chem Cam

Chemistry at Cambridge Newsletter

Summer 2010

Making inorganic macrocycles A new strategy for the department **Predicting** molecular properties Simulating how **proteins fold**

As I see it...

Cambridge chemistry alumnus Julian Huppert was elected as the LibDem MP for Cambridge in May. He spoke to Sarah Houlton about the election, and what his early days in parliament have involved

Tell me about your chemistry background. I started as an undergraduate at Cambridge in 1996, studying NatSci at Trinity, and specialising in chemistry. After a gap year working for a financial software company in the City, I came back for a PhD with Shankar Balasubramanian on DNA structure and function. I then got a research fellowship at Trinity to work at the Sanger Centre, returned briefly to chemistry in the Unilever centre, and then in 2007 started a research group in the Cavendish lab – my work had become so biological it didn't really fit in the chemistry department, so I moved to physics!

How did you get involved in politics?

I'd always been interested in what was happening in the rest of the world, and my interest was initially with the United Nations – I ran conferences including simulations of the UN for school and university groups, and set up a Cambridge university UN society. In the sixth form, I started to get more interested in domestic politics, and joined the Liberal Democrats, as I discovered by watching Prime Minister's Questions (PMQs) that I kept agreeing with the LibDem position. I got involved in the student campaign in Cambridge in the 1997 election, and then in 2001 stood for Cambridgeshire County Council as a LibDem, and was elected for East Chesterton, close to where I grew up.

I spent eight years on the council, and had been the leader of the LibDem opposition group, before standing down last year when my term was up. I'd found that running a research group was more than a full time job, and leading the LibDem group took up at least another two days, and it was getting hard to combine the two! But then the LibDem MP for Cambridge, David Howarth, decided to stand down from parliament at this year's election, which got me thinking. I'd already stood for parliament once, in 2005, but that was in Huntingdon, John Major's old seat, which used to be the safest Tory seat in the country. Cambridge was a very different proposition.

I was already an approved candidate, and was one of very many who applied for the seat. Six of us were shortlisted, all locals, and then in December and January we had a month to go round all the LibDem members in Cambridge to canvas votes, through the ice and snow! I had a great team helping me, and it climaxed in a packed hustings meeting – the room was full to bursting – and I was selected as the candidate.

What was campaigning like?

It was very intense, and pretty much a full-time thing. I enjoyed it much more than the unsuccessful campaign in Huntingdon as it involved a lot more people, and there was a real buzz of energy. I took part in a huge number of hustings meetings – 35 – with the other candidates. That was probably too many, but it was interesting, especially those focused on specific topics like disabled issues and homelessness. Preparing for them made me think more about those issues. It was an exhausting process!



I guess the election day itself was a very long one?

It was, but because I had such a large team of people – including some from the chemistry department – it wasn't too bad! The result was declared after 5am, so it was a very late night. From the piles of ballot papers the result was clear for quite some time before it was declared, so there was an odd sense of hanging around for a while, knowing I couldn't actually celebrate yet. But I was very pleased with the result – Cambridge has 13 wards, and I won 12 and came close in the 13th, so it does feel like I represent all of Cambridge. I managed to get a few hours' sleep after that, but because of the election result no-one actually knew what was happening next.

Those few days of uncertainty must have been fascinating.

They were, yes. On the Monday and Tuesday during the coalition negotiations, unlike the other parties the LibDems were totally involved as members. We met many times and knew what was happening at every stage, and ultimately we had to vote on whether to accept the deal. It was a real shock introduction to parliament – there was no time for 'this is your office, this is your phone' – it was more 'we'll do all of that later, just do this first and then we'll tell you where to sit'.

We voted as a party at about 1 am on the Wednesday, but while we'd all seen the full text of the agreement, many of the Tory backbenchers didn't see it until it was published at 10am. But I'm glad I'd seen it - it's a big thing, and I needed to be able to say that it was broadly OK; of course there are bits I disagree with, and if it were a LibDem-only government I'd be horrified, but of course, it's not as we didn't actually win the election! The fact that we all saw it was an important buy-in process.

You were pretty quick to make your maiden speech, weren't you?

Yes, I gave it on day 2 of the Queen's Speech debate. I wanted to get on with it – you're not really supposed to do numerous other things until you've given your maiden speech. So I got it in early, speaking about science, wellbeing and sustainable transport – I'm probably the only MP who cycled home from their count!

What have you been up to since then? A huge amount! I've already asked a lot of questions and spoken in various debates, and even asked a PMQ of David Cameron about Trident – he didn't agree with me! I was also the first LibDem to ask Nick Clegg a PMQ when he was standing in for Cameron; it was about child detention, and he announced that the children's unit at the immigration removal centre Yarl's Wood was being closed, which was a fantastic result. That was on my birthday, too! I've asked questions in parliament about plenty of other topics, as well – the military, homelessness, the digital economy act, student visas and, of course, science funding.

While of course I want to champion science I don't want to be pigeonholed, and although I am the LibDem backbench science rep I'm actually on the home affairs select committee rather than the science and technology one – another LibDem Cambridge NatSci graduate was keen to do the science committee. But home affairs subjects like the immigration cap are a big issue for science – how can we keep science and high-tech businesses in places like Cambridge going if we say to people outside the EU that we don't really want them here? It's an awful message to send, and we have to find a way of dealing with that. It applies to student visas as well, so it's a really big thing.

Is it what you expected?

People said it was like this, and I didn't believe them! It's a bit of a madhouse – the hours are ridiculous. On Monday and Tuesday, for example, we're supposed to finish at 10pm, but actually that's when the votes start, and because each takes about 15 minutes it can be difficult to get home, as I'm commuting from Cambridge. The 11.15 train is just about doable if there aren't too many votes, but we can be much later – one day we were still sitting at 2.30am! A couple of times I've had to stay in a hotel or with friends, but it's tough on them as you show up after midnight and leave again at 7am.

The general scientific understanding among MPs is abysmal. Of course there are exceptions, but many seem to think it's acceptable not to understand science – they'd never dream of saying they don't know any Shakespeare, but think it's OK not to know any science! There are even some who are completely anti-science, and the recent report on homeopathy was a disgrace, as they seem to have given up on the concept of evidence.

One thing I am having to get used to is changing from one topic to a very different one and getting up to speed on new subjects quickly. And planning the diary is a nightmare, as timings change – a 3.30pm debate can actually start at 6pm. We even had something on the order paper that said it would happen at, before or after 7pm.

It makes planning meetings difficult, and you often have to move them at the last minute, which looks unprofessional. But it's very exciting, as well as being very hard work, and I'm not regretting it - yet!

Colloid absence

Dear Editor

My Cambridge chemistry was in 1959-Nov 1961 when I qualified for my PhD, working with Denis Haydon at Free School Lane. I find Brendan Carroll's article in the Spring 2010 issue of Chem@Cam and the group photograph there very nostalgic. I remember each face and most names, though I do not appear in the photograph myself as I had had to dash off to Ghana to take up teaching in a new university named after President Nkrumah.

I met Brendan in 1966 when I went back to the department on a sabbatical leave, soon after the Ghanaian president had been deposed in an army coup d'état. I was Denis's first student at Cambridge, and met him and his wife Primrose when they were setting up their new home at Great Wilbraham, a few miles away.

Yours sincerely,

Byomkesh Biswas,

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What an atmosphere

Dear Editor

The latest issue of Chem@Cam has just popped through the door, and as per usual I take great pleasure in its mix of scientific and people stories. This issue, with feature on Neil Harris, struck a particular chord with me as I was involved at the Centre for Atmospheric Science from 1993-2000, firstly with a PhD on a novel broadband lidar supervised by Rod Jones, and secondly as a postdoctoral researcher.

Since leaving the department I have had something of a career change and am now working as a musician in Glasgow, playing and teaching the clarinet. However, Chem@Cam always brings back the memories of several happy years spent on Lensfield Road.

The reason I'm getting in touch is to tell you of a sponsored cycle ride I am doing this summer with friend Oliver Rundell, another Cambridge alumnus and musician living in Glasgow). Together we will be cycling 1500 miles from Gothenburg to the North Cape (the northernmost point of Europe), in order to raise money for the National Deaf Children's Society and a new film about the profoundly deaf Scottish cyclist James Duthie, who cycled solo to the Arctic Circle in the 1950s. We have a website at www.ollyandalex.com with further details of the trip, if readers are interested.

Yours sincerely

Alex South; alex@scq.org.uk Chem@Cam is always interested in hearing about the exciting exploits of alumni and hopefully next time Alex will let us know how they got on!

Burning down the house

Dear Editor

David Howells' suggestion (Spring 2010) of a reunion for surviving occupants of Lab 287 is a great idea. If I can persuade Steve Quarrie to bring the Cornish pasties, I'll bring the fire extinguisher. Peter Baker (1967-70) Peterbaker61@googlemail.com

Electronic alternative

Dear Editor

I greatly enjoy the magazine, so excuse me in advance if this sounds picky. Is there not an e-version? I would forgo the paper copy if there were, and surely this would save the department nx£1000 in postage etc if the majority of people were to take it up?



Letters

For curiosity I tried to find recent back numbers (I'm ashamed to say I don't store them) - and failed. Cordially.

Bryan Slater (France)

And the good news is - as part of the impending relaunch of the departmental website, a full archive of pdf versions going back to the redesign in Summer 2006 (issue 25) will be available to download on the site. At the moment, we don't have the capability to replace individual paper copies with emailed pdf files, but if a lot of readers would like to receive the magazine that way instead of as a hard copy, we'll look into it. Let us know if you'd be interested at news@ch.cam.ac.uk

chemacam

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Photograph:

a year by the University of Cambridge Chemistry Department. Opinions are not necessarily those of the editor,

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News

A pair of leadership fellows

Matt Gaunt and Jonathan Nitschke have been awarded Leadership Fellowships by EPSRC. The fellowships are designed to support researchers with the most potential to develop into international research leaders. The hope is that, by the end of the award, they will be setting and driving new research agendas.

The competition is fierce – typically every year EPSRC receives 250 applications for these fellowships, and only about 20 are awarded. This year, just 16 were given out across the whole spectrum of science and engineering. The five-year awards cover salary and also provide support for the recipient's research team.

Jonathan is delighted to have received one of the fellowships. 'With it, we will build on work that we published last year in *Science* on molecular encapsulation,' he says. 'We are interested in seeing how "hiding" one reactive molecule inside a capsule, then letting it out later, can cause a chemical system to evolve in a different direction and produce different products than it otherwise might have done.'

Matt is also very happy with the award, and the support it will provide for his chemistry. 'Through this fellow-ship, I hope to be able to develop a new synthesis blueprint by using transition metal catalysts to unlock the reactivity of latent C-H bonds in organic molecules,' he says.

'This will hopefully bring about a step-change in how chemists think about making molecules. We are aiming to develop new synthesis concepts that enable us to develop effecient, fast and "green" ways to make biologically interesting molecules and modify medicines, proteins and functionalised materials.'

A sensor achievement



PhD student Tanya Hutter and colleagues won nearly £30,000 of funding in the recent CamBridgeSens Network Grant competition. CamBridgeSens is the university's EPSRC-funded network for uniting sensor research across departments, and the competition was open to multidisciplinary teams working on the development of sensors.

The idea of the competition is to foster innovative ideas for sensor research, from the initial proof-of-concept stage into a strong and competitive bid for funds from external funding bodies. Tanya's group was awarded £28,300 for developing portable handheld integrated sensors. The project is a collaboration between chemistry and the Centre for Advanced Photonics and Electronics (CAPE) in the electrical engineering department, and included Tanya's supervisor Stephen Elliott and postdoc Lei Su, as well as Nikos Baimedakis, Richard Penty and Ian White from CAPE.

The goal of the group's project is to design and develop a portable handheld

Stephen Elliott, CAPE postdoc Nikos Baimedakis, CamBridgeSens project director Clemens Kaminski, Tanya Hutter, Mica Green and Lisa Hall from CamBridgeSens, and chemistry postdoc Lei Su

From the left:

device that incorporates all the components needed for sensing applications. The device will contain all the optical, electrical chemical and biological components required on a single printed circuit board – the optical source and detector, the optical waveguides, the microfluidic channels and the electronic circuitry. It will be functionalised with sensitive receptor groups such as dyes, self-assembled monolayers or polymer brushes, which selectively bind to the desired analytes.

As they are so small, a large number of different optical sensors can be integrated into a single chip allowing simultaneous detection of different molecular species. It should be widely applicable – its functionality can easily be adjusted simply by substituting the reactive agents.

'We're really delighted to have won,' says Tanya, who's in the first year of her PhD in Stephen Elliott's group. 'The money will give a real boost to our research, and will allow us develop the idea further so we can attract external funding for the project.'

Olympic gold!



This year's chemistry Olympiad took place in Tokyo – and the GB team were awarded a rare gold medal, plus two silvers and a bronze. Peter Wothers, David Wade, Joshua Stedman, David Edey, Ben Pilgrim, Andrew Worral and Ruth Franklin, plus a selection of medals

Peter Wothers accompanied the team once again. As usual, the students spent time here in Cambridge practising in the labs with Mykola Karabyn and the lab techs and going over theory papers before heading out to Japan, under the watchful eye of Peter and fellow mentors Ben Pilgrim from Oxford and Andrew Worrall from Harrow School.

The students – David Edey (Alcester Grammar School), Ruth Franklin (Manchester High School for Girls), Joshua Stedman (Abingdon School) and David Wade (Northgate High School) – spent 10 days in Tokyo. Ruth was the first female British student to win a gold medal – only the sixth gold won by any British student ever – and distinguished herself by coming 8th overall.

As well as the long exams and practical sessions, they got to see something of the city and Japanese culture. 'We saw a lot of shrines, and were even introduced to Prince Akishino, who's second in line to the throne, and studied biology at Oxford,' Peter says.

He also reports that some of the toilets, in particular, were eye-opening. 'They were automatic, with sprays, heated seats, and the lid even opened and closed automatically!'

Academic changes

There was good news for the chemistry department in this year's round of academic promotions. Professorships have ben established for Jane Clarke, Michele Vendruscolo and Dominic Wright, while Matt Gaunt becomes a reader and Andy Wheatley a senior lecturer.

In October, we'll have a new inorganic lecturer, Erwin Reisner, who is joining us from Manchester. We're also bidding farewell to Jeremy Rawson, who's to be a professor at the University of Windsor in Canada.



The seminal paper that announced the presence of the Antarctic ozone hole was published 25 years ago, and the department held a symposium to celebrate the anniversary in May.

All three of the paper's authors – Joe Farman, Brian Gardiner and Jonathan Shanklin – were in attendance, and all the speakers spoke about some aspect of ozone research, including Nobel prizewinner Paul Crutzen, and former Linnett lecturer Susan Solomon, who chaired one of the Intergovernmental Panel on Climate Change's working groups.

The conference was organised by Neil Harris, John Pyle and Peter Braesicke, and Neil says it was an obvi25 years of the ozone hole

ous idea to hold a symposium celebrating the paper's publication. 'It's one of Nature's top-10 most cited papers, and while I don't like to use the word iconic, for that paper, it's true,' he says. 'The measurements were simple but the results were stunning.'

The talks covered a range of current ozone research and historical background, and Neil reports that they proved inspirational. 'I had a couple of emails from young PhD students after the event, who said the conference had really inspired them to do their own research rather than just following what they had been told,' he says.

About 130 people attended the meeting, and around 50 of them went on to a dinner at St Catharine's. 'Brian Gardiner, who hadn't given a talk during the day, gave the after dinner speech,' Neil says. 'He told us beforehand that he'd speak for about half an hour and we were alarmed – but he was really entertaining and we wouldn't have minded if he'd spoken for longer!'

Left: Joe Farman gives his lecture

Right: the 'supporting cast' of lecturers. Front row: Jonathan Shanklin. Susan Solomon, John Pyle: middle row: Brian Gardiner, Paul Crutzen, Michael McIntyre, Keith Shine: back row: Jean-Pierre Pommereau. David Fahey, Archie McCullogh Neil Harris



Facilitating chemistry research



The latest addition to the department's academic-related staff team is Isabelle de Wouters, who joined us in June as research facilitator. This newly created post was put in place to support the department's research strategy, and aid academic staff in identifying funding opportunities, and developing research applications.

Isabelle grew up in Tasmania and Africa, and has lived in the UK for the past 18 years. Her background is scientific – she has a PhD in the biological sciences from the Open University.

She's spent her career working in academia and for research funding bodies, including three years at BBSRC as senior programme manager responsible for biochemistry, cell biology and a range of cross-council initiatives.

In 2008, she moved to the National Institute for Health Research in Leeds, which manages the Department of Health's research funding streams. While there, she was primarily responsible for medical and dental clinical academic careers, and the institute's research methods programme.

This experience of both academia and research funding councils will prove invaluable in helping our academics secure funding in the current difficult climate. 'I'm really excited by the new challenge of working in the chemistry department,' Isabelle says. 'I look forward to meeting all the academic staff and discussing their research interests..'



Mark Eddleston, a PhD student in Bill Jones' group, tasted success in May – his talk at the Young Crystallographers session at the British Crystallographic Association's meeting in Warwick was adjudged the best. The talk, entitled 'Transmission electron microscopy of pharmaceutical materials', won him £100 and a bottle of champagne. He's pictured receiving his prize from Judith Shackleton of the University of Manchester

News

Prizes for Cambridge chemists

We've got another great crop of prizes to report this issue. First, several Cambridge chemists are on the list of Royal Society of Chemistry award winners for 2010. Chris Dobson is the recipient of the Khorana Prize for his 'outstanding contributions to the study of the structure and properties of biological molecules, especially proteins, and their relationship to biological evolution and disease'.

Daan Frenkel was given the RSC's Soft Matter and Biophysical Chemistry Award, for his work on 'development and application of computational methods that have transformed our understanding of soft and biomolecular materials'.

The third RSC winner is Clare Grey, who has been awarded the John Jeyes Award for her work on solid state NMR and functional inorganic materials. This isn't her only recent prize – she's also received the Ampere prize in recognition of her 'seminal contributions to the elucidation of ionic conduction and electrode processes in batteries and fuel cells by solid state NMR'. She gave her prize lecture for this award at the Euromar conference, which was held in Florence in July.

A prize from the American Chemical Society is heading Richard Lambert's

way – he's been given a Langmuir Lectureship Award of the American Chemical Society. He will be giving his Langmuir Lecture on catalytic chemistry and self-assembly on metal surfaces at the forthcoming ACS meeting in Boston.

Younger members of the department have also been recognised. Felipe Garcia has been given a Corporate Associates Junior Faculty teaching award, and Andreas Bender won the European Federation for Medicinal Chemistry's 2010 Prize for Young Medicinal Chemist in Academia. Andreas will be giving his prize lecture at the EFMC symposium in Brussels in September.

Chemist – and biochemist!

A list of the past decade's top-20 most cited biochemists in the Times Higher Educational Supplement contained a familiar name – Chris Dobson.

Chris is number 11 on this list, but on another list of biochemistry citations, with the data counted and analysed in a different way, he's second, behind Dundee's Philip Cohen.

What makes this achievement even more remarkable is the fact that Chris actually publishes most of his science in non-biochemistry journals. As a result these rankings are based on less than half of his papers.



The 14 August issue of the journal *Physical Chemistry Chemical Physics* features Graeme Day's chemistry on the cover. He was invited to submit a paper to this themed issue of the journal on solid state and cluster structure prediction, and he wrote up the results of an informal blind test for the issue.

'One of the big challenges that we are working on in our group is the development computational methods for predicting the crystal structures of molecules,' Graeme explains. 'We do a lot of method validation on molecules where the crystal structure is known in advance and then make claims that we can predict structures in advance of experiment. So we have to give ourselves a real test every so often to keep ourselves honest.'

Graeme was speaking with crystallographer Carl Henrik Görbitz about what they are doing in this area, and Görbitz offered him some unpublished crystal structures as a challenge. 'He told me the molecules, but kept their crystal structures under wraps, and then I came back with my predicted crystal structures,' he says. 'These are some of the most challenging systems that have been studied to date using crystal structure prediction methods, so I was thrilled when the predictions for two of the three crystal structures were spot on. The third structure was pretty close as well, so these results really prove that the predictions work.'

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Pharmaceutical Services

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 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.

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:

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access to departmental research lectures;
Ability to hold 'Welcome Stalls' in the department entrance hall;
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Preferential conference rates;
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A new department strategy

Recently, there have been significant changes in the way research funding is allocated, and the information demanded of us by the university, research councils and even industrial companies has changed, making it increasingly complex to meet their demands. A couple of years ago, it became clear that the way that we were structured as a department was proving a hindrance, and we began to look at what we should be doing differently. Planning ahead in terms of research was clearly an important part of this, but by no means the only factor - we also wanted to look at how we supported staff development, whether academic, academic-relatedor support staff, and encourage our people to get to know each other and their fields of expertise better.

Two groups were set up, one to look at research strategy, chaired by Steve Ley, and the other, which I chaired, to look at departmental strategy. On the research side, with several recent senior professorial appointments and several retiring in the next few years, we had the opportunity to think about the areas of science we want to focus on going forward. At that time, we had just appointed John Pyle to the 1920 Chair of Physical Chemistry, reinforcing our commitment to atmospheric science as a research theme, and Daan Frenkel to the theoretical chair, so there was a focus on computational materials and soft matter. More recently, the appointment of Clare Grey to the Geoffrey Moorhouse Gibson Chair emphasised the importance of energy research.

CORE CHEMISTRY

Most of our chemistry now falls into one (or more) of five core areas: chemical synthesis, computational and informatics, materials, atmospheric, and biological chemistry. It became clear to us that chemistry is moving away from the traditional concept of sectors, and while the familiar demarcations of chemistry organic, inorganic, physical, theoretical will remain important for teaching purposes and ensuring a good interface with school chemistry, they do not really describe modern chemistry research as there is so much blurring at the edges. This distinction is particularly important as far as the research councils' activities are concerned - they will put out a call for, say, chemical biology, but without a chemical biology sector, we found it hard to create a coordinated response. This could lead to future funding opportunities being lost.

So, from October, the old sectors will be replaced by five research interest groups. This does not mean there will always be five – there is no reason we cannot add further groups in future as chemistry develops. For example, we might Big changes are ahead in the way Cambridge chemistry is organised, explains head of department Bill Jones



want to look at other areas such as sustainability if the government and research councils believe that is a future priority. The new structure will make this easier for us to prepare for and respond to calls for funding.

An important advantage of the new groups will be that they will help the department prepare bids when initiatives come up in that area. So, for example, Clare Grey might take the lead on an EPSRC call on energy, and she would have a much better idea of who was working in relevant areas as they would be part of the same interest group, rather than being spread across sectors.

Some people might sit in more than one interest group – some will have interests in both materials and computational analysis. for example, and some of our synthetic chemists clearly will also be important in developing new materials.

Another new initiative involves crossdepartmental academic teams. These groups of eight to 10 staff would not necessarily be linked by common research interests, but would include a spread of subject and seniority. One of our concerns was that, with about 45 tenured academic staff, and an additional 15 or so nontenured PIs, a lot of our colleagues do not know each other that well. The idea was that if we had academic teams that weren't focused on research, it would be a way of making sure people mix more. Making links across different disciplines could be important in sparking future creativity.

We also felt that as we're such a big department, with 150-200 postdocs, 280 PhD students and 110 support staff, issues like staff development and career progression are another issue. And because we're so big there is an impression that we are not 'friendly'. Chem@Cam does a great job of telling people what w're doing, but do we have a welcoming atmosphere for new people coming in? We want to encourage them and retain them. We believe the new structure will help with this, and with staff development at all levels.

We have already reorganised our support staff, with Andy Middleton in charge of the buildings, Marita Walsh heading up the support staff, and the creation of Tim Dickens' role as head of IT, which has had a huge impact. This has enabled us to take better care of our support staff in terms of how we train them, and make it possible for them to move into new areas as science develops and priorities change. We are also focusing on how IT can improve the way we communicate, and are soon to launch a more helpful website.

As of October, the sector heads will be replaced by a senior management team which will, in effect, be the department's executive body under the head of department. Below this will be five new committees, whose heads will be members of the SMT. The new committees are research strategy, led by Steve Ley; teaching, which will continue under director of teaching James Keeler; David Wales will lead the resources and support committee; staff management, chaired by Jane Clarke; and David Klenerman will head the safety committee. All other department committees, such as library, IT, buildings and finance, will report to one of these committees. We hope to make it much easier to identify individuals who will take responsibility for any issues that might come up. So if we needed information about research output. say, it would be the research strategy committee's responsibility.

SCIENTIFIC LINKS

We have worked closely with the School of Physical Sciences and its strategic research plan. It is important that our research overlaps as much as possible with theirs – all academic appointments in the department now have to link in with the school's plan in some way. That way, there won't be lecturers isolated in one department; rather, further links will be built across different scientific disciplines. In the coming few years when resources will be stretched having these joined-up activities will be to our advantage.

Ultimately, the aim is that the head of department will have time to think more strategically, rather than being snowed under by day-to-day paperwork that would be better dealt with elsewhere. And given the likely significant government cuts we are likely to face in coming years – 20 to25% would not be unexpected – the department and whoever succeeds me as its head next year, will be much better placed to respond with the new structure, as there will be a much clearer picture of where our priorities lie.

I have enjoyed my time as head of department, and the process of reviewing how we move forward. I have had a lot of assistance from my colleagues over these past two years or so, and there is a general feeling of optimism and support to make the new structure work.

Inorganic synthesis: not

Inorganic synthesis can be notoriously unpredictable. Dominic Wright is trying to create inorganic structures in a more predictable way

> Figure 1 (below left: Structure of the host-guest compound [{P(µ-N^tBu)}₂(µ-NH)]₅I[−], viewed from the side of the molecule. The Ianion is H-bonded to the five N-H bridges in the ring

Figure 2 (below): Structure of a 'doped' Ti7Co cage

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methods for the doping of bulk and molecularly constrained titanium oxide. 'It all came out of a conversation Richard and I had in the teaching lab four or five years ago,' he says. 'He was wondering whether it would be possible to make large amounts of titanium dioxide doped with nitrogen, to make low band-gap semiconductors.'

TiO₂ is interesting as it's a very cheap material - it's the main white pigment in paint for many different applications - but it also has the ability to destroy pollutants. 'If you excite the electrons from the valence to the conduction band, provided the recombination rate is not too great, you can get migration of the resulting holes and electrons to the surface of bulk TiO₂, where they can oxidise and reduce organic molecules on the surface.' However, Dom says, the big problem is that only about 5% or so of the light energy at sea level is available to do this, as it's a UV process with

a reasonably large gap between the conduction and valence bands, so by doping it in a conventional way extrinsically with nitrogen, you can lower the band gap. This makes the TiO₂ active with visible light.

In the past, the problem with these sorts of approaches was that making an active material very much depended on the synthetic process,' he says. 'We've developed a very simple approach where you could, in theory, make kilos of the material. We've already made hundreds of grams of it, and not only is it

Born: Gosport; moved to Cumbernauld in Scotland at <u>Dominic Wright</u> the age of 10.

Education: Studied chemistry at Strathclyde University, then moved to Cambridge in 1986 for a PhD with Ron Snaith on battery materials, funded by Octel.

Career: After two years as a college research fellow at Gonville & Caius, he was appointed lecturer in 1991, reader in 2002, and in October will be made Professor.

Status: His wife Carol is an English graduate – 'Like most of my family, she's on the artsy side!

Interests: Swimming and growing vegetables on his allotment

Did you know? He's the odd one out in an arty family, with one brother a violin maker, another a folk musician, and his brother Richard is the artist who won this year's Turner Prize. 'The awards evening was a great night out – an alternative reality!' he says. He has a few other family connections to the arts – his great-uncle was the actor and playwright Arnold Ridley, better known as Private Godfrey in Dad's Army, and his great aunt the actress Patricia Hayes.

In organic chemistry, it's the norm to be able to design a synthesis and have a fair idea what you're going to make. For inorganic chemistry, particularly of the main group elements like phosphorus, sulfur and nitrogen, it's often less easy to predict what you're going to get. Dominic Wright is trying to change that.

'We can make quite complex inorganic macrocyclic systems, for example, in a planned way, rather than just boiling a mixture up to see what happens, which is the more stereotypical inorganic approach!' he says. These new inorganic macrocyclic systems are analogous to organic structures such as crown ethers, calixarenes and porphyrins.

'These organic molecules are made using metal or anion templates, which enables the size and shape of the ring system to be fixed,' he says.

'But to make inorganic macrocycles, it's a little more complicated as there are other issues to consider. These include variable oxidation states, sensitivity, and size mismatch between orbitals. 🧉 Generally, the bonds are

weaker and more ionic, so they are more reactive. So when you're trying to establish a precise molecular arrangement, it is more difficult as the molecules are more flexible, and more likely to break open and react, rather than remaining in the ring structure. In particular, they are prone to polymerisation because of the dominance of single bonding between the atoms over double bonds. It's very difficult to do!'

These difficulties aside, the peculiarities of inorganic structure can work to your advantage, he says. 'For example, if you take simple dimers of the type $[XP(-NR)]_2$, where X is a leaving group and R an organic group, it turns out these are really good precursors for making macrocycles because the cis forms of these rings are more stable than the trans. So, in a sense, they pre-organise to cyclise rather than polymerise.' Various macrocycles, such as the pentameric host-guest complex $[{P(\mu-N^{t}Bu)}_{2}(\mu-NH)]_{5}I^{-}$ shown in figure 1, can be produced with different anion binding capabilities.

'The pattern of chemistry follows quite closely what you'd see in organic chemistry,' Dom says. 'By putting different templating agents into the reaction, such as different metals and anions, you can determine the size of macrocy-

cle that is formed. Even without a template, unusually, just one type of macrocycle is made, in pretty much 100% yield, because of this preorganisation. So there are no extraction or separation problems.'

Another research area, funded by EPSRC on a joint grant with Richard Lambert, is applying simple inorganic

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such a black art?

active, it's also very cheap and easy to synthesise – it's relatively trivial chemistry, reacting titanium chloride with water and ammonia in a round-bottomed flask.'

However, where it starts to get more interesting is if, instead of looking at bulk samples of TiO2, you look at doped molecular fragments of Ti_xO_y. 'Various people have made titanium-oxygen cages of this type containing up to 18 titanium atoms, which are essentially little chunks of titanium dioxide with a ligand periphery around them,' he says. 'These can be used as building blocks for hybrid materials, by cross-linking them to each other with organic linkers, either with or without conjugation. These have the effect of sterically trapping or encasing these titanium dioxide units, so they can be used in photovoltaics and other light-activated processes.'

In particular, he says, if you can develop methods to dope these cages with other metals or non-metals, in a manner analogous to bulk TiO₂, then you could use these new molecules as little 'engines' for photochemical reactions. 'In an organic medium, it might be possible to use sunlight to drive some types of oxidation and reduction reactions,' Dom speculates. 'This could be very interesting in a practical sense, as well as from the purist inorganic point of view.

'One obvious idea is to dope the transition metal, which absorbs in the visible spectrum, and use d–d transitions to mediate the formation of holes and electrons within the material of the cage itself. We've made a series of these new types of compounds now, using transition metals right across the spectrum of



metals. Potential applications include making hybrid materials, but it's also possible to hydrolyse the cages themselves, and so use them to deliver a given amount of transition metal within a titanium oxide dispersion, which again could have applications in photovoltaics.'

An example of such a transition metal doped cage is shown in figure 4. He's collaborating with Andy Wheatley in the department on this, and while it's still early days he says it's looking promising. 'If you hydrolyse these cages in the presence of a reducing agent, you get the metal itself trapped within the titanium dioxide, either atomically or in the form of a nanoparticle. That could be used for catalysis.'

Another project involves applying main group elements in catalytic bond formation. 'Initially, we're looking at dehydrocoupling in which two P–H bonds to give P–P plus hydrogen,' he says. However, 'This also has the potential to be applied to the formation of other bonds, both homoatomic such as Si–Si or C–C, and heteroatomic bonds such as C–P and B–N.

The starting point in these studies was a series of p-block metal phosphinidene compounds, which contain RP^{2-} ligands. Nitrogen analogues containing RN^{2-} , doubly deprotonated amines, are stable



Francesca Stokes, Vesal Naseri, Robert Less, Salvador Eslava, Dominic, Silvia Gonzalez Calera and Rebecca Melen

Scheme 1 (above): Typical decomposition of phosphinidene complexes into P-P bonded products and metal phases

Figure 3 (below): a ferrocenesubstituted cyclophosphane – although N–N bonds are short (about 1.45Å) they are weak as a result of lonepair repulsion (about 167kJmol⁻¹). In contrast, the P–P bond is about 2.1Å, but considerably stronger (about 201kJmol⁻¹) because of the lower lone pair repulsion.

'We've found that if you make metal compounds containing RP²⁻ they are thermodynamically unstable compared to phosphorus-phosphorus bonds and the metals themselves,' he says. 'For example, the heterometallic cage [{Sb(PCy)₃}2Li₆.(Me₂NH)₆] decomposes into the cyclic phosphane [PCy]₄ and the Zintl compound [Sb₇Li₃] at 30°C, as shown in Scheme 1.

This new type of reaction can be harnessed in two ways. First, the phosphinidene compounds can be used as single-source materials that decompose from solution into the metals or alloys. They can be sprayed onto a hot surface, whereupon they decompose directly from solution into the metal phase, with the P-P bonded byproducts being pumped off. Alloy or metal films have broad-ranging applications in the electronics industry in a host of devices, such as photomultipliers like those used as one of the major components in the

Hubble telescope. Indeed, this technology has been patented in collaboration with Electron Industries for light-detecting photomultipliers.

Phosphorus-phosphorus bonded products are also of interest in their own right, however. For example, strained cyclophosphane ring compounds like the unusual ferrocene-substituted compound in figure 3 are potential precursors for ringopening polymerisation into novel P-P bonded polymers. Notably, this compound cannot be made in any other way than via dehydrocoupling of the phosphine FcPH₂, where Fc is ferrocene, using a series of main group reagents developed in his group.

'There's a lot of interest in making unusual types of polymers, such as boron-nitrogen or phosphorus-carbon,' he says. 'Wherever there's a thermodynamically stable bond that can be formed, there's potentially a precursor molecule that could be made to engineer the formation of that bond in a thermodynamic way. The aim in the future is to develop a general methodology for the synthesis of a whole range of bonding types.'

The greatest challenges in inorganic chemistry, he believes, are the development of new synthetic methodologies capable of providing the sort of control that organic chemists take for granted in their systems, and the use of controllable methodologies in the building of large-scale inorganic macromolecular and structures.

Science



Right: the protein villin in both its unfolded (above) and folded forms

South African native Robert Best first arrived in Cambridge more than a decade ago for a PhD with Jane Clarke. While his PhD on protein folding was experimental-based, during his two postdocs and now as a Royal Society university research fellow, he gradually moved away from the lab, and now is firmly based in the world of computer simulations.

'In my PhD, I was using an atomic force microscope to unfold proteins by pulling on them, which gave an alternative picture of the energy landscape to more traditional methods,' he says. 'I then moved on to doing structure calculations, representing the protein as an ensemble of different structures, rather than just a single static structure. In my postdoc at NIH I used coarse grain models to try and interpret some of the experiments we'd been doing. Although I still use coarse grain models to some

Best Born: Cape Town

Status: Single

Robert

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Education: Degree in chemistry at the University of Cape Town, then moved to Cambridge for a PhD with Jane Clarke in 2000

Career: After a six-month postdoc here with Michele Vendruscolo, he spent three-and-a-half years on a second postdoc at the NIH in Bethesda, MD, US. He returned to Cambridge in October 2007 as a Royal Society University Research Fellow.

Interests: Rowing – something he started doing during his PhD – and sleeping!

Did you know? Coming as he does from a city that's dominated by a mountain, he was inspired a few years ago to go trekking in the Himalayas. He plans to return – but claims he probably won't make it quite as high as the summit of Everest...

Protein folding: a case of simulation

Protein molecules fold up very precisely into complex tertiary structures, but what happens during the folding process? Robert Best is simulating what takes place

extent, I'm now mostly using atomistic models, which is a lot more challenging, but should also be a lot more accurate.'

Proteins are strings of amino acids, and while on paper they look long and thin, in practice they fold up into very precise tertiary structures. When protein folding in the body goes wrong, the result is often disease, from cancer to Alzheimer's. So being able to predict how a protein will fold - and misfold in different environments can give important insights into their activity and what happens when the folding process fails.

Coarse grain models make the simulations easier because they reduce the number of variables involved in the calculations. A more accurate picture can be obtained if all the atoms are included, but the calculations instantly get much more difficult - every atom that is added increases

the level of complexity, and of course there are very many atoms in a protein. Even the simplest amino acid in a protein - glycine - contains eight atoms, and many of them contain 15 or more atoms. Multiply this by the large number of amino acids in a protein, and the number of atoms rapidly becomes enormous, and the calculations to simulate how they might fold are rendered extremely complicated.

'A lot of the proteins we look at are chosen because they are sufficiently small to make the calculations a little more manageable,' he says.

'Typically they have about 35 amino acids, so they're barely even long enough to class as proteins. But this makes the calculations practical, both from the point of view of sampling configuration space and how rapidly you can run a simulation of that size.

'The computer programme runs classical dynamic simulations, with some additional techniques to enhance

sampling methods. It's essentially solving Newton's equations of motion with an empirically parameterised energy function.'

He's just starting to look at proteins whose normal state is unfolded, but when they bind to a target in the body they then fold up. 'There are many examples of these intrinsically unstructured proteins,' Robert explains.

'They are often involved in signalling, where "messages" are passed between different processes in biological cells, for exam-

ple in regulation of transcription. Because of their role in sig-

nalling, they are potential targets for drugs to treat diseases like cancer. The improvements we have made in the energy functions used in the calculations should allow us to better address this type of problem.'

This combination of simulations and experimental data gives a good picture of what is happening when a protein folds.

'Most of the time, a protein sits in a stable state, whether that's folded or

unfolded, and its properties can be measured using techniques like NMR,' he says. 'But in an experiment, it's very difficult to look at the precise mechanism of how the protein goes from one stable state to another from unfolded to folded - as it doesn't

spend long enough at the different points along the folding pathway.

'There are indirect experimental techniques that use kinetic information to give some insights, such as the ϕ value analysis developed by Alan Fersht. But, apart from single molecule methods, most experiments measure an ensemble average, whereas simulations can give an insight into the reaction mechanisms between the stable states.'

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Pharma property predictions

Andreas Bender is exploring how past experiments can inform the future design of active molecules – as he explains to Sarah Houlton, there's a huge amount of data to mine

Scientific research creates data, and often huge amounts of it. And this poses a challenge for scientists – how can data from many different experiments and projects be exploited to inform future science? Andreas Bender is trying to do just this in his work predicting the properties of molecules in the life science field.

'In recent years, the genomes of many different organisms have been sequenced, and those biological data have always been public,' he says. 'In chemistry, this really wasn't the case. Pharmaceutical companies test molecules against proteins to see how they interact, but this kind of data about biological activity was always proprietary, and remained within the companies' own databases. But in the past five years or so, these data have started to become public, with databases like PubChem in the US, and ChEMBL in Europe containing millions of compounds whose structures are connected to bioactivity data. That's a lot of knowledge!'

Photo:

This knowledge of what type of molecules inhibit a particular enzyme, for example, can be used to design better molecules in the future, he explains. 'Essentially, we mine these databases for ideas. Say a new biological target is discovered that might be useful in medicine, but no molecules are known that bind to that receptor. How could we use existing knowledge as a starting point?

'We can go into the databases and look for receptors with a similar shaped binding pocket. Might molecules that bind to the receptors we find also bind to the new one? So the idea is to exploit previous knowledge to design bioactive compounds more easily than before. Of course it doesn't work in every case, but it's better than random – and twice as good as random is already an improvement as you save 50% of resources!'

Another focus of his research involves finding ways of predicting the properties of molecules. Many proteins in the body are associated with adverse drug reactions. A good example is the hERG potassium channel, which can cause cardiac side-effects when it's inadvertently activated. Medicinal chemists now try to design compounds that don't activate it, and looking at molecules that are known hERG channel activators is a good starting point.



'There were even drugs that had to be withdrawn from the market because of this side-effect,' Andreas says. 'It turned out that they looked very similar to known inhibitors of hERG. So we can build computer models that tell you if a molecule looks like known inhibitors, and warn you to take care. If you can predict early on that a compound might cause problems, it will save a lot of time and money later on.'

This work is all built on chemoinformatics software tools that enable statistical models to be created around chemical features. 'These fingerprints describe parts of the chemical structure,' he says. 'As an example, a molecule might have a carboxylic acid, an aromatic ring and a hydrogen bond donor a certain distance away from the aromatic ring. We take these combinations of features, put them into statistical models, and these models predict which combinations are most likely to be active, or cause side-effects, based on previous knowledge. In this example, it also recognises the distance to the aromatic ring.'

The model is also trained to learn which features are more important, and weight them all accordingly. 'The ChEMBL database used to be commercial before it was handed over to the European Bioinformatics Institute at Hinxton, and it contains a large amount of useful information about molecules and drug targets,' he says. 'It has close to a million data points in it, but we can train our model using those data points in a couple of hours. If we put a new molecule into our model, it will go through all those different proteins, and tell you which the molecule is most likely to bind to, based on real-world experimental data.'

BINDING PREDICTIONS

A long-term aim is to connect different 'layers' of data to get a bigger picture. 'Right now, databases like ChEMBL connect molecules and proteins, and others connect proteins and biological pathways,' he says. 'Pathways can then be linked to phenotypes, or observable characteristics in humans, but this is currently the weakest link.

'Going forward, we want to be able to predict which molecule binds to which target, which pathway this alters, and then what phenotype this gives. This might also help in predicting pathways that might cause side-effects – you know which chemical features cause the side-effect, and the adverse reaction at the end, so by looking between the two it could be possible to find which targets and which pathways contribute to that adverse reaction.'

Born: West Berlin – the wall came down when he was 16

Education: Studied chemistry at the Technical University of Berlin, followed by a year as an exchange student at Trinity College Dublin and a summer working in a chemoinformatics startup company near Berlin. After a masters degree at the University of Frankfurt, he came to Cambridge in 2002 for a PhD with Bobby Glen on molecular similarity.

Andreas Bender

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Career: In 2006, he moved to Novartis in the US for an industrial postdoc in their lead discovery informatics group. His independent

research career began as an assistant professor at the University of Leiden in 2008, and he returned to Cambridge as a lecturer in the Unilever Centre this May.

Interests: Spending time in the pub, and shopping. However, unusually for a German, he's not a big fan of Pilsner – he has developed a deep and abiding love of real ale

Did you know? He teaches in a private bioinformatics institute in Bangalore every summer, and his time in India has made him an expert in the essential skill of haggling.

Science day

The flash side of chemistry!

Our annual open day gives schoolkids the chance to find out that chemistry can be fun. Nathan Pitt and Caroline Hancox took the photos of this year's event

This year's chemistry department open day in March was another resounding success, with hundreds of schoolchildren and their parents visiting the department to find out more about chemistry.

Peter Wothers' demonstration was even more dramatic than usual this year. Entitled 'Burning issues – flame and fire', it looked at the process of combustion, and as you'll see from the photos offered plenty of opportunity for flashes and flames. Particularly impressive was the 80 foot long tube filled with hydrogen and oxygen hanging from the ceiling of the BMS lecture theatre!

As well as a display from the Nanoscience Centre, there was the usual array of chemistry experiments for the kids to try. There were plenty of old favourites and a few new ideas among the experiments. These included extracting DNA, the incredible erupting and dry ice volcanoes, lava lamps and rainbow water, shiny pennies and zinc plated coins, disappearing coffee cups and liquid nitrogen icecream, making nylon and, of course, those old favourite messy ones, blue goo and the cornflour slime tank.

Thanks to the organisers, led this year by James Keeler and Emma Graham, and of course Eric and Katharina Walters, without whose generous financial support the day would not be able to happen. And finally, thanks to all the students and postdocs who supervised and ran the experiments, and the teaching technicians for their help with all the activities, and making Peter's lecture possible.

































Alumni

Reminiscences of 1960s colloid science



Gentlepersons:

I was pleased to find the article 'Colloid science – 1960s style' in your Spring Newsletter. This revived good memories of my postdoctoral year at Colloid Science in 1949-50.

I recognized a few of the people in the 1960 photo including Len Saggers, who was a great help with my research equipment and the Head, Prof. F.J.W. Roughton. However, many of my contemporaries had left including my research advisor, Prof. G.B.B.M. Sutherland (who some jokingly called 'Gordon Boom Boom'), who was a pioneer in infrared spectroscopy and the use of infrared polarization.

Several of my colleagues included Tom Robinson, an able technician, who subsequently married postdoctoral fellow Britta Davidson, from Sweden whom we visited at a later trip there. Also, there was Norman Sheppard, Leonard Bovey, Alister Valence-Jones from New Zealand (who subsequently moved to Canada, and with whom I went hiking in Switzerland, and the late Maurice D'Hont from Belgium, with whom I went youth hostelling throughout England and Scotland.

Maurice, after a stay in the US, became director of the chemical division of the Belgian Atomic Energy Commission, where I visited him in Mol and enjoyed swimming in the warm cooling water from the nuclear reactor. We had lectures by illustrious British

scientists like Paul Dirac, Max Perutz,

Prof. Lennard Jones (whom the students believed had great potential) and Fred Hoyle, who was in the midst of controversy about his concept of a steady-state universe. This was balanced by great philosophy with Bertrand Russell, with whom the small group of American students enjoyed having as a guest for a Thanksgiving dinner.

Britain was still recovering from WWII, and life was a bit austere, but the cool digs that the hundredweight a month coal ration allowed were a benefit in that it encouraged me to spend more extended hours in the centrally heated laboratory which was much warmer.

Equipment was primitive by today's standards, and I recall, the rescue session for the rock salt optics of our infrared spectrometer when the basement laboratory became flooded. However, for a spoiled American, this was a good experience since it prepared me for the early days at the University of Massachusetts in Amherst which was also somewhat ausere in that it was then small and had just become a university, having been an agricultural school.

Also, considering the energy-starved future that many predict, it offered the reassurance that life can be enjoyable, even under austere conditions. Sincerely Richard S. (Dick) Stein Goessmann Professor of Chemistry, Emeritus University of Massachusetts, Amherst, US

That's my father!

Dear Chem@Cam,

I recognised the person second from left on the front row of the 1961 Colloid Science department photo as my father, Dr John Chipperfield. He went on to become a lecturer in inorganic chemistry at the University of Hull. Sadly, he died a couple of years ago.

However, my mother recognises the person on his left as Denis Haydon. She also spotted the person third from the right on the front row as John Kernohan. He became a lecturer at Dundee University and is still living there in retirement. The person on the left end of the second row is Ian Saggers.

I followed in my father's footsteps and did my degree and PhD in Chemistry at Cambridge (1984–1990). Dr Ann K. Keep

keepa@matthey.com

A handful of names

Dear Editor

I was interested to see the 1961 departmental photograph of the department of Colloid Science, and to see old faces. I did my PhD there under Paley Johnson from 1957 to 1960. I find I still remember some faces. The ones I remember and can name are:

Counting from the left, number 5 on the back row, the name has gone but he was an assistant to Paley Johnson; he ran the (Beckman) ultracentrifuge.

First on the middle row is Len Saggers who ran the machine shop, number 5 is Sara Suchet from Argentina; she went to Princeton, New Jersey for postdoc, and then got a job, I think in Buffalo, New York. Number 11 is Cyril Smith, who I think was a glassblower. He distinguished himself by blowing out the wall of the glass blowing room by exploding toluene while making a toluene regulator.

On the front row, number 4 is lecturer Paley Johnson, 5 is Prof Roughton, 6 is Ron Ottewill, whom I think was a reader and went to Bristol, 7 is an Irish man whose name I forget – it might have been Callaghan – and number 8 is Arthur Rowe, a contemporary of mine. He went to Leicester.

I had already left, and was doing a postdoc at Princeton under Jacques Fresco in 1961. Later, I went to the biophysics department at King's College London.

I hope this helps. Yours sincerely Ted Richards 2 Peckarmans Wood, London SE26 ted@ricswal.plus.com

The early days in Lensfield



Yusuf Hamied (left) and Brian Tyler (right) pose in their new Lensfield Road lab

Dear Editor

These photos were taken in the UG labs at Lensfield Road in 1956. At the time I was in my final year at Christ's with Yusuf Hamied and David Bronnert. The photo on the left shows a very young Yusuf . In both cases, in the background is Mike Burnett (Pembroke I think). The photos show the typical light approach to safety of that time, as I was the only one with safety glasses on!

Mike and I both did PhDs with Sandy Ashmore, sharing a lab on the mezzanine floor of the new labs overlooking the car park. We had some amusing times there (they would now be considered irresponsible and alarming). We brewed coffee in the lab and Mike would turn up about 10am with some pastries to go with the coffee I had been instructed to have brewed about then.

He smoked a pipe and would wander over to my bench to chat, throwing his spent match into my bin which often contained ether soaked cotton wool (from cleaning the Apiezon grease from the taps of my vacuum system). A ball of flame would rise towards the ceiling. But no one came to harm. Regards

Brian Tyler

S&T Consultants, Handforth, Cheshire

Dear Editor

Recent comments about Ernie Cox, the physical chemistry storekeeper in the 1950s and 60s, reminded me how the Christadelphian Society played an important role in the interpretation of the rotational spectrum of chlorine dioxide.

This spectrum, lying in the microwave region, was one of the studies in the theses of myself and J.G. Baker under Morris Sugden. The spectrum is unusually complex because of the interaction of electron spin and nuclear quadrupole moments with the rotational energy levels leading to a wide splitting of each rational transition into up to 14 components. This, together with the two abundant chlorine isotopes, gave a profusion of lines which defied analysis.

Our best hope of making progress seemed to be to identify the spectra of the two isotopes, and we decided to prepare chlorine dioxide from HCl, enriched in a thermal diffusion column. The only problem with this idea was that the thermal diffusion apparatus required many long lengths of uniform bore glass tubing, and we knew that any request for Ernie to sort through his huge stock of glass would be met with his famous blank stare and thin smile which he reserved for ridiculous requests.

The breakthrough came when I noticed on his desk a pamphlet on the Christadelphian Society, and expressing

an interest I was given a handful of leaflets to read. A few days later, after careful study and some discussions with Ernie about the Society, I broached the subject of glass tubing, and was allowed to enter the sanctum of the storeroom with my verniers, and go through the stock of glass.

The thermal diffusion column which we subsequently built enriched the HCl isotope ratio from 3:1 to 10:1, and allowed the two chlorine dioxide spectra to be identified, and eventually led to the full analysis of both.

Another recollection of that time is the near-panic caused by John Goodings during the laboratory's opening day. After the official opening performed by HRH Princess Margaret, a tour of the laboratory took place. John, Roger Kewley and I were standing by our microwave spectrometers in the lab, next to the lift on the second floor of physical chemistry, when the word came that she was coming. We hastily put out our cigarettes - in those days, almost everyone smoked - and John dropped his in the waste paper bin by the door. A few moments later, clouds of smoke emerged from the bin, just as the procession reached the door. In the lead was the Lord Lieutenant of Cambridgeshire who, sizing up the situation, drew his ceremonial sword and gave the contents of the bin a thorough stirring. Amazingly, this put the fire out and, as you can see from the photograph, I was just able to regain a straight face as Her Royal Highness entered through a haze of smoke, followed by the departmental professors. Yours sincerely Dennis Jenkins, demonstrator, physical chemistry 1959–64 Manor House, Littleton, Chester drlittleton@aol.com



Alumni

A picture from Pembroke Street



Dear Editor:

The recent issue of chem@cam (Summer 2009) brings back to me memories half a century ago when I came up to King's (1953) on a scholarship from the Bombay University. Then the Chemistry building was located on Pembroke Street till I left in 1955.

My downstairs laboratory housed over 30 doctoral students and postdoctoral fellows. In the upstairs laboratory going through a spiral staircase, 10-12 chemists had their work benches. These laboratories had students of Professors Sir Alexander Todd, Alan Johnson, George Kenner, John Harley-Mason, Kipping, and B.C. Saunders.

My contemporary chemists had come from all parts of the world: Donald Hayes (Ireland), Dan Brown (later FRS) (Scotland), R.J.W. Cremlyn (Wales), Frederich Cramer (Germany), Albert Langemann, Andre Giddey (Switzerland), Miha Tišler (Yugoslavia), Laslo Szabo (Hungary), G. Baluja (Spain), Françoise Baron (France), Brian and Dorothy Armitage, Ronald Breslow, Murray Goodman, Jay Kochi (USA), Ken Carroll (Canada), F. Feigl (Brazil), Kenneth Hays (South Africa), Jack Cannon, David Magrath, Jeff C. Watkins (later FRS) (Australia), Peter Grant, W. G. Hanger, R. Basil Johns (New Zealand), S. Varadarajan (India), S.A. Faseeh (Pakistan), and Percy Wannigamma (Sri Lanka) were doing their Ph.D. or postdoctoral work.

Among other chemists from UK were: Ben Brown, Eric Bullock, Basil Chase, Malcolm Clark, Neil Hughes, A. M. Michelson, George Miller, Fred Newth, Colin Reese (Later FRS), Bob Sheppard, John Turner, and Reg Webb. The only woman chemist from UK was Helen Higson (M. Langemann). The laboratory From the left: Jeff Watkins, Bob Sheppard, Bal Joshi, George Miller, John Wren, R. Basil Johns, Neil Hughes, Colin Reese, Ken Carroll, Ken Hayes, Bill Hanger (Taken after George Miller's prank in the lab) assistants were Woodcock and Cyril Smith (glassblowing). A.R. Gilson was the laboratory manager and also designed many useful pieces of laboratory apparatus.

I remember lectures from Robert Woodward and Carl Djerassi on their recent work. I attended the series of lectures by Professor Todd on vitamins and hormones. Professor Dorothy Hodgkin used to come to the laboratory to discuss the collaborative work on vitamin B12. Professor Todd gave me the problem of structure determination of the aphid pigments. Bert Holmes would scout on his bicycle and let us know when the willow trees and the pea farms were infested with aphids. The team on the aphid problem consisted of Alan Calderbank, Ben Brown, Jeff Watkins and R.I.T. Cromartie.

The only instruments then available in the laboratory were UV and IR spectrometers and a polarimeter. I spent considerable time in determining the number of C-methyl groups in erythroaphins by Kuhn-Roth estimation.

When I left Cambridge to work with Professor Morris Kharasch at the University of Chicago in 1956, the structure determination problem was continued by Yusuf Hamied, Eddie Haslam and D.W. Cameron. The structures of all the aphid pigments were finally completed when NMR and mass spectral facilities became available. Lord Todd showed me the series of papers on aphid pigments and gave me a copy of his lecture published in Experientia when I visited the Lensfield laboratories in 1963. Yours sincerely,

B. S. Joshi (King's 1953), Athens, GA, US bsjoshi1228@bellsouth.net

Cleaning up the southern basement

Removing the radioactive contamination from the southern basement posed a significant challenge, as safety officer Margaret Glendenning explains

The basement of the department's southern wing has been unused for years, a legacy of its days as Alfie Maddock's labs. Maddock's work on radioactive isotope protactinium-231 left a radiological contamination legacy, as ³¹Pa is an alpha-emitter with a half life of more than 32,000 years. Work stopped in the lab in 1965, and although the lab was finally fully decommissioned in 1993, it was too difficult to decontaminate the riser – Riser Q – which took air out of the lab, and so the labs were left untouched.

Within days of starting as university chemical safety adviser in August 2001, I was told about Riser Q, and its asbestos and radiation contamination issues. My then boss in the university safety office, Will Hudson, had been handed the project, and I was brought in as I had 'special responsibility' for chemistry. It was obvious to both of us that the university had neither the appetite nor the desire to spend the money required to undertake the necessary decontamination – after all, it was in a safe condition and the Environment Agency was aware of the issues, but were not applying any pressure for the legacy to be removed. In 2001, the projected cost was in the region of £300,000.

However, when I became safety officer for the department in August 2004, I began to see the legacy as a liability that posed a significant risk if there were a major fire in the southern wing. I had visions of headlines regarding a radioactive and asbestos smoke cloud over Cambridge. I was also concerned about how, as asbestos duty holder for the department, we could manage the redundant Urastone ductwork within Riser Q, which was so tightly packed together. Urastone is sectional ductwork fabricated from asbestos cement, where the male and female joints are packed with loose asbestos, which is wrapped or sealed to prevent the packing material coming away.

In January 2006, I went to the Safety Office and met with Will Hudson and David Plumb, the university radiation protection officer, and asked if we could revisit the proposal to remove the filter housing and associated ductwork within the riser. I felt it was only a matter of time before the regulatory authorities started to put pressure on the university to tackle the legacy, I was concerned about ensuring a safe working environ-



ment for maintenance personnel – we have been clearing asbestos ductwork from within risers and plant rooms as funds have been made available – and development of the southern wing would only be possible if Riser Q was cleared. I also had to develop the department's Emergency Response Action Manual, and I had a huge question mark over the riser and filter housing. How would we respond? I was beginning to get obsessed! So I set myself the goal of achieving this project, much to David Watson's amusement.

Several options were possible, but they were all costly - decommissioning, decontamination and disposal costs had spiralled and we were warned to be looking at nearer £900k. The preferred option was to remove just the radiologically contaminated duct from within the riser and the filter housing from within the fourth floor plant room, but I knew that this was never going to be possible. I believed the duct was tucked behind several other redundant Urastone and, given the restricted space within the riser, I didn't think it would be possible to remove it without damaging the other ducts, which would give a further risk of asbestos release.

But which ducts were which? They snaked and twisted up through the riser, so asbestos consultant Matthew Goldsmith was sent into the riser with cans of various colours of spray paint to trace each duct up through the riser and into the plant room. The coloured spots that he sprayed proved my suspicions were correct – the radiologically contaminated duct was tucked tightly behind the others.

The job then became primarily an asbestos clearance, with the added complication of a radiological contamination thrown in. And, of course, Clare Grey was joining the department and the space was earmarked for her new labs. So the decontamination project became essential.

What made this project so unusual was that we were dealing with two types of licensed removal work asbestos and radioactive - in one project, and the method usually employed for each were, in some ways, in direct opposition to each other. For example, you would never purposefully break up asbestos where it can be avoided because of the potential for fibre release, but you aim to compact radiological waste. So what do you do if the radiological waste is asbestos-based? The hunt was on for a company who had experience of working in both these fields. Two were identified, both of which undertook asbestos clearances in nuclear power stations - somewhat different to our issue but they had the infrastructure in place to tackle the job in hand.

Given the complexity of the project, the regulatory framework within which we would be operating, and the controls that would need to be applied, Harry Percival from estate management spent a lot of time and effort in selecting the design and management team, which consisted of the asbestos consultant Matthew Goldsmith, radiological consultant Keith Stevens, project manager Carl Fox, CDM co-ordinator Greg Brown, and myself.

The project brief to the contractor made even more challenging as the research activities within most of the laboratories adjacent to Riser Q were to continue throughout the project. Our plans had to be scrutinised by Cambridgeshire Fire and Rescue



Above: the riser, complete with coloured spray paint dots

Below: The Riser Q Musketeers – Harry, Carl, Margaret and Matt

Service, the Health and Safety Executive, the Environment Agency, and the University's own specialist advisers. There was no room for mistakes.

It is worth pointing out that none of the labs affected were going to benefit from this project, and all labs adjacent to the riser (354, 290, 180 and G55) were going to be inconvenienced. Lab 180 was likely to lose half its fume cupboards, the fume cupboards in G55 were going to be shut down, and all lost space while the work was on-going as enclosures had to be erected in their areas. By some miracle, we were able to keep the fume cupboards up and running in Lab 180, but it was only because the building is a sieve that we were able to achieve the make-up air required to keep them running! All lab users in the affected areas were brilliant and supportive of the project, and I cannot thank them enough for their help and understanding.

For me, not only did I achieve a personal goal, but I got to work with some amazing people. I will never forget the day I stood in the fourth floor plant room where the filter housing had once been and looked down the riser into the basement below. I cried as I never thought we would achieve it! I spat blood for the project - literally and definitely took one on the chin for the department! Harry, Carl, Matt and myself all lost weight because we were living the project, working silly hours, cancelling leave and in at weekends. I nicknamed the four of us 'The Riser O Musketeers'. But I made some brilliant friends on this project and the sense of achievement was incredible.

Chat lines



Jeremy takes the cake

Jeremy Sanders was vice-president of this year's Burgenstock conference in May, and a little bird told the organisers it was his birthday. So a rather impressive cake was wheeled out after the evening lecture, which he had to cut into with a terrifyingly huge knife.

Jeremy says Matt Gaunt gave a 'stellar' lecture at the conference. 'Everyone in the audience was on the edge of their seats as he unveiled ever more astonishing and exciting results,' he says. 'The discussion afterwards was one of the best I have seen here.'

Brian bows out after 49 years



The department's NMR supremo Brian Crysell retired at the end of June after an astonishing 49 years in the department.He was adamant he didn't want any fuss, but there was no way he was going to get away without some recognition. So a collection was organised anyway.

Those who know that the NMR machines are all named after malt whiskies won't be surprised to learn that his gifts included two bottles of Dalwhinnie Distillers Special Edition whisky, and a couple of Waterford crystal glasses to drink it out of. He also got a flight in a Tiger Moth from Duxford, and £110 in garden vouchers – one of his retirement plans includes spending time on his new allotment.

Brian's also partial to the odd pint, and while the last thing he wanted was the fuss of a buffet and presentation ceremony in the department, he did quite fancy a lunchtime pint to celebrate his final day. So a fuss was most definitely not made in the Regal pub on St Andrews Street. And the photograph above of everyone wishing him farewell – Brian aside! – was taken in reception.

However, Chem@Cam is delighted to be able to report that Brian hasn't cut his ties with the department entirely – he's agreed to continue as a member of the editorial advisory board. So we will still be able to call on his exceptional knowledge of the department's people when trying to identify faces in photos! Comings & goings New staff Kate Nix

Zac Rudder-Logan Arwen Tapping Alice Wood

Retired Brian Crysell

Leavers Silvio Fusiello Martin McLean



We've had a couple of milestone birthdays among the assistant staff recently – librarian Judith Battison (above) celebrated her 60th, and Vicky Spring (right) from the print room was 65



Emily's gold and green wedding



This issue's Hello magazine moment goes to Emily Valentine and her hubby Simeon Dry. Emily, a PhD student in Jonathan Nitschke's group, first met Simeon as an undergraduate – they were both in the same year doing NatSci, and got to know each other better through the City Church Cambridge. Simeon studied physics and has just finished his first year teaching at Comberton Village College.

The wedding took place at Brickfields, which Emily describes as a blue warehouse next to Tesco on Newmarket Road, but is actually the building owned by the church, and where they meet on Sundays. 'I had great fun designing green and gold decorations to make it look more wedding-y inside!' Emily says. 'Lots of friends and relatives had helped me to preserve autumn leaves to go in the bouquets, flower arrangements and to use as name cards for the reception. I had all the beading on my dress done to match the green theme, too. It was a beautiful day!'

They moved on from the church to Emmanuel for photos in the cloisters and fellows' garden, and the reception was held at Anstey Hall in Trumpington, which she describes as a rather quirky manor house. 'It was quite a long day, which meant I felt able to actually say "hi" to most people, which was really important to me,' she says. 'It was perfect!'The evening entertainment featured a mini-cabaret, including a silly song entitled 'You make all my clichés come true' by poet Jude Simpson Brown, and a gospel-style song composed by the bride and groom themselves.

For honeymoon, the happy couple headed off to the south of Spain, to a little village called Bubion where one of their family has a flat. 'We enjoyed a couple of mountain walks when it wasn't foggy, and went to Granada for some sightseeing at the Alhambra,' she says. 'It was wonderfully relaxing.'

Last issue's winners

ChemDoku

Correct solutions to the 'Where on earth...' puzzle came from Jim Dunn, R.N. Lewis, Robin Foster, John Turnbull, Nick Broughton, A.J. Wilkinson, Bill Collier, Robin Cork, Audrey Herbert, John Anderson, Helen Stokes, Keith Parsons, Alison Griffin, Steve Sunderland, Dave Stone, Ian Threlfall, Morgan Morgan, Tim O'Donoghue, Neil McKelvie, Karl Railton-Woodcock, Tom Banfield and Annette Quartly.

To pick the winner, this time we took our inspiration from Paul the Psychic Octopus, who proved remarkably successful at picking winners of World Cup games from his tank in a German zoo. Chem@Cam doesn't have an octopus hanging around, but she does have a cat called Ginola (ah, those thighs). So by dint of laying out a line of catbiscuits and seeing which one she ate first, the winner is... Tim O'Donoghue. Congratulations!

Orienteer

David Wilson's puzzle had some readers stumped. For example, Jonathan Sayce reports that every time he attempted the puzzle he got a different answer, whether or not he heeded our admonishment to eschew calculus. 'As for physical chemistry, my equilibrium has certainly been disturbed,' he says. Perhaps the phase rule has some bearing on the two phases of our hero's journey, or perhaps he showed a balanced reaction in choosing his optimum route. Or perhaps this answer would not have found favour with Professor Norrish or Dr Sugden, two of my mentors in the early 1950s.'

We also had some incorrect answers. Bill Collier and Steve Sunderland both thought the answer was 133.3m, the former reaching the solution using a combination of Pythagoras and v=s/t, and the latter using Hess's Law as an analogy. And Dave Stone had the right idea, but the wrong answer.

Several readers reported correct answers, however. It's based on Snell's Law, with the situation being modelled by a ray of light at grazing incidence, as light takes the fastest path between two points. Sin θ /sin90 = speed of orienteer in wood/speed of orienteer in open ground =1/2. $\theta = \sin^{-1}(0.5) = 30$, i.e. the angle of a triangle whose sides are in the well-known ratio 2:1: $\sqrt{3}$. So $\tan\theta = x/100 = 1/\sqrt{3}$, or $x = 100/\sqrt{3} = 57.7$ m.

A correct solution came from Ian Potts, who said it was similar to the 'Baywatch' problem - where should the lifeguard enter the water when she (Pamela Anderson!) can run twice as fast as she can swim? Paul Stickland was also correct, although he claimed that it uses a physical rather than a physicochemical principle... He added that David should not have expected a quiet half hour, as it should only take such a class a few minutes to derive an expression for t in terms of x, to differentiate and find the stationary value of t, and solve to give the correct answer. 'It took a rising 80 rather longer, with recourse to a calculus textbook!' he says. Karl Railton-Woodcock was also correct - though he claims the very wellknown physicochemical principle he used wasn't quite the one we had in mind. 'Plugging Pythagoras into a spreadsheet and starting with the obvious 3,4,5, it took me about three minutes of trial and error to spot a root 3!' he says. 'I know this is cheating and eagerly await being told what I probably should have remembered.

Correct answers also came from John Wilkins, John Carpenter, Martin Stentiford and Annette Quartly. And Ginola picked the catbiscuit representing John Carpenter. The $\pounds 20$ will be on its way to you.

Drunkard's Walk

This one proved much more difficult, but we did get a couple of correct solutions from persistent readers: Annette Quartly, Karl Railton-Woodcock and Dave Stone. And the feline assistant picked Karl Railton-Woodcock's catbiscuit. Email jsh49@cam.ac.uk if you want to see the solution!

Elementary recognition

Graham Quartly's elemental recognition puzzle a couple of issues ago went down so well, he's come up with another one for us. Hurrah!

By tracing out a path of knight moves visiting all 25 squares of the grid once only, spell out the names of two wellknown scientists and a brief description of why they are famous. Spaces between words have been suppressed, and some elementary symbols thus stretch across adjoining words.

The usual £20 prize will go to one randomly selected correct solution.

Na	Ι	U	Al	Ι	
Nd	Те	Nd	Cr	0	
С	0	Ρ	Rn	С	
At	He	At	F	Nd	
S	K	Na	Li	W	

An alchemical ChemDoku

	Pb	Cu						Hg
Sb			As	Cu				
Hg					Sn	Cu		
	Cu					Sn		
	Au						As	
		Fe					Pb	
		Hg	Sb					As
				Fe	Au			Sn
Sn						Ag	Cu	

And finally... here's another ChemDoku to titillate those brain cells. This time, we've gone way back into history for our inspiration, and all the elements in the grid were used by the alchemists. The alchemists may not have managed to turn lead into gold and create untold riches, but one lucky reader will turn a correct solution into £20. Now that's... magic!

£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



If only all lectures were as exciting as Peter's on Science Day...



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