Whittle and George Porter. The most recent Cambridge recipient before Jean-Pierre was Dave King.

'I'm extremely pleased, and I really didn't expect to receive this award!' he says. The medal itself is a rather splendid silver gilt affair, and came with a cheque for £1,000 which Jean-Pierre has spent on old books. 'These include a copy of Gibbons' "Decline and Fall of the Roman Empire", which I'm looking forward to having time to read,' he says.

Jean-Pierre was in good company at the ceremony, with other recipients including physicist Stephen Hawking



Bill takes over as head of department



Bill Jones: a new man at the helm

New head of department Bill Jones took over from Jeremy Sanders at the beginning of January, and is already looking to the future.

Taking on the department headship represents a whole new challenge for Welshman Bill, who has been in the department since 1978, and works at the interface between chemistry and materials science in the materials chemistry group and the Pfizer Institute for Pharmaceutical Materials Science.

'At the moment, I'm busy making sure I'm known to the department as a whole,' he says. 'But there are many things that are going to keep me busy in coming months, such as recruiting three new professors to replace the chairs being vacated by Brian Johnson, Jean-Pierre Hansen and Dave King.

'We're also recruiting for lecturers in inorganic and the Melville lab. With this and all the other issues that are always around, it's not been a gentle entry into the job! However, one of the things that has greatly impressed me is the high standard of the young people who are applying for fellowships, and it bodes very well for the future.'

Other issues that will be keeping Bill and his team busy include the impending refurbishment of stores, and the extension work to the south-east of the department.

As far as the research labs are concerned, the Melville lab is expanding onto the floor below, and David Spring's group has moved into the space on the second floor vacated by the GlaxoSmithKline group.

We are sad to report the death of two eminent chemists with links to the department.

Nobel Laureate Alan McDiarmid, who was Linnett Professor in 2003, died in February.

And Al Cotton, an honorary fellow at Robinson College and regular visitor to Cambridge, also passed away in February.

Fame comes calling for Stuart

Little did Stuart Mackenzie know when we wrote about his chemistry in the last issue of *Chem@Cam* that it would lead to an appearance on BBC Radio 4.

He was featured in the station's 'Material World' programme in early March, talking about cluster chemistry. The programme goes out at 4.30pm, and is aimed at schoolteachers who, apparently, are likely to be driving home that that time.

'I got an email from the producer who had seen *Chem@Cam*, and said he wanted to do a 15-minute feature on cluster chemistry,' Stuart says. 'They like

to have two guests, and so I suggested that Tony Stace from Nottingham should come along too.'

The programme goes out live, and they had to turn up at Broadcasting House just half-an-hour before transmission. 'We were still in the foyer at 4.10pm, but finally met presenter Quentin Cooper just before the show. They like to do it live because, apparently, it makes it more spontaneous – but it was nerve-wracking!

Go to www.bbc.co.uk/radio4/science/thematerialworld_20070308.shtml to hear what Stuart had to say.

A musical end to the year

Jeremy Sanders' final annual head of department talk to staff before Christmas was hijacked by a farewell concert, with various members of the department displaying their talents to a packed lecture theatre.

Ablly MCed by Brian Johnson, it featured performances by Rebecca Penkett on the harp, and a musical group, Los Elementos, who came together specially for the event and enjoyed it so much they are continuing to make music together. There was also a choir made up of Jeremy's research group, and Dudley Williams fair made Jeremy blush with his rendition of 'When Jeremy sang in Lensfield Road'.

It was also a good excuse for Pete Wothers to demonstrate his skills with nitrocellulose again. Rather than the traditional bunny, he got into the festive mood and a snowman met a fiery end.

The event had been cooked up by Jeremy's secretary Liz Alan, and amazingly he remained in the dark until he turned up in the Bristol-Myers Squibb lecture theatre to give his talk.

'I was really touched at the amount of thought and effort that went into it,' Jeremy says. 'It certainly made my final annual talk very memorable.'

Right, clockwise from top left: Jeremy and incoming head of department Bill Jones speak, Rebecca Penkett plays the harp, and Brian Johnson MCs



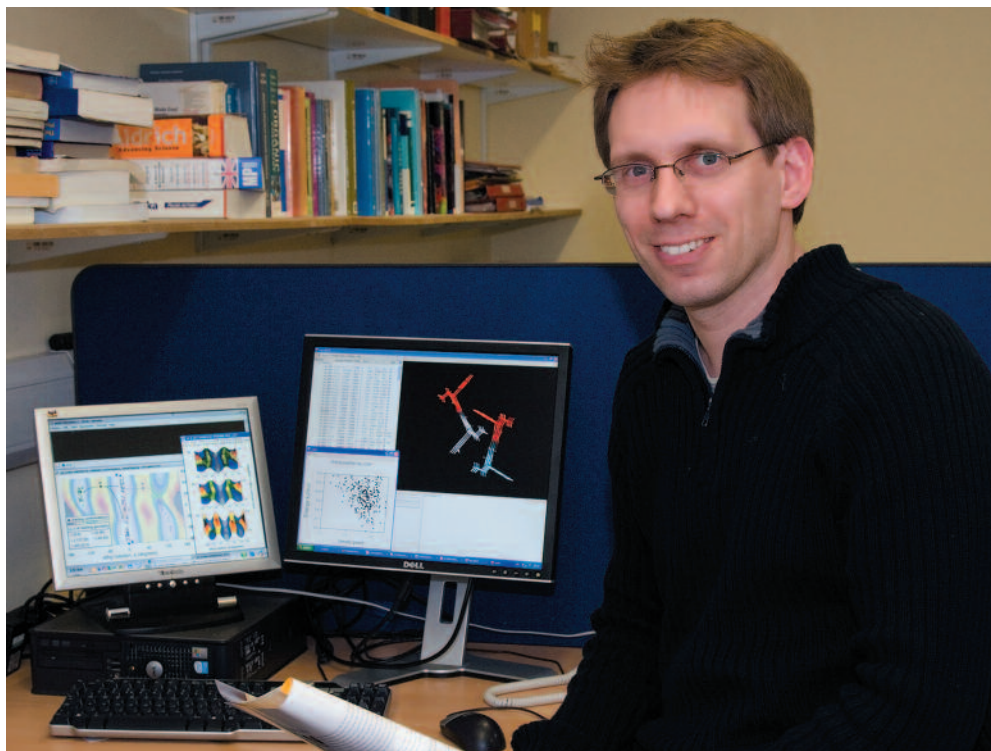
Below, clockwise from below left: Pete Wothers and his snowman – and its conflagration, Dudley Williams sings and plays, Jeremy's group in musical harmony, and Los Elementos make music



Photo: Nathan Pitt

Prediction: the future

Photo: Nathan Pitt

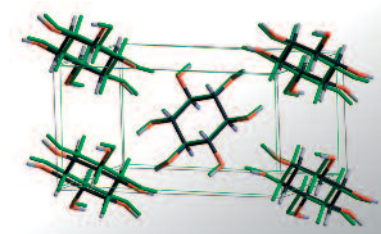


If it we could predict crystal structures, it would be an extremely powerful tool for industry. Graeme Day is trying to achieve this

The way molecules crystallise has a huge bearing on their properties, and in sectors such as the pharmaceutical industry the crystalline form is critical. Yet it is not obvious simply from their chemical structure what structure their crystals will take when they form. Graeme Day's research is focused on the complex area of trying to predict how molecules will crystallise, and thus how they will behave.

'If you can do all this on a computer, it would save a lot of lab time!' Graeme says. Much of his work is within the Pfizer Institute for Pharmaceutical Materials Science, which has projects in the chemistry department, materials science and the Cambridge Crystallographic Data Centre. Predicting crystal shapes and properties is particularly important in the pharma industry, where the choice of solid form for a drug molecule can have a great bearing on the properties of the final product.

It's very much early days still for crystal structure prediction, but Graeme is already having some success. 'We're getting good at it for some simple molecules,' he says. 'A few times in the past year or so we've taken the results of our calculations and are confident that they are pointing to a particular structure, and have then confirmed our prediction



Predicted (green) and observed crystal structures of scyllo-inositol, a potential new therapeutic for Alzheimer's disease

by going into the lab and making it. It's beginning to get reliable enough now to guide experiments, which wasn't the case in the past – at first we were looking at calculations and how they were wrong if they didn't agree with observations, but now it's often the other way about.' The close link with the experimental projects in Bill Jones' materials chemistry group has been vital in validating the computational methods; it's important to be able to look for structures that the calculations suggest should exist.

Predictions have thus far assumed that the molecules are static. But, in the real world, they move about, and this has an impact on the way they pack as crystals. 'I'm working on trying to understand how molecules move in crystals and the influence of their dynamics on the relative stability of crystal structures,' he says. 'If we can then feed the results back into our crys-

tal structure predictions, it will help us understand how the molecules will crystallise and how stable they will be.'

He is already finding that by including entropy in his calculations it is helping to make the predictions better. 'By assessing how the molecules pack and how the dynamics affect this, we are trying to work out exactly which interactions we need to model to get the best results, and what effects they have on the predictions.'

'It's difficult enough analysing the static structures, and adding the dynamics makes it much harder,' he says. 'Looking at the influence of specific interactions on dynamics is my pet project! Some ideas will work, some won't, but those that prove useful will be fed into the predictions to make them more accurate.'

Graeme's work so far has been on simple model systems as the models are being worked out and refined. In future, the intention is to move on to more complex molecules that look more like real drugs. 'We are starting to look at salts and co-crystals, incorporating a second molecule into the crystal lattice and see if we can predict what effect that will have on the lattice structure. Ultimately, it would be fantastic to be able to predict, for example, the best salt form for any drug molecule.'

There is still some way to go before the predictions reach a stage where a company like Pfizer could use it as a general tool. But Graeme's already making great progress. 'I'm sure that the dynamics calculations will have a huge impact on the effectiveness and usefulness of the predictions,' he concludes. 'And I'm confident it will keep me busy for a while!'

Graeme Day

CV

Born: Halifax, Canada

Education: His first degree was from Saint Mary's University, Halifax, in chemistry and maths. He came to the UK in 1997 for a coursework-based masters degree in theoretical chemistry at Oxford, which was followed by a PhD with Sally Price at UCL.

Career: Graeme made the move to Cambridge in 2002 for a postdoc with Bill Jones, and was made a Royal Society University Research Fellow in October 2005.

Status: He's been with his girlfriend Aileen since their PhD days in London. She now works in Cambridge for a materials selection software company.

Interests: Graeme plays football, and still goes to London every week to play as a goalie for his old team there. He's now contemplating cricket – perhaps a goalie to wicketkeeper transition could be on the cards! He also goes to plenty of live indie and alternative music.

Did you know? As a student in Halifax he used to do Irish set dancing – not Riverdance, but a rather more pub-based activity...

The incredible power o

Bobby Glen and his colleagues in the Unilever Centre are using informatics techniques to solve a host of chemistry problems



Photos: Nathan Pitt

Since it was set up in 1999, the Unilever Centre for Molecular Sciences Informatics within the department has gone from strength to strength. Its initial five-year funding was extended by Unilever for a further five a couple of years back, and substantial cash has also been received from other firms such as the drug companies Boehringer Ingelheim, AstraZeneca and Pfizer. It has also received a large collaborative grant from the EU, as well as a whole host of UK research council grants.

'The scientific areas we focus on are all centred around informatics,' its director, Bobby Glen, explains. 'My colleagues and I in the Centre are developing an underlying set of techniques in informatics such as molecular simulation and text mining, and this also means we collaborate with a wide variety of external partners, helping them handle complex datasets.' The range of software tools they have at their disposal allows them to address problems as diverse as molecular design and knowledge management.

One of the projects utilising molecular similarity that has been running in Bobby's group recently involves traditional Chinese medicines. The objective was to connect western and Chinese

medicines, as there is very little correlation between the Chinese system and western pharmacology. 'Chinese medicines are empirical in the sense that they have been formulated and tried out on people over thousands of years – there is no measured scientific basis for their activity,' he says.

'The products are made up of a diverse set of plant extracts, coupled with a method for making them, and there's a very large placebo effect for many of them. But the assumption is that over the centuries some of the products that have been put into the medicines do actually have therapeutic benefit distinct from the placebo effect. We are trying to identify some of the key compounds that are present in Chinese medicines, which are typically natural products, and then link them to western pharmacology.'

They have constructed a virtual screen of about 120 pharmacological drug targets, like ion channels and enzymes, that are familiar from medicines such as antidepressants, antibiotics and cholesterol-lowering agents. 'We now have this screen on our computers, and can take a Chinese medicine, identify the key components using chromatography, and pinpoint their chemical structures,' Bobby says.

Bobby Glen: helping collaborators handle complex datasets

'We then take these chemical structures and feed them into our model, which then predicts the biospectrum of each molecule, made up of predictions of its activity at each of these 120 targets. This "signature" is then compared with the biospectrum of known drugs. We know, for example, that a beta-blocker lowers blood pressure. So if the Chinese medicine component had a similar biospectrum to the beta-blocker, it would also be expected to lower blood pressure.'

They have already looked at extracts from about 50 different Chinese medicines, and have come up with some fascinating predictions. While some of them don't appear to have any effect at all, perhaps because no target that is sufficiently clear has yet been identified, some very interesting correlations have been found.

One example is the compound rhynchophylline, a component of the Chinese herb Gou Teng which has neuroprotectant properties. The virtual screen predicted that rhynchophylline would be kappa opioid agonist, which would account for this neuroprotectant effect. It also predicted that it would act as a calcium channel blocker, agreeing with a previous study that found the herb to have a negative inotropic effect, and also as a dopamine D2 antagonist, which ties in with its sedative, anticonvulsant and antispasmodic effects.

Other interesting tie-ups include monakolin K, a constituent of red yeast rice, which acts in the same way as the statin drugs, and isoerubicin B, a constituent of garlic, which appears to be active in cholesterol distribution. This fits with garlic's known role in lowering plasma cholesterol. It also has a similar activity to a group of compounds that is currently being investigated to treat Alzheimer's disease.

This work is being funded by Unilever, whose aim is to identify new functional additives with beneficial health effects that might be included in food products. 'It might be that it's cholesterol-lowering, it's antidepressive or it has some effect in lowering blood pressure,' Bobby claims. 'The hope is that in the future some of these compounds we have identified will appear on the supermarket shelves'

A very different project, also being supported by Unilever, is to develop a polymer mark-up language, or PML, that provides an effective way of making polymer data searchable. It's rather like chemical mark-up language, which was developed to make it easier to man-

f chemical data mining

Bobby Glen

CV

Born: Alexandria, beside Loch Lomond in Scotland

Status: This year, he and his wife Anne celebrate their 25th wedding anniversary. Anne used to be a nurse, but the arrival of triplets Abigail, Harriet and Oliver put paid to that! They're now 16, but none are likely to end up in the chemistry lab – Abigail's considering studying English and history, Harriet is fascinated by geography, and Oliver wants to be a pilot. 'I think all 16 year old boys want to be pilots – I did!' Bobby says.

Education: He studied chemistry at what was then Paisley Tech, followed by a PhD in X-ray crystallography at Stirling with Peter Murray-Rust – now one of his colleagues in the Unilever centre.

Career: He initially joined Wellcome to set up a computational chemistry group, and after a short stint at ICI returned to Wellcome before heading to the US to join Tripos. He was involved in the setting up of three biotech companies, one of which is still going strong, and came back to the UK in 1999 to set up the Unilever centre.

Interests: He loves scuba diving, and occasionally goes flying.

Did you know? Back in 1972, Bobby was paid the princely sum of £10 to play the guitar in a pub on Loch Lomond one evening. And his partner in musical crime that evening? A banjo player by the name of Billy Connolly.

age information on chemical compounds, but it is, necessarily, somewhat more complicated.

'Polymers are very difficult to deal with because there is a range of molecular weights and structures within the same material,' Bobby explains. 'So we're developing a language to define polymers that would allow databases to be searched to answer very complex queries, taking into account the large molecular weight range and the structural differences of polymers. Even the way they are manufactured has an effect on the polymer's properties, such as how they are extruded.'

'We are looking at ways of storing those data, and also annotate existing literature data to make them more useful, and making it easier to find the right polymer to include in a food or personal care application, for example.'

If a polymer within a washing powder formulation, for example, were to be deemed by the EU as no longer acceptable because of the length of time it takes to biodegrade, it would leave the manufacturer with the problem of finding an alternative that has similar properties. Being able to trawl polymer data to quickly identify a suitable replacement polymer would save huge amounts of time and money.

'Questions like this are complicated,

but we believe that if we structure the data in the right way, we can answer them,' he says. 'We have constructed for the first time a very comprehensive dictionary of the information that's required to describe a polymer. This helps us understand what information needs to go into the database, and how it is connected, in order to make it easier to search for the right information.'

A third area Bobby's group has been working on is understanding why proteins fold – not what shapes they fold into, but why they do it in the first place. This is being carried out as part of a large EU collaboration, the EMBIO project, with six other groups from around Europe.

'We are asking some very basic scientific questions,' he says. 'What is the role of water in the folding process? How can water reorganise itself during folding? What influence do the dynamics of the process have? What are the roles of ions and intermolecular interactions? And how do the dynamics of the system change as the protein folds?'

They have started off by looking at small peptides – protein fragments – and even though they are much smaller the calculations required are still ferocious, 'We've got some very interesting evidence already,' Bobby claims. 'For example, we can calculate the "dynamic memory" of water, and it turns out it retains its dynamic memory for much longer than we'd anticipated after the system has evolved – up to at least five

nanoseconds after the folding event we still see its dynamic memory being propagated throughout the water. That's very interesting.'

'We've also found that very small changes to the structure of the water at a large distance from the folding event perturb the whole system and stop it folding. So the folding event involves not just the water right next to the folding protein – the whole system is part of the folding event.'

'Intriguingly, you can interfere with the dynamics of the water molecules as much as fifteen water molecules away from the folding event, and it will stop it folding. The whole system is in a dynamic, concerted motion in which all the particles are interacting with each other.'

They are applying computational mechanics to the problem, which Bobby says means they can look at how the dynamics of the system evolves over a long period, and how the memory of the system evolves.

'For example, if there is a fast folding event and a torsion angle suddenly shifts across a large distance, why does that happen? The only way it can happen is if lots of particles are moving in the right direction at the right time. Otherwise, it wouldn't go anywhere – it would just continue to vibrate randomly around its original position. The whole system works together to fold the protein in a very precise way.'



Bobby and his group pictured outside the Unilever Centre. From left to right: Charaka Goonatilake, Donatas Zmuidinavicius, Christian Jenson, Max Macaluso, Dmitry Nerukh, Bobby, Sam Adams, James Bell and Hamse Mussa

If a synthetic material is going to be made with carefully defined properties, then it's important that the polymer chains it's made of join together in the right way. While chemists have become expert at assembling synthetic polymers selectively in organic solvents or with no solvent, it's a very different matter in water. And this is one of the focuses of Oren Scherman's chemistry.

'In different solvents, the polymers have different kinetics,' he says. 'They can stick together or fall apart much more rapidly in one solvent than another, and a lot of the dynamics of this process is well understood in organic solvents. But if we really want to promote the concept of green chemistry and also be able to incorporate new synthetic polymers into biological applications, we want to be able to do polymer chemistry and make new materials in an aqueous environment.'

Take, for example, a block copolymer, where a number of A monomers are joined together, and then the monomer changes to B, so you are left with a single polymer chain where the first half is all A and the second half all B. If A likes water and B doesn't, then in water all the Bs will clump together leaving the As on the outside in a micelle structure. But what about more complicated polymer chains with more complex functionality?

TERTIARY STRUCTURE

While the properties of commodity polymers and many block copolymers are well understood, as are the ways of making them assemble into well-defined shapes, Oren claims this is only really well understood for polymers where the repeat units are fairly simple.

'Biology has shown us that you can take a whole variety of amino acids and, when they're put together exactly right, you get a unique tertiary structure which leads to its biological function,' he says. 'It's that beautiful folding of a protein into a perfect shape that allows it to be an enzyme, for example. And it assembles spontaneously. Wouldn't it be cool if we could make synthetic polymers that are more interesting in an aqueous environment?'

This has fascinating possibilities in the biological realm. 'Drug companies sometimes attach polyethylene glycol, or PEG, to a biological entity they want to get into the body because it makes it more water soluble,' he says. 'But there are so many other synthetic scaffolds that might be useful and biocompatible. We might even be able to add some form of scaffold as a targeting group to get it into the right place in the body, and once it's there the scaffold comes away and is metabolised, being excreted without invoking a negative immunological response.'

Dynamic possibilities



Photo: Nathan Pitt

Oren's group is trying to discover ways in which well-defined diblock or even triblock polymers can be designed that have some form of selective molecule at the end of the chain, and these selective parts find each other and assemble in a pre-determined way. 'How can we go about getting the chains to assemble to form an interesting architecture?' he says. 'I'm really interested in finding different ways of getting these molecules to interlock. In some systems we're trying to build, the

The way polymers assemble in organic solvents is pretty well understood. Oren Scherman is looking at what happens when they are in water

small molecules attached to the ends of the polymer chains ensure they will find each other and pair up.'

He's also looking for even more complex systems containing further components. 'What about having a third molecule in the mixture that acts as a "switch"?' he says. 'If the two chains have selective molecules that don't interact with each other directly, then a third one could be designed that acts as a pair of handcuffs, attaching to one end of each chain and binding them together. You could even introduce a fourth factor – maybe the handcuffs don't clamp together unless the pH is in a certain range, so this external stimulus could act as the key to the handcuffs.'

As well as biological applications, this sort of system has a variety of potential uses. 'You could use a pH switch like this to change the system's viscosity,' Oren says. 'This could be done, for example, if the linear polymers are separate to start with, but as you increase the pH the chains elongate and get entangled, then the viscosity will increase as they self-assemble. I really believe that non-covalent interactions working together like this will be very important in the future.'

Oren Scherman

CV

Born: Norman, Oklahoma, US

Education: Oren studied chemistry at Cornell University in the States as an undergraduate, including stints abroad at Bayer in Leverkusen, Germany and at the Technion Institute in Haifa, Israel. His PhD was with Bob Grubbs at Caltech, working on catalyst design and polymer synthesis.

Career: He spent two years working with Bert Meijer at the Technical University of Eindhoven as an NSF International postdoc fellowship. He was appointed as a university lecturer in the Melville lab last summer.

Interests: His passion is travel, having spent time hiking in South America, and travelling around Asia and Europe, and claims to have had two extra sets of pages added to his passport to accommodate all those stamps. A highlight was Bolivia, where he went above 5,500m, and needed oxygen to cope with the thin atmosphere. 'It may be completely flat in Oklahoma where I grew up, not to mention here in East Anglia, but I love the mountains!' he says.

Did you know? While in Bolivia, he helped out with the coca harvest, again a far cry from the wheat prairies of Oklahoma...

Preserving the chemical past

Department archivist Ruth Horry, who works in the Whipple Museum, reports on her recent trip to Lisbon for a conference on chemistry heritage

In February, a group of historians, chemists and museum professionals convened at the Museum of Science at the University of Lisbon, Portugal to discuss the scientific heritage of chemical sciences. The conference provided a forum for discussing the future of chemical collections and apparatus held in universities and laboratories.

I was able to report on ongoing projects within the University of Cambridge to preserve scientific heritage. Chemistry was presented as a key example of a university department that is committed to celebrating and preserving its history through projects such as the departmental archive and Todd-Hamied room displays.

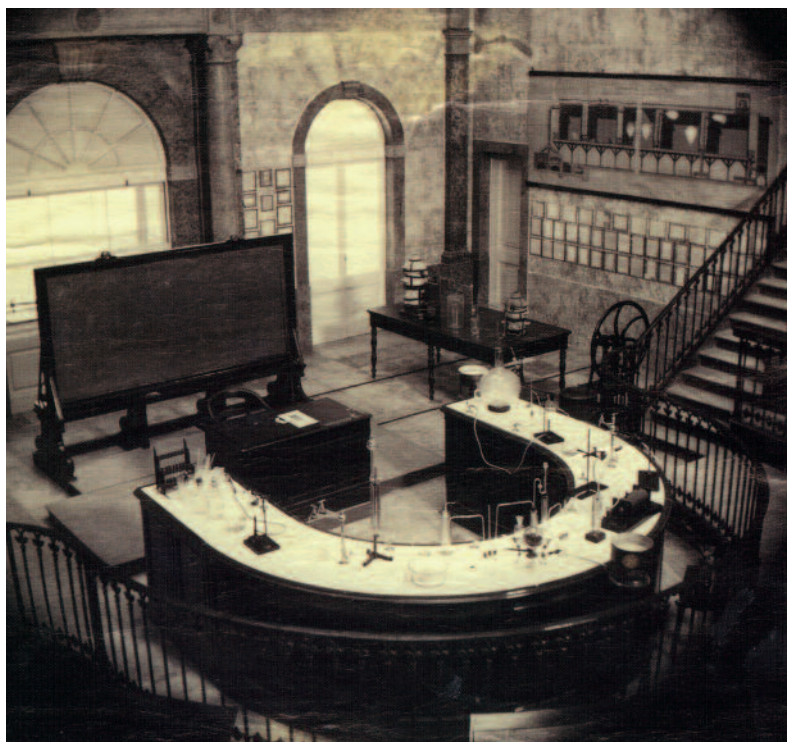
The Whipple Museum of the History of Science collaborated with the chemistry department last year on the displays of material related to the work of Lord Alexander Todd in the Todd-Hamied Room. Building on previous work by Chris Haley and the Museum Group, the displays are designed to inspire students through the history of their subject, and celebrate the rich past of chemistry in Cambridge.

In addition, by housing departmental archives in a dedicated space that was established in 2002, Cambridge chemistry has shown how university departments can work together with historians to ensure the material culture of science is preserved for future study.

I received an extremely positive reaction to these projects, and made good contacts with several institutions undertaking similar work. My introduction on Lord Todd and his work was particularly warmly received, as many chemists were present in the audience.

Fellow delegate Professor Bernardo Jerosch Herold told me how, as a student in 1958, he had the pleasure of meeting Lord Todd at a gathering of Nobel Laureates in Lindau, southern Germany. The meeting was one of several arranged with the idea of bringing together Nobel Laureates who had been separated by war and emigration. He described his great joy at sitting for dinner at the same table as Lord Todd and Leopold Ruzicka, listening to the stories they told about their experiences as students and as scientists.

Amphitheatre of the laboratório químico, Escola Politécnica, Lisbon, in about 1890



Museu da Ciência da Universidade de Lisboa

He particularly recalls one of the stories Todd told him, dating from his postdoc in Frankfurt, about the German professor Julius von Braun. One day, a terrible explosion was heard in the basement of the lab; everybody rushed downstairs and found a student lying on the floor and a lot of shattered glass. When von Braun entered the room he stepped over the prone body of the student, asking, 'Where is the substance?' before even looking at the student. It seems that the student had been trying to ozonise a compound.

Professor Herold also recited a limerick that recalls the strong and charismatic leadership for which Todd is remembered:

*Pray, don't you think it is odd,
That Sir Alexander Todd
Writes his name, if you please,
At the end with two ds,
When one is sufficient for God.*

It was written by Nobel laureate John Cornforth, according to David St. Claire Black of the University of New South Wales, Australia.

The conference also gave opportunities to see what other institutions were doing to preserve their chemical heritage. In particular, our hosts at the Museum of Science, Lisbon gave delegates a sneak preview of the newly restored laboratório químico – the 19th century chemical laboratory within the museum, which will open to the public later this year.

The site that now houses the Museum

of Science has been used for teaching science for more than 150 years. In 1837, the building became the Escola Politécnica where students were trained in experimental methods in chemistry, pharmacy, medicine and engineering. Chemistry teaching was centred on the large chemical laboratory with its adjoining amphitheatre, where up to 200 students could be seated to view practical demonstrations and lectures. The laboratory itself held up to 50 students undertaking practical work and was equipped with high quality fume cupboards and apparatus.

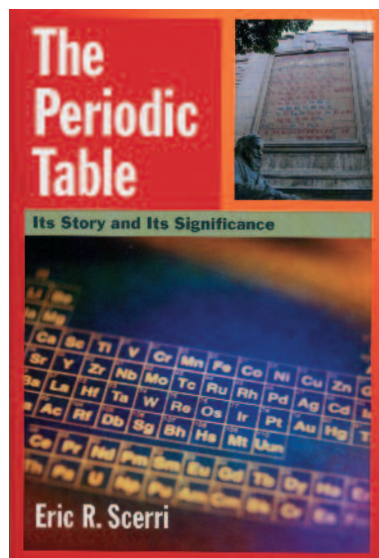
The laboratory survives today as a very rare example of a practical setting for university chemistry in the 19th century. It is particularly important as much of the original instrumentation and apparatus is still intact. The site has much to offer as a source of historical information on the teaching of chemistry in the period. Consequently the Museum of Science has been undertaking a programme of restoration work and historical research that will return the space to how it looked in the 1800s.

Original instrumentation and glassware will return to the lab benches for visiting members of the public to experience a unique and real setting for teaching chemistry in the 19th century. I hope that this project is one of many schemes that will continue to preserve and present histories of chemistry for the enjoyment of students, specialists and the wider public.

Lord Todd, as photographed in 1958 by Bernardo Jerosch Herold



Elementary, my dear Eric



The Periodic Table: Its story and significance

Eric Scerri

Oxford University Press, £19.99

ISBN 0-19-530573-6

Ask a non-chemist what images the word 'chemistry' brings to mind, and chances are they'll say bubbling coloured liquids, mad scientists in white coats, or the periodic table.

The periodic table in its medium-long form has become an iconic image of science, and we take it for granted today that the elements are arranged in order of increasing atomic number, starting with hydrogen and ending with a string of elements that have only ever been created in tiny amounts in the lab.

But this was not always the case, and back at the end of the 18th century and well into the 19th, scientists were struggling to bring order to the chaos. Eric Scerri's book tells the fascinating story of how ideas about the similarities between the properties of the elements led them to start arranging them in some semblance of a pattern.

Some of the ideas were ridiculed at the time, such as Scottish physician William Prout's hypothesis of 1815 that

elements are all multiples of hydrogen, but history has shown him to be not far from the truth. Others were just plain wrong.

While the Russian Dimitri Mendeleev is generally given all the credit for devising the table, in fact various other far less well-known figures played crucial roles, despite Mendeleev's unlikely claims that he hadn't seen the work of his contemporaries.

Many different tables were proposed in the years leading up to Mendeleev's diagram, from the logical to the slightly surreal. It seems remarkable that a table that so successfully arranges the elements was developed half a century before the proton and atomic number that are the key to the system were discovered.

I read much of the book on aeroplanes, trains and airport lounges, and (despite some good-natured teasing by British Airways staff about my choice of reading matter) it kept my brain well occupied, even if the chapters on quantum mechanics and the physicists' attempts to

explain the table in terms of atomic structure proved a bit of a struggle for an erstwhile organic chemist. But Scerri succeeds in interweaving the history and science with thought-provoking philosophical strands.

He concludes by suggesting that, out of the thousand or more different periodic tables that have been proposed, the 'left-step' table where the elements are aligned to the right (and based on the quantum number $n+1$), with the first four elements in pairs and the third line starting with boron and ending with magnesium, and no large 'gaps' in the middle as in the table we're familiar with.

Scerri believes that this shows the greatest degree of regularity combined with an adherence to the deepest available principles relating to the elements as basic substances. There is a good deal of logic in this idea, but whether chemists, wedded as they are to the medium-long form of the table, would agree is another matter entirely. SH

The Corporate Associates Scheme

Accelrys

Akubio

Amura

Astex Therapeutics

Astra Zeneca

Biotica

Boehringer Ingelheim

BP

BP Institute

Bristol-Myers Squibb

Cambridge BioTechnology

Cambridge Display Technology

CambridgeSoft

Dow

ETRI

GlaxoSmithKline

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, plans are afoot to provide new undergraduate chemistry exam prizes, departmental summer studentships, and new faculty teaching awards.

Corporate Associate membership not only provides essential support for the department, but also provides numerous benefits to help members work with us and achieve their business objectives. Members enjoy many benefits through their enhanced partnership with the Department, such as:

- Visibility within the department;
- Invitations to recognition days and networking events at the department;
- Access to the department library and photocopying/printing facilities;
- Regular communications about upcoming events, colloquia, and updates about the department;
- Complimentary subscriptions to

Department publications, including Chem@Cam;

■ Access to emerging Cambridge research via conferences, special briefings and various publications;

■ Priority notification of and free access to departmental research lectures;

■ Ability to hold 'Welcome Stalls' in the department entrance hall;

■ Preferential conference rates for Corporate Associate members;

■ Free access to the teaching lectures held within the department;

■ The full services of the Corporate Relations team to facilitate interaction with students, staff, and other parts of the University of Cambridge to help achieve your corporate objectives.

The next Corporate Associates Scheme meeting in the department will be on Friday 27 July, with a focus on state of the art synthetic chemistry.

If your organisation would be interested in joining the Corporate Associates Scheme, then please email Jane Snaith at cas-admin@ch.cam.ac.uk, or call 01223 336537.

We look forward to hearing from you!

Insense

Jeol

Johnson Matthey

Kodak

Merck Sharp & Dohme

Research Laboratories

Novartis

Pfizer

Proctor & Gamble

Roche

Shell Global Solutions

The Society of

Chemical Industry

Shell Global Solutions

Solexa

Syngenta

Unilever

Another bunch of rogues...

Dear Editor,

I wonder if you would like another rogues' gallery for your next issue of *Chem@Cam*? I came across this long-forgotten photo when I decided to digitise some old slides in my collection. The picture was taken at Lensfield Road in 1973 (I think).

It may look like a meeting of the problem hair self-help group, but in fact shows members of the Alan Battersby, Jim Staunton and Ted McDonald groups. I think it was one of several pictures taken by Professor Battersby and given to members of the three groups.

I am particularly grateful to Peter Sheldrake who provided the names of several people whom I did not recognize. The key is given below the photo. Any mistakes are mine.

Kind regards,

David Griffin, Wokingham, Berks



Lensfield Road, Cambridge, 1973. Members of the groups working for Alan Battersby, Jim Staunton and Ted MacDonald. Left to right: Dennis Buckley, John Beck, Eric Hunt, Bruce Middleton, Peter Sheldrake, Elaine George (secretary to Alan Battersby), Neil Westcott (rear), Jane Stephenson (front), Phil Strange (rear), Gordon Hodgson, Ray Jones (rear), Andrew Stachulski, Rachel Rayner (behind), Robert Hill, John Milner (rear), Ralph Whitney, Brian MacCarry, Andrew Kus ? (rear), Rob Bryant, David Griffin, Apichart Suksamran and David Grayson

...and some more theoretical ones



Jean-Pierre Hansen supplied this photo of the theoretical sector, which we're pretty sure was taken in the early 1960s. Between Jean-Pierre and David Buckingham, we've managed to identify quite a few of the suspects. Theoretical chemistry was clearly a male-dominated practice in the 60s!

Front row, from the left: Mark Child (retired Coulson professor at Oxford), Ruth Lynden-Bell (now retired and back in Cambridge), John Murrell (retired from Sussex), the late Christopher Longuet-Higgins, Lionel Salem from Paris, Ian Mills (retired professor at Reading), ?, ?.

Middle row: ?, Anthony Stone (recently retired at Cambridge), Alan Carrington (just retired from Southampton), Andrew McLachlan (now retired from the LMB, ?, ?, the 'other' Bill Jones, who moved to Aberystwyth when 'our' Bill Jones moved here.

Back row: All unidentified.

Let us know if you recognise anyone else in the photo!

A letter from LA

Former student Eric Scerri sent *Chem@Cam* a copy of his recent book to review, so we asked him what he's been up to since his Cambridge days...

I was a PhD student with David Buckingham, and arrived not knowing what research in theoretical chemistry entailed and spent most of my time on some rather speculative philosophical ideas having to do with quantum mechanics and relativity.

After a while Prof Buckingham began to despair of me and once said, 'You can't keep going back to Aristotle on everything' by which he meant, 'Stop being so philosophical and just get on with using quantum mechanics.'

But I persisted until he finally suggested that I take some of my writings over to the department of History and Philosophy of Science. They were not over-impressed since I lacked any background in the field. I had, after all, studied nothing but chemistry, physics and mathematics since starting my A-levels in the classic British educational tradition of 'deep and narrow'.

So I left Cambridge and took a year off before starting a masters degree in Physical Chemistry at Southampton which I completed but which was still not really to my liking.

Finally in 1986 I began what became the first PhD in the new field of the philosophy of chemistry at the University of London and thus took up Buckingham's

suggestion of many years previously. My topic was to examine the relationship of the periodic system to quantum mechanics. Does the latter explain the former and, if so, to what extent?

For the past seven years I have been a lecturer in the Department of Chemistry and Biochemistry at UCLA in Los Angeles where I teach large general chemistry classes of about 350 students. I also teach courses in the history and philosophy of science. I have founded and continue to edit the journal *Foundations of Chemistry* which is now in its ninth year of publication.

Recently, Oxford University Press published my book 'The Periodic Table: Its Story and Its Significance' which sold out of the first print run of 2,500 copies

The UK government's recent proposals for carbon emissions to be cut by 60% by 2050 means there is a real need for new low-carbon technologies, whether for energy generation or more energy-efficient devices and processes. Ideas range from the practical to the wacky, but unless they emerge from the research centres of large companies with big development budgets, how can they get funding?

Devotees of the TV show 'Dragons Den' will know just how difficult it is to get investors to stump up cash to fund projects – they're very good at picking out the flaws in the pitch. Having a carefully prepared proposal that has considered everything that might be relevant is essential, with research done and credible people in place. And without experience, it's not as easy as it sounds. This is where organisations like business incubators come in, such as the one managed by Angle Technology on behalf of the Carbon Trust. Its mission is to get low-carbon technology ideas into a position where the investors are more likely to hand over the money.

Based in a Guildford office, Angle's staff includes an ex-Cambridge chemist (and former *Chem@Cam* cover star!), Malcolm King. He works as a consultant, helping academics and small companies prepare that all-important pitch, giving advice about what further research and development they need to do to increase their chances of success.

Malcolm's career change was born out of his own experience. Towards the end of his PhD with Dave King, he and Victor Ostanin came up with an idea for a new type of computer mouse. 'We put it to venture capitalists, and rapidly discovered we had a lot to learn!' he says.

He'd been on a one-week entrepreneurship course organised by the university during the summer at the end of his PhD, and while his mouse idea may have died a death – it was a nice idea but the barrier proved to be access to market – contacts he made on that course ultimately led him to his job at Angle, helping other people and organisations put their ideas into production.

'When a company comes to us, the most important factor to start with is that they must have a good carbon reduction case,' he explains. 'This can be directly by displacing fossil fuels in energy generation, or by using energy more efficiently. For example, if you can reduce the energy consumption of an electric motor by one-sixth, that could have a substantial impact, if you consider that electric motors and systems are responsible for about 40% of global electricity consumption. When you think of low carbon energy, you think of solar panels or wind turbines, not necessarily a motor!' Another example is a novel bioprocess, developed by a

Investment aims

How can a good idea for reducing carbon emissions gain funding? Malcolm King works with the Carbon Trust Angle Incubator helping to turn ideas into pitches that will appeal to investors

From Cambridge to Guildford: Malcolm is now helping inventors attract the attention of venture capitalists



Didcot-based company, that makes fermentation and biotransformation products in a preconcentrated form, so less energy is expended removing water.

The value of an idea at the outset depends on its features, benefits, advantages, the size of the market and its growth potential. 'If you're really lucky, 10 years down the line you'll get a 100 times return on the initial investment, but getting there is the difficult part,' Malcolm says. And whether you get there depends on both money and management. 'It's a chicken and egg situation. To be able to attract the management you need the money, and to attract investment, you need good management. The result is a repeated process of pitching for money to get the business to the next stage, until if all goes well it reaches the stage of being self-funding.'

SPOTTING PITFALLS

If an academic has managed to take an idea to the proof-of-concept stage with a research council grant, showing that it works at the lab scale, Malcolm says there's a danger that all they will see is the pound signs and not the pitfalls.

'We worked with a university group that had developed a high efficiency motor with an EPSRC grant,' he says. 'We engaged with the customers really early on to develop a market-led design specification. The process helps academia turn their ideas and research into products for a real customer as well as published papers. It may take the form of simple alterations to the design, or a substantial

rethink once we find out what a customer will actually be willing to buy.'

The next step is to engage a contract r&d house or an engineering firm to develop the specification and a plan for achieving it, and then work together with the academic to develop that customer-defined prototype.

In its three years of operation, the Carbon Trust Angle incubator has already successfully incubated 15 companies, which have gone on to raise a total of £27m in funding, £15m of that by Oxford Catalysts alone.

'Once the project is ready, we match it with venture capitalists who have a specific interest in investing in that space,' he says. 'We'll prepare them for their interrogation by firing all the nasty questions the potential investors would so that they are less likely to be caught off guard.'

He stresses that it's not good enough just to have an idea – it's essential that all the planning and, most importantly, the right people are there. 'If you just turn up with the technology, the venture capitalists are likely to say no,' Malcolm concludes. 'We tend to be involved with companies who are burning cash and need to go through several funding rounds before they become cash positive. But without all the right people and plans in place, that is very unlikely to happen. You have to be able to convey the idea to the investor in the structured format that makes them feel comfortable enough to put their money into the venture.'

■ carbontrust@angleplc.com

Happy ever after – eventually!

Here at Chem@Cam we love a romantic happy ending. But for Thanasis Karapanayiotis, who's just finished his PhD with Andy Holmes, it looked for a while like his happy ending might be in doubt – or at least somewhat delayed.

His beloved, Rui Zhang – who's also just finished a PhD in chemistry, with Christine Willis at Bristol – is Chinese, and the wedding was taking place in China in February. Their 'adventure' started before they were even due to travel, thanks to the British Airways strike that, ultimately, didn't happen. But they had to make other arrangements, and were forced to fly to China on different days using alternative airlines. 'This seemed inconvenient at the time, but was nothing compared to the trouble that was to come,' Thanasis says.

Their internal flight from Beijing to Harbin in the north of China was forced to land at Changchun airport instead thanks to very heavy snow which started only moments after they took off. They had no idea until they landed that they were in the wrong place – he says the air crew told them shortly after he remarked, 'Finally, let's go home and get some sleep!' Chance would be a fine thing... As it turned out, they were lucky

The happy couple looking rather more awake than might be expected



Thanasis posing next to the not-so-cleverly-concealed taxi sign, which should normally reside on top of the vehicle rather than in the passenger's lap...



to have got as close as Changchun – theirs was the last flight that was diverted to that airport, and later flights were sent even further away from Harbin.

Two hours later, they found out that the family couldn't come and collect them because the highway was closed because of an accident, so the only option was a five-hour train journey to Harbin. But that meant getting to the railway station. 'Predictably, the taxis were ordered to stay put because of the bad weather,' he says. 'We managed to bribe one of the drivers to take us, which took about two hours driving in the heavy snow. He removed the taxi sign and put it inside the taxi to hide it – we couldn't resist taking a photo!'

By this time, the pair were beginning to get a little stressed as the ceremony was due to take place the next morning. They managed to get a train, though for three hours they were standing and the other two were spent looking for seats, they finally arrived in Harbin, only to find that the highway they needed to use was also blocked. 'The normal hour-and-

a-half cruise to Da Qing – which would have allowed us about six hours sleep before the ceremony – turned into a seven-hour ride through hell, as we travelled through villages and off-road areas. Fortunately Rui's cousin, who had collected us, is an expert navigator and somehow managed to get us there without driving off a cliff.'

They arrived an hour late for Rui's makeup and hair appointment – and the family were wondering if they would make it at all. 'To add insult to injury, we lost even more time because our hotel room door was jammed, and the management had to give us another room,' Thanasis says. 'Surprisingly, however, we managed to start the ceremony only an hour late. What's even more amazing is that we didn't actually feel tired, despite having had no food or sleep for two days!'

Fortunately, the wedding went without any further hitches, and they got their happy ever after in the end. They're now off to work in Montreal – hopefully the journey to Canada will prove less eventful!

A spate of new arrivals

The department has been keeping the midwives busy in recent months, with several new babies to report.

Amazingly, two of them were even born on the same day. Tanya Radic, head of purchasing and accounts had a baby boy on 10 January. He's called Marko, and weighed in at 3.8kg (that's 8lb 5oz in imperial baby-units).

At the same time as Tanya was giving birth to Marko, Stuart Mackenzie's wife Christiane was also busy producing a

baby boy. To add to the coincidences, little Fraser Robert – Stuart and Christiane's first child – also tipped the scales at a healthy 3.8kg. He's pictured on the right, looking remarkably peaceful. Bet he's not always so quiet!

Meanwhile, a few weeks later on 26 February, Michal Sharon, a Dorothy Hodgkin research fellow working with Carol Robinson, has had a third baby – a healthy little girl named Ronnie, who weighed in at 3.9kg.



Alan sees a ghostly apparition



Alan Battersby continues to defy the years and enjoy his retirement by spending much of his spare time hiking the hills. He spent Christmas in the Lake District, climbing the fells around Buttermere, where this photo was taken.

'Lovers of the Lakes should be able to work out which summit I was on from the background and the sun's angle – it was early afternoon,' he says. 'The weather was remarkable, with the valleys full of cloud and rather dull, yet by climbing to around 1,500 feet there was brilliant sunshine. It was spectacular.'

Coming off Red Pike in this same weather, he saw his image as a Brocken spectre projected onto the clouds below.

The image appears as a shadow surrounded by a circular rainbow halo. Sadly he didn't have his camera with him that day, but seeing the spectre made his week.

'I first read about this phenomenon as a boy of about 10 years old, in a children's general knowledge magazine called *World of Wonder*; older readers will remember its excellent quality,' Alan says. 'It took umpteen decades to pass before I saw the real thing for the first time, and I was thrilled.'

If readers are curious about what a Brocken spectre looks like, then there's a pretty good photo at www.atoptics.co.uk/droplets/globrock.htm

Jeremy has a cracking time

He doesn't do things by halves. No sooner had Jeremy Sanders retired as head of department but things were thrown into disarray by a freak bike accident that left him with a badly injured left arm.

'I didn't get hit by a car or even fall off,' he says. 'I fell off as I was getting on!' When pushed for further details, he admitted that it was entirely his own fault – rather than climbing on and setting off like any sensible person might do, he started pushing the bike down the drive before launching himself boyishly into the saddle. Unfortunately, the saddle had other ideas, leaving Jeremy in a rather painful heap with an arm that was broken in several places.

After an operation in Addenbrookes to repair the damage – and a rather nasty reaction to the antibiotics – he's now on the mend, but won't be cycling again for a while yet. 'And when I am, I don't think I'll be trying to get onto the bike while it's moving again!' he says.

Comings & goings

New Staff

Terri Elston
Senior secretary
Catherine Jordan
Senior secretary

Leavers

Irene Derungs
Ollero
Ashleigh Matthews

Welcome back from maternity leave

Christina Akosile
Cleaner

Anyone for cricket?



The department's cricket team is looking for players, scorers and umpires for the up-coming season, which gets going in May.

We play in the University Inter-departmental League against other departments, the games are played mid-week. They usually start at 5.45pm, with both teams hoping to bat for 20 overs.

All members of the department and

friends are eligible to play. If you're interested, email Matthew Brooker on mb466@cam.ac.uk or come along to the free net sessions at Fenners Cricket ground. There are four net sessions booked from 6-7pm on 4, 11, 18 and 25 April.

For more info, look out for notices in the Cybercafe, or visit our website at www-leeper.ch.cam.ac.uk/CrickTeam.html

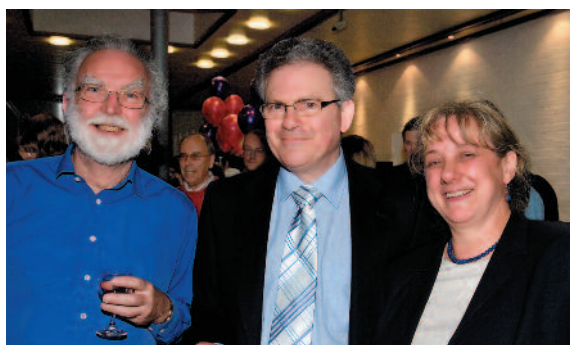


Photo: Caroline Hancox

If the tree surgery pictured in the last issue wasn't scary enough, how about this? Photographer Caroline Hancox spotted them at work high above Lensfield Road, removing diseased branches. Apparently, the council wouldn't let them get to work on it until they'd proved that the tree really was sick, but finally allowed them to remove the manky bits before it spread to the rest of the tree. It's not a job for people with vertigo!

A drop of festive spirit

The annual staff Christmas party is a great excuse for current members of the department to catch up with some old faces. Photographer Caroline Hancox was on hand with her camera



Above: Chris Forman, David Palmer, Aurora Cruz, Angel Orte and Dudley Williams; above left: Anthony Stone, Jeremy Sanders and Deborah Easlick; left: Peter Wothers and Sebastian Müller; right: Brian Johnson sneaks a kiss with Deborah



Above: Tim Layt and a glass of wine (of course) with Nic Davies and Sue Johnson; right above: Tony Gray, Tiger Coxall and Jim Watson; right Pete Proctor, Don DiFranco and David Miller; left Irene Derrungs Ollero, Mykola Karabyn and Chris Blackstone



Photos: Caroline Hancox

Last issue's winners

Chemdoku

As ever, Chemdoku proved popular with Chem@Cam readers. Correct answers to last issue's puzzle came from Keith Parsons, Robin Foster, Philip Blake, Jim Dunn, Wendy Annan, Michael Aicken (whose postcard this time featured oast houses rather than pubs this time, but at least he kept up with the beery theme, Tony Pike (who admits to being 79), Peter Keefe, A.J. Wilkinson, L. Taylor-Brown, Tim Edwards, Cris Walker, Stephanie Walker (who put in a plea for another elementary crossword: your wish is our command, Stephanie!), Robin Pope, John Salthouse, R.N. Lewis (who was here between 1943 and 1946, which probably makes him older than 79 – he claims he's still going strong! – do we have any older readers?), G.E. Hall, Oliver Taylor, Helen Stokes, Annette Quartly, Robert Broughton, Tom Banfield, John Carpenter, Richard Brown and Peter Grice.

And the winner, chosen at random (sadly without the aid of a footballing mug this time as they're all in the dishwasher) by Chem@Cam's glamorous assistant and random number generator, otherwise known as David Husain, is... R.N. Lewis. Congratulations!

Transmutation

Keith Parsons' anagrammatical puzzle also produced a handful correct solutions. In it, Keith asked if readers could transform the letters of chromium, indium, iron, neptunium, palladium, rubidium, sulfur and ytterbium into eight other elements.

The correct answer was bismuth, dubnium, fluorine, iridium, mercury, platinum, plutonium and radium, and correct solutions came from Michael Goodyear, Richard Brown, Robert Broughton, Annette Quartly and Roger Duffett. The lucky winner is Michael Goodyear. Congratulations!

Richard Brown described the puzzle as 'fiendish', and borrowed his son's 'superior computer skills' to work it out.

'It appears that there are 8,302 possible solutions, i.e. potential combinations of eight elements that use only the letters from the eight original elements,' he says. 'However, there is only one solution that used all the available letters.'

'Incidentally, it took about three days to run the computer programme, which tested each element in turn, subtracted it from the available letters, subtracted the next element, and returned to the list when any letters ran out. Chemdoku was a bit easier!

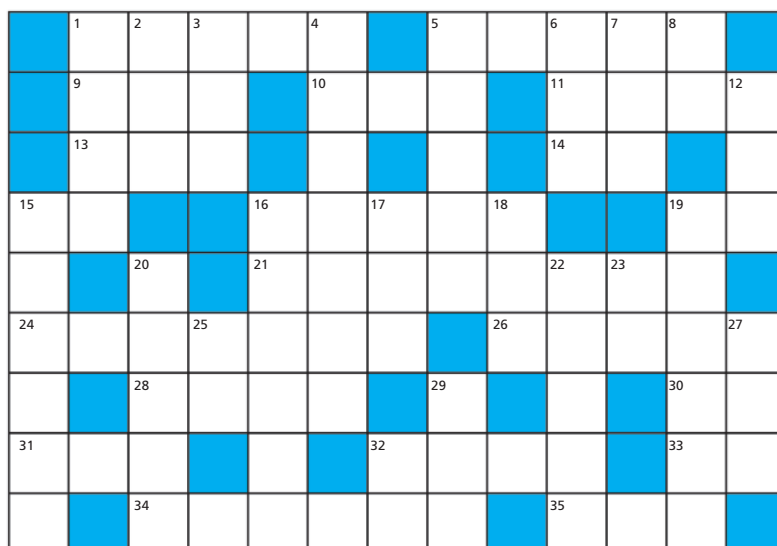
This issue's puzzles

Graham Quartly has set us another Chemical Crossword. 'This time, I've included more chemistry in it,' he says.

As before, each square in the grid has to be filled with the symbol for a chemical element in such a way that the resulting words fit the clues. For example, 'European language' requiring six

elements could not be either FRENCH or SPANISH as they are too short, but it could be SPANISH or ICELANDIC.

The usual £20 prize will go to the first correct solution randomly drawn. Hopefully Chem@Cam's washing up will be done by then and the football mugs will make a reappearance.



Across

1. Excellent
5. Chemical for the garden
9. Bears
10. This rascal could be an oriental sailor
11. Bends the rules
13. Layers
14. Paddle
15. Genuine
16. Basic
19. Water pot
21. Man of the world
24. Rays of light
26. Neither here nor there
28. Place for phoning or voting
30. Seaweed
31. Hot air balloon
32. Restricts
33. Slender
34. Over sweet
35. Kill

Down

1. Of space
2. Below
3. Gap in range
4. Iron worker
5. Vegetable
6. Mexican dish
7. Clip
8. Item of clothing
12. Part of ship
15. Start again
16. Contains ethanol
17. Sole
18. Noble gas
19. Ill
20. Black sacks
22. Queen of the jungle?
23. Large marble
25. Simple note
27. Get back
29. Bear
32. Form of transport

Hidden identity

And finally... another puzzle from Keith Parsons. The solution to this puzzle is a nine-letter noun. To solve the puzzle requires lateral thinking and letter-manipulation skills. In addition to identifying the noun, the solver must explain why it is correct and thus account for the somewhat stilted wording used in the puzzle. £20 to the first correct answer, as ever.

HI !

SIX AND II - YOUR LUMINOUS GUIDING CLUE

BE ELEMENTARY

HMM ! HMM !

LO ! NOUN

£20 prizes are on offer for both puzzles. 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

People matters

Our roving reporter Don Flory talks to assistant academic secretary Christine Wilson about her human resources role

Photo: Nathan Pitt



Increasing employment legislation from the government and European Union and a growing awareness of employees' rights in the workplace has led many UK businesses to employ specialist human resources personnel, to deal with the complex problems these issues can present. The university is no exception, and here in chemistry, assistant academic secretary Christine Wilson is the 'trouble-shooter' looking after this vital area.

ADMISSIONS MATTERS

'I've been working in the department since November 2005, preceded by a period of secondment from the personnel division for one day a week,' she says. 'My day-to-day work is rarely prescribed or scheduled, and a typical day may include admissions matters, staff performance issues and departmental training programmes. It's also my job to interpret the impact of changes in employment law, new or revised university policies, procedures, rules, and regulations, and recommend how such introduction or revisions should be interpreted here in the department.'

She finds the wide and varied remit of her job very stimulating, and at times demanding and challenging, not least when she becomes involved in conflict management issues that require considerable tact, diplomacy, and discretion. 'I may provide initial advice and support

to managers, staff and students on welfare matters. I also ensure that correct procedure is followed, and maintain a monitoring and facilitating overview of issues such as an employee's phased return to work after maternity leave, workplace modifications to cater for disabilities, or a student's return after a break because of ill health.'

Christine explains that, in the case of contract research staff, for example, there is a lot of mandatory legislation surrounding the use of fixed-term contracts, which are issued because of the fixed amount of funding provided by sponsors for the undertaking of specific research-related project work.

One of the principal roles for Christine and her colleagues involves postgrad admissions. 'Julie Lee and I also arrange and review an annual programme of transferable skills training courses/activities, which run from the time a student arrives in the department up to the time they leave,' she says. 'This includes the essential health and safety training that must be undertaken before a student is allowed into a lab,' she said.

'The programme requires first years to attend a number of compulsory courses in life-skills that will better equip them for their study, and also for their future careers. While it might seem that students compete with each other in trying to get out of as many transfer-

able skills training courses as possible, and their feedback can at times be negative, this contrasts with largely positive feedback received from postdocs to whom we offer a similar continuing professional development programme.'

Christine was brought up and spent her early schooldays in the small Cambridgeshire village of Great Chishill near Royston, and later attended Melbourn Village College. On leaving school in the early 1970s, her first job was as a secretary at Premier Travel Agency, Rose Crescent.

During this time, she married and brought up two daughters before changing her career. 'Once they were both settled in secondary education, I felt the time was right to re-focus on me and my career aspirations – something I had put on hold because of the many commitments bringing up a young family entails.'

A job in the employee benefit section at Cambridgeshire County Council attracted her, and while working there she embarked on a three-year day-release course offered by the Chartered Institute of Personnel Development at Anglia Polytechnic University. This led to a chain of job changes in the finance, personnel and education divisions.

In the mid 1990s, she moved on again, to set up personnel procedures in Downing and Pembroke colleges, where she supported the work of both bursars. She said they were the only colleges who then recognised the overdue need to bring their working practices up to date, and found herself in a unique position that had materialised thorough an initial speculative enquiry letter. In 2002 Christine made the move to the university's personnel division, which was undergoing reorganisation.

ADVANCED CERAMICS

In her spare time, Christine is a keen ceramicist, and has recently gained a City and Guilds Certificate in Advanced Ceramics. She is also a competitive mid-range tennis player, and tries to play friendly tennis fours regularly as a member of the Next Generation Tennis Club in Cambridge. 'I also try to get Wimbledon tickets each year through the annual ballot,' she says.

However, during last year's tournament, Christine had more on her mind than tennis, as this is when she and John, an environmental health officer were married. She is delighted that they now have a collective total of four daughters – two still at university and two married, plus two grandchildren, which she says means life is never dull or boring. They spent their honeymoon travelling across a distant and romantic area of the world – Vietnam and Cambodia! It was a far cry from Lensfield Road.



When I said, 'Let's try wave power,' that wasn't quite what I meant...



UNIVERSITY OF
CAMBRIDGE

Chem@Cam is written,
edited and produced
by SARAH HOULTON

Printed by Cambridge Printing,
the printing business of
Cambridge University Press