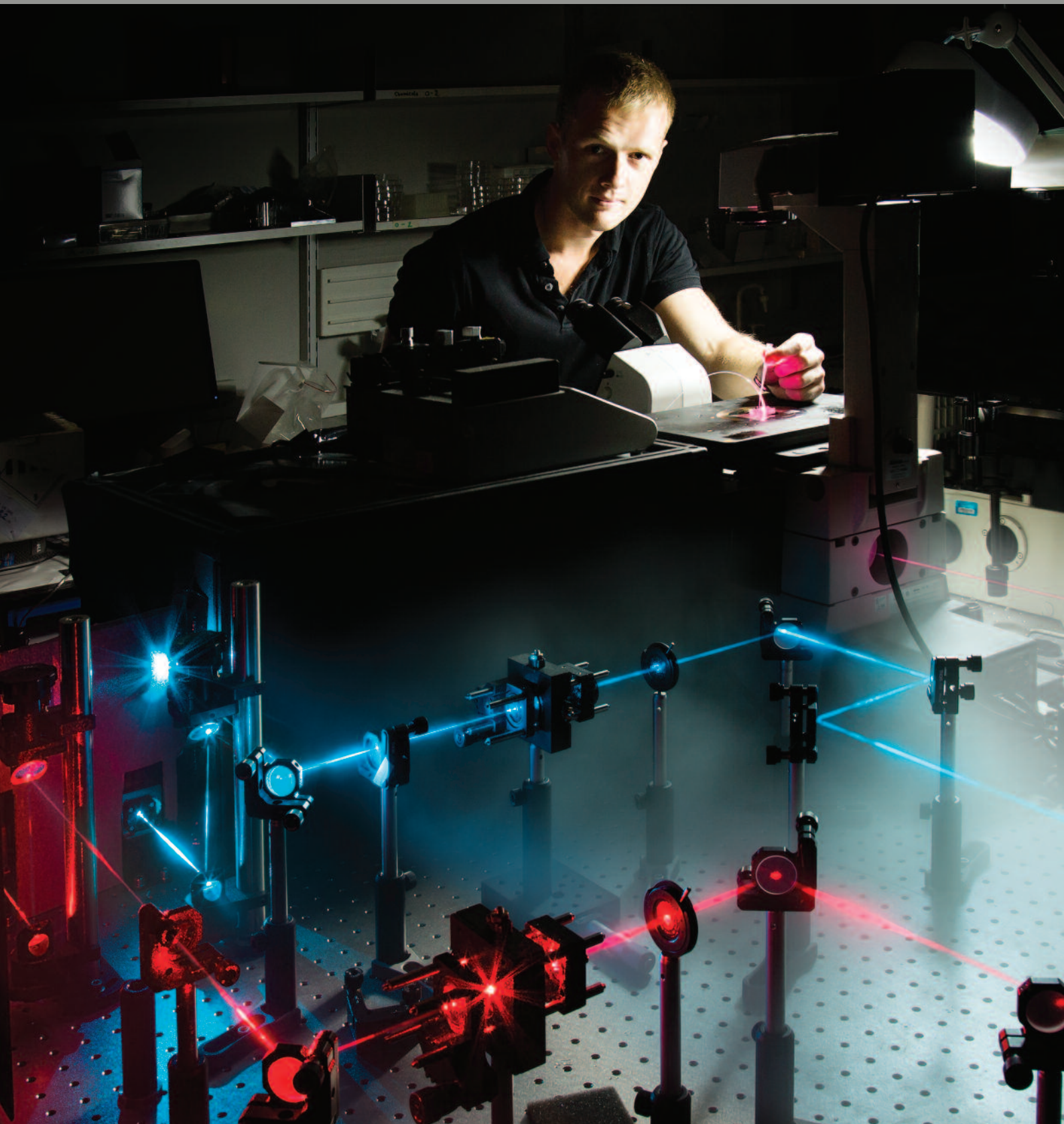


# chem@cam

Chemistry at Cambridge Newsletter

Autumn 2013



**Predicting 3D protein structures**  
**Back to the 1950s – explosively!**

**From Lensfield Road to Brisbane**  
**Calculations using wavefunctions**

Cambridge chemistry alumna Mary Garson has been in Australia since the 1980s, working on marine natural products. In January, she takes office as president of IUPAC's organic and biomolecular chemistry division. She tells Sarah Houlton about her chemistry career

### How did you become interested in chemistry?

It was through my high school teachers – Miss Armstrong, whom we called Miss Angstrom and, before her, Mr Jones. He loved doing chemistry demonstrations and was always blowing things up, such as the day he blew out the lab window after mixing the contents of balloons containing hydrogen and oxygen! I was hooked from the start. We also did quite a lot of organic chemistry, and I was captivated by carbon and all the bizarre reactions it did. I was mystified by how the changes happened, and I liked the detective component of mechanistic studies, for example pushing curly arrows to work out how an alcohol can become an ester.

### So chemistry was an obvious choice to study at university?

Yes – natural sciences at Cambridge. I matriculated in 1971, so I was one of the last group of students with a choice of only three women's colleges, and I went to Newnham. I benefited from the nurturing and supportive environment in college contrasting with the largely male population in the chemistry labs – there were five women in Part II out of a class of 80 or so. My supervisors were with Delia Agar and Ruth Lynden-Bell – Ruth remains a friend and professional colleague to this day.

I never thought about doing anything other than staying on for a PhD, which I did with Jim Staunton on polyketide biosynthesis. I worked on some of the early carbon-13 and deuterium labelling methods that became commonplace in biosynthetic investigations, and Jim was a fantastic mentor and supervisor. Most of my contemporaries applied for NATO fellowships and headed off to north America, but I wanted to have a cultural experience in Europe, inspired by the Italian postdoc working on the next bench to me.

I was awarded a Royal Society fellowship to go to Rome, where I spent a year. It has turned out to be invaluable – 35 years on, I have a collaboration on marine sponges with researchers in Naples, and being able to communicate in Italian has really helped. Next, I returned to Cambridge and a three-year fellowship at New Hall, working alongside Jim again, continuing with the biosynthesis work from my PhD.

Opportunities for advancing in academia at that point were limited, so I took a position at SmithKline French in Welwyn, which proved an interesting exposure to medicinal chemistry. However, I learnt that industry was not



for me, as the only way to advance involved leaving the lab, and there was little opportunity to follow up interesting results that take you off on a tangent. But I enjoyed making compounds and interpreting data!

### Australia's a big move – how did you end up emigrating to the other side of the world?

For personal reasons, I needed to find a job in Townsville in north Queensland. I applied for a Queen Elizabeth II fellowship and – to my surprise – I was offered it.

I'd written a proposal about studying biosynthesis in marine sponges, having discovered that they contained bioactive compounds with unusual isocyanide functional groups. Then I realised I'd have to collect the sponges myself so I'd have to learn to scuba dive – yet I could barely swim! This was just one of the many challenges that I had to deal with when I arrived in Australia; I've now done more than 400 dives, and I am aiming to reach 500 before I retire.

There is also a little marine animal named after me, which I'm really proud of. I was diving off Heron Island with a colleague whose wife was a flatworm

specialist, and he asked me to look out for specimens for her. Almost immediately I got under the water, I saw a flatworm that didn't look like anything I'd ever seen before, and I pointed it out to him. To identify a new species, you have to collect two specimens and, luckily, later on the same dive I found another.

That evening, over a bottle of wine, his wife said they'd like to name it after me, and we had to decide on the Latin name. And that is why there is a flatworm named *Maritigrella marygarsonae*. It's even a new genus – 'maritigrella' means 'little female sea tiger', acknowledging the beautiful tiger markings on the worm's back. But I also like to think it's suitable for someone like me!

After two years in Townsville, in early 1986 a number of lectureships were advertised around the country, and I moved to the University of Wollongong near Sydney. It turned out to be a great place, with a terrific new head of department who was a wonderful mentor, Leon Kane-Maguire, and a very collegial working environment. I'd done some teaching in Cambridge, including college supervisions, and I realised at Wollongong that I found teaching extremely rewarding.

I moved back north to the University of Queensland in 1990, and I'm still here – I love living in Brisbane, and it's very convenient for fieldwork on the Great Barrier Reef. I progressed through the ranks and was appointed professor in 2005. I spend about half my time teaching and the other half on research, and I've always been involved in a range of external activities, as well.

### What external projects have you found most rewarding?

Well, I chaired the Australian science Olympiads organisation that looks after our teams in physics, chemistry and biology, and we hosted the international biology Olympiad in 2004. This involved setting up a partnership between three Brisbane universities, government and industry, and it was one of the most rewarding things I've ever done.

While it's nothing to do with chemistry, it drew on the organisational skills I developed running field trips to remote islands – you can't get to Lizard Island, a spectacular remote field station at the top of the reef, and discover you don't have enough glass pipettes! Everything has to be carefully pinned down – experiment list, equipment list, even food list as there's no supermarket. I think a lot of the organisational skills I apply to high-level project management

Mary received the 'Distinguished women in chemistry or chemical engineering' award at IUPAC's meeting in Istanbul this year. She says the award – a framed portrait of Marie Curie really brightens up her office!

Right: *Maritigrella marygarsonae*, the flatworm that bears her name

emerged from my research activities.

I also organised a women's networking breakfast for the International Year of Chemistry a couple of years ago. I felt the obvious focus would be to celebrate Marie Curie, with women coming together for breakfast events in time zones that matched – in Australia we connected with events in New Zealand and China. We arranged for women in New Zealand and Hawaii to connect across the international date-line, completing a worldwide chemical 'handshake' via Skype. It was a great success – more than 5000 women chemists were involved and some of these networks continue. I even met Marie Curie's grandchildren afterwards!

Oddly, the breakfast that I hosted in Brisbane almost didn't happen in the aftermath of some major floods. The venue was in the flood zone, the university was closed, and I had no electricity – so no internet – at home. Fortunately I have an old-fashioned rotary dial telephone, which allowed me to continue finalising arrangements!

### How did you get involved with IUPAC?

In the mid 1990s, my academic mentor at the University of Queensland, Jim O'Donnell, became ill. He had been leading a bid for Brisbane to host the IUPAC General Assembly – now the World Chemistry Congress – which is held every two years. He was passionate about putting Brisbane on the world chemistry map – as well as the benefits for research, he wanted our



students to be exposed to the world's best chemists. When he died, I took over, and with Graham George here in Brisbane and Bob Gilbert in Sydney, we set up a three-way leadership team, of which I was the executive secretary.

The meeting was a huge success, despite the opposition from many people beforehand who were worried about the cost. Afterwards, I became a member of Division III, organic and biomolecular chemistry, and quickly became involved, eventually as secretary keeping the communication 'web' together. It's much easier now than in the past when we relied on fax and post! And now I am about to take up the presidency of the division for the next two years.

### What are your aims for your presidency?

I want to ensure that organic chemistry is taken seriously in the IUPAC organisation. There are cross-divisional activities that, today, appear stronger than the 'traditional' disciplines. For example, the green chemistry network originated in the organic division, there's an interdivisional materials group, and a strong biotechnology group that's emerged in the past five or so years. We mustn't forget that these all have their roots in organic chemistry! Another concern is the low representation of women, and I want to address this, too.

### Do you have any other concerns?

One is the leaky pipeline for women chemists. Appointments and awards absolutely should be made on merit, but more women need to put themselves forward. Yet they can be reluctant to do so. This is why it is important to publicise when women win awards and promotions – much as we may hate self-promotion, it is essential that other women see that they, too, can win.

The American Chemical Society has 'rising star' awards, and I think other chemical societies should think about putting similar schemes in place to recognise and acknowledge younger women chemists. I've been looking closely at the Athena Swan awards in the UK, and I'm starting to wonder if, via IUPAC, we can promote it more widely across the world. I would certainly like to

## eChem@Cam

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

If you would like to swap your paper magazine for an e-version, then please send an email with the subject line 'eChem@Cam' to [jsh49@cam.ac.uk](mailto:jsh49@cam.ac.uk), and we'll start to send you the mag electronically from the next issue. Don't forget to tell us your postal address so we can check that the correct person is being removed from the mailing list for the paper magazine.

get something set up in Australia.

Another important message for women thinking about careers in chemistry is that a lot of mentoring schemes assume they will go into academic careers. We need to broaden the definition of academic success. Yes, I'm a successful researcher, but that's not all I do – I'm also a successful teacher, and am involved in all those external activities.

There's much celebration of the culture of successful 'grantsmanship' and publishing papers – let's also celebrate the role of teaching. It's also about training the next generation of scientists, regardless of whether they work in academia or industry. We need to celebrate diversity in chemistry – and chemistry achievements.

### You've had an interesting career path...

My scientific journey starting all those years ago in Lensfield Road has been very much about opportunity. I had a loose plan that I was going to be a scientist, but it wasn't well defined and I followed my instincts. But every time there was an opportunity I seemed to sense what would work for me and, as it turned out, I made good choices. Academic jobs opened up in Australia about two years after I arrived here, and so I never returned to England. I'd become an established researcher in marine natural products, and while there are beautiful sponges in the Irish Sea, I'd much rather scuba dive off the Barrier Reef!

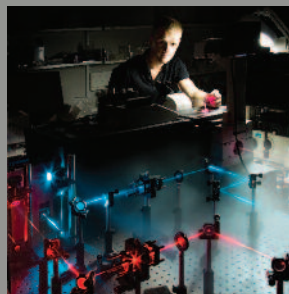
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Chemistry at Cambridge Newsletter

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### Cover



Mathew Horrocks, a PhD student in David Klenerman's group, setting up a microfluidic device that can be used with single-molecule confocal microscopy to look at biological complexes

### Photograph:

Caroline Hancox & Nathan Pitt

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

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## Energy symposium



Photo: John Rogers, RSC

The importance of renewable chemical energy was highlighted this summer when Cambridge hosted a big RSC-organised International Symposium on Advancing the Chemical Sciences, or ISACS12, meeting on the topic. Erwin Reisner was one of two co-chairs, Clare Grey was a member of the scientific committee, and two of Erwin's post-docs, Christine Caputo and Ahu Dumanli, organised workshops before and after the three-day symposium.

More than 350 people from all over the world attended the conference, where topics ranged from photovoltaics, new battery materials and fuel cells, to solar fuels and molecular catalysis. 'Energy is one of the department's priority areas, and it was excellent to have so many great researchers in the field here in Cambridge at the same time,' Erwin says.

Speakers and attendees pictured in the lecture theatre



Photo: Nathan Pitt

Every so often, companies who supply chemicals or lab equipment visit the department and highlight their offerings via a trade stand in the CyberCafé. In November, there was a slightly different presentation – our own photography department was showing off the services they offer to department members. Nathan Pitt, Caroline Hancox and Gaby Bocchetti (who's pictured in action above) took it in turns on the stand, explaining what they do and how they can help members of the department – from photography to poster production. 'Our latest capability is printing posters on thin inkjet cloth,' Nathan says. 'This gives posters that are much more portable than the old laminated ones. They can be folded up (and are ironable!), so poster presenters don't need to worry about leaving the poster tube on a train or plane, being hassled at airport security, or being forced to relinquish a precious poster to the hold of the plane as it's too large for hand luggage!' If you want to know more, give them a shout – they're on photography@ch.cam.ac.uk

## A safe pair of hands

The department has a new safety officer. Martin Maunders is a biochemist by training, with a degree and PhD from Leeds, and joins us from the biotech industry. He started his industrial career as a bench scientist making biochemical reagents, and gradually moved away from the lab into management.

Martin developed an interest in safety issues and gained a NEBOSH occupational health and safety certificate, and ended up in charge of safety at BAT's Cambridge plant biotech site.

He joined us at the beginning of November. 'Moving from industry into academia is an interesting challenge!' he says. 'However, it is good to find that so many people here realise how important safety is, and I'm very appreciative of everyone's patience as I learn the ropes.'



Photo: Caroline Hancox

This year's BP Lecturer was James Tour of Rice University in Houston, TX, US. He spoke about the growing importance and widening sphere of applications for graphene, the single-layer form of carbon

## New Herchel Smith professor elected

Chris Hunter has been elected as Herchel Smith Professor of organic chemistry. Chris started his chemistry career as an undergraduate here in Cambridge, followed by a PhD with Jeremy Sanders.

After a spell at the University of Otago in New Zealand, he was appointed a lecturer at Sheffield, where he has been ever since, being made professor in 1997 and elected FRS in 2008. Chris will be joining us in October 2014.

### Awards & prizes

Jonathan Nitschke has won the 2013 Bob Hay lectureship, awarded by the Royal Society of Chemistry's Macrocycles and Supramolecular Chemistry group. He gave the lecture at the RSC's annual macrocyclic and supramolecular chemistry meeting in Glasgow in December.

And Gonçalo Bernades received an RSC/BMOS young investigator award, enabling him to attend the 15th Brazilian meeting on organic synthesis in São Paulo back in November. He gave a presentation on his work at the meeting – immediately before Nobel Prize winner Bob Grubbs!

## The PWF is back in action!

Earlier this year, the PWF (or personal workstation facility) in G30 got a major make-over, and the room is now looking magnificent.

Not only has it been given a new lick of paint, the five-year-old computers have all been replaced with new machines running Windows 7. The 10 PWF machines in 154 and the 22 in the library were replaced at the same time.

'It was a bit of a rush getting everything ready in time, but we managed to

reopen the room the week before term started,' says computer technician Dave Pratt. 'We also replaced the printers with Konica Minolta multifunction devices, that not only print but can send scanned documents to email.'

And the name has been updated, too – it's now not the PWF but the MCS, or managed cluster system.

Those who remember the old G30 won't recognise it from the way it now looks in the photo!

Spot the difference: unrecognisable from the way it was!



Photo: Nathan Pitt

# Synthesis and catalysis in action



The Pfizer-sponsored Chemical & Biological Synthesis & Catalysis meeting we held in November was a huge success. Six students from different groups gave talks about their science, alongside guest speakers Igor Larrosa from Queen Mary, John Bower from Bristol and Ian Storer, one of the three organising committee members from Pfizer. Organiser

Clockwise from above: poster presenters line up for their flash talks; Daan Frenkel at the prize-giving, Alan Brown of Pfizer gives Yu Heng Wu his best talk prize; and participants voting for the best poster



In November, we held an afternoon synthesis and catalysis symposium, with two guest speakers. Tim Jamison from MIT (right) spoke about continuous flow multistep synthesis, and Kenichiro Itami of Nagoya University (below right) about catalyst-enabling chemistry toward transformative molecules



Photos: Caroline Hancox

Deborah Longbottom also gave a presentation about her research with the O'Reilly group in Warwick.

A poster session attracted 23 posters, with all the presenters also giving a flash talk about their work – one slide, one minute. Only one overran and found the screen went blank! The poster session itself was held in the CyberCafé during the wine-and-nibbles reception, and as everyone had already had a taster of what they were about, presenters were deluged with people wanting to talk about their posters.

Several prizes were on offer. Yu Heng Lu from David Spring's group and Katie Deigan Warner (Abell) won the judges' prizes for best talk and best poster respectively. Symposium participants also voted for the best poster, and this prize went to Elise Cahard (Gaunt).

'About 120 people from the department registered in advance to attend the symposium – and more showed up on the day,' Deborah says. 'The atmosphere was excellent, and there has been lots of very positive informal feedback. We are now planning a similar event for the next academic year.'

Deborah and Matthew Gaunt were ably helped with the departmental organisation by five students and post-docs – Louis Chan (Balasubramanian), Alison Choy (Glen), Dean Holt (Gaunt), Feilin Nie (Spring) and Nadia Shivji (Klenerman). The EPSRC impact acceleration account and the synthesis RIG provided top-up funding for the



Photos: Nathan Pitt

symposium, and logistics would simply not have worked without the tea, coffee and lunch shuffling done by Shirley Allen and Sue Begg, as well as invaluable organisational advice from Julie Lee.

Head of department Daan Frenkel was delighted with how well the day went. 'This symposium was almost too successful: during the day many labs were virtually empty,' he says. 'But it was worth it: the programme was fabulous.'



## Simulation award for Jean-Pierre



Jean-Pierre Hansen has won the Berni J. Alder CECAM prize, which recognises exceptional contributions to the field of microscopic simulation of matter.

Jean-Pierre was among the first to demonstrate the power of computer simulation as a reliable test-bed for simple theories that can be used to understand complicated phenomena.

The award was made jointly to Jean-

Pierre and Herman Berendsen, emeritus professor at the University of Groningen in the Netherlands.

The photo shows Jean-Pierre and Herman flanking Berni Alder, the inventor of molecular dynamics, who made the trip in August at the grand old age of 92 to present them with their award at the Computational Chemistry and Physics conference in Moscow.

## An insight into the workings of government

Michelle Cain, a postdoc in John Pyle's group, has just finished an 18-month part-time NERC policy placement fellowship with the UK Department of the Environment, Food and Rural Affairs, or Defra. She was working with the air quality evidence team, managing a modelling project involving many different universities, consultancies and research centres.

'My work in Cambridge focuses on modelling the composition of the atmosphere, and they were looking for a modeller to work with the team as they had little expertise in that area,' she says. 'It was a fascinating experience finding out how a government department works from the inside, as we normally only see a tiny fragment of what they do in news stories.'

The EU requires member states to report air quality data and where pollutant thresholds are exceeded. Most countries just use direct measurements,

but in the UK and the Netherlands, data from sensors is supplemented by modelling, which can give a more detailed picture of what is happening. During her two days a week in Westminster, Michelle was largely working on a modelling intercomparison exercise, evaluating the strengths and weaknesses of the different models that could be used to complement air quality measurements or to evaluate policy options.

'A monitoring station only gives a picture of one specific point, whereas the levels of pollutant can be significantly different from one side of the road to another thanks to air recirculation effects,' she says. 'Models help to fill in the gaps.'

Michelle says she learnt a lot about how evidence is used within government. 'From the outside, it can seem from news reports that they are ignoring the evidence,' she says. 'But that's not the case. There are many different forms

of evidence that policy makers have to take into account in addition to the science, such as social impacts and costs. For example, the worst air quality is usually in city centres, and one of the worst culprits is the exhaust from diesel engines. Should we ban lorries – or even all cars – from these areas? While it may help air quality, it might not go down well with the voters!'

The two reports she was involved in have just been published, and are available for download on the Defra website (<http://tinyurl.com/q3cmqtu>). And she's now back in the department full time. 'As well as learning a lot more about the health effects of the emissions I model, I was surprised to find out how technically difficult the policy side is,' she says. 'The papers are full of legalese and often harder to read than a scientific paper. It was a real eye-opener to see what they need to know, and work within their constraints.'

Photo: Nathan Pitt



This year's first year chemists all received shiny new labcoats, courtesy of BP. Many thanks to BP for their generosity!

## A change of (scientific) scenery

Alex Archibald, a Herchel Smith research fellow working with John Pyle, has just got back from a five-month sojourn at the Natural Center for Atmospheric Research in Boulder, Colorado. His scientific focus is on modelling the chemistry in the atmosphere and its impact on climate, and he's been spending time in Colorado working with a group who have a different model, trying to assess the importance of the chemistry of factors that affect air quality, such as particulates and ozone, in their model.

'It's been a really interesting and valuable experience,' he says. 'They're working in an area that's at an interface with what I do here. I've benefitted from looking at a new model and a working with different people, and being able to pick their brains about problems we have, and I hope they've gained something from my input, too.'

The NCAR has a fantastic group of climate scientists, but there was an added attraction for Alex in spending time



Taking advantage of the great outdoors...

there – enjoying the great outdoors, Rocky Mountains style. 'It's been a great opportunity to go out hiking and biking and, now that the snow has come, skiing and snowboarding,' he says. 'And the microbreweries around Boulder make some wonderful beer!'

'It's been a phenomenal experience – if you can get the chance to spend a few months somewhere else learning a new skill, increasing your professional network, and exploring somewhere new, you really should take it.'

## Jason's Hall of Fame induction

Jason Chin has been inducted into the European Inventor Hall of Fame at a ceremony in Munich celebrating 40 years of the European Patent Convention.

The Hall of Fame is a travelling exhibition that honours outstanding creativity and innovation among the finalists and winners of the European Inventor Award. Seven innovators and innovation

teams, whose work exemplifies invention's sweeping impact, have been selected for recognition.

Jason was nominated for his work in synthetic biology, and the patented new form of ribosome that works with a more complex genetic code than that found in nature to create novel proteins. Potential applications of this new 'pro-

tein factory' include the development of therapeutic medicines.

He's been busy – in October he gave one of the annual Solvay Public Lectures in Brussels. These lectures are part of a public event that is part of the Solvay Institute's mission to popularise science. In his lecture, Jason spoke about his work on reprogramming the genetic code, enabling new proteins to be made.

Previous lecturers include Jean-Marie Lehn, Harry Kroto and George Whitesides.

# Keeping up with the wavefunctions

The wavefunction is the first object students learn about in quantum mechanics – everything about a system is encoded in this one mystical function. But when chemists are trying to calculate properties of large condensed phase systems, it is normally thrown out straight away in favour of simpler objects as it is so complex.

However, much potentially important detail is lost when it's thrown out. George Booth is looking at ways of retaining the concept of a wavefunction in electronic structure calculations, and its associated accuracy, in his high-accuracy materials modelling experiments.

The wavefunction is a function of all the electrons in the system – in triplicate, because they move in three-dimensional space. In reality, this makes it far too complicated to try to expand and optimise this function using brute force for large systems.

'Physicists will generally throw it out straight away, and build theories around something much simpler like a density,' he says. 'But we know from quantum chemistry on small molecular systems that if we are able to work with the wavefunction directly, we can get incredibly accurate results. If we can find ways of compressing the information stored in the wavefunction and 'unzipping' the important bits when they are needed, then, potentially, we can transfer the accuracy to much larger solid-state systems. This is the aim of my research – to marry ideas across two disciplines, condensed matter physics and quantum chemistry, in order to make progress in the accurate simulation of "strongly correlated" bulk materials.'

However, all the reasons physicists discard the wavefunction remain – it's simply not possible to use the brute force of a supercomputer with anything other than very small and simple systems. The answer lies in making clever approximations. 'We can take out a chunk out of the middle of an extended solid and treat it with accurate wavefunction methods,' he says.

If you remove a part from a quantum system, it would not, in general, contain an integer number of electrons, and wavefunctions are only defined for whole numbers of electrons. This is where ideas from chemistry and physics can be merged to define a quantum-mechanical 'entanglement' from the accurately described portion of the material to the rest of the bulk system. 'Once we have this, we can get around this issue of defining wavefunctions in this portion with non-integer numbers of electrons, and correctly stitch this correlated portion back into the full environment of the material,' he says.



Photo: Caroline Hancox

**Theoreticians make calculations simpler by reducing the number of parameters they use. George Booth wants to keep the most complex – the wavefunction**

An alternative is to coarse-grain the wavefunctions, reducing the number of degrees of freedom needed to describe them. 'Monte Carlo techniques can be used to stochastically sample the wavefunctions, so they never have to be stored in all their glory at the same time,' he says. 'If we time-average these samples over a simulation, we can extract meaningful information.'

## STRANGE MATTER

It would be untrue to claim that all materials need to be modelled to this level of accuracy, but there are many systems where this additional level of detail is absolutely essential. 'It has been hypothesised that a system with a graphene structure could exist in a very exotic "spin liquid" phase, where even at zero temperature the magnetic moments of the electrons remain disordered because of strong quantum fluctuations from the interactions of the electrons,' George says.

'These are strange, non-conventional phases of matter whose collective excitations create particles which do not obey normal quantum statistics. Traditionally, the Pauli exclusion principle ensures that exchanging particles leads to a sign change in the wavefunction. However, if

these strange particles do emerge from the lattice, exchanging them could lead to deviations from the Pauli exclusion principle, and could have far-reaching consequences that could be exploited in quantum computing.'

However, to find out whether or not they do exist requires both a very accurate resolution of all the interactions between the electrons, as well as access to huge system sizes so that the system realistically models the bulk solid – a difficult combination of challenges. So the electrons cannot be ignored, and George's ideas to build new electronic structure theories around the wavefunctions of the system could help provide this extra, vital, detail, and give a greater insight into what's going on compared to alternative approaches which try to avoid this wavefunction explicitly.

Another potential application concerns investigating the process of singlet fission. This could, theoretically, allow solar cells to have efficiencies in excess of 100%, with one photon giving rise to more than one electron worth of potential difference. For each photon absorbed, the energy would be split between two different chromophores in the material, which would separately create charge transfer states, each giving rise to the voltage.

'The large pentacene crystals in the cells are difficult to simulate, and require careful resolution of the electronic interactions,' George says. 'The actual mechanism is still under debate, and the solution will require input from both theorists and experimentalists. Hopefully these tools are mature enough now to begin to make headway, and the computational techniques made to work in conjunction with experiments to shine light on these important problems. The successes of quantum chemistry should no longer be restricted to molecular systems.'

**Born:** South-west London, where he grew up and went to school.

**Education:** Studied physics at Nottingham, coming to Cambridge in 2006 for a PhD with Ali Alavi.

**Career:** He was awarded a JRF at Trinity in 2010, then spent a year at Princeton with Garnet Chan, returning to Cambridge as a temporary lecturer in August.

**Interests:** Watching football (he has a season ticket at Chelsea) and a variety of other sports. He's also a bit of a film buff, and loves live music.

**Did you know?** In his childhood, he acted as tenor José Carreras in reconstructions for a Channel 4 documentary. He also confesses that this isn't the first magazine article he's featured in. 'In the 1990s, I was the subject of a piece in the teenage girls' magazine "Bliss",' he says. 'I'll keep quiet about what the article was about to save myself further embarrassment!'

George Booth  
CV

# The statistics of protein structure



Photo: Nathan Pitt

**Proteins are complex, long molecules whose 3D structure is not obvious from the sequence. Lucy Colwell is applying a technique borrowed from maths to predict how proteins will fold up**

Proteins comprise long chains of amino acids that fold up to form complex tertiary structures. Normally, a protein always folds in the same way, and while these complex folded structures can often be determined using NMR spectroscopy or x-ray crystallography, predicting how they will fold just from the sequence of amino acids is another matter entirely. Lucy Colwell is looking to change this.

She didn't start out in chemistry – a Cambridge maths degree was followed by a PhD in applied maths at Harvard. 'I wanted to apply mathematical thinking to problems in the real world,' she says. 'The amount of data being generated in biology fascinated me. How could information be extracted from the sequences of biological molecules like proteins and DNA?'

Lucy is now using statistical analysis to look at correlations in protein sequences. 'There is a natural variation

in proteins between different people and organisms, yet unless there is a major problem with the sequence, these small changes do not affect the way they fold up,' she says.

## SEQUENCE ALIGNMENT

She is comparing the sequence alignment – how similar the amino acid chains are – for thousands of different versions of the same protein, in a search for pairs of amino acids that change together. 'If you take, say, the amino acids at position 50 in the sequence across all of these versions of the protein, and compare those at position 100, is there a correlation in the way they change between different sequences?' she says.

It became apparent very quickly that a technique borrowed from statistical physics was an extremely powerful way of extracting information from the protein sequence alignments to predict the

3D structure. She has now managed to predict the structure of several large transmembrane proteins, including the adiponectin receptor 1 which mediates antidiabetic metabolic effects and is important for obesity, insulin resistance and Type II diabetes, and had not been solved experimentally.

Some amino acids are completely conserved, while there is a lot of variation in others. For each residue in the sequence, statistical analysis of many protein sequences gives an insight into the mutation pattern of each position. Then, comparisons between correlated changes in pairs of residues can be studied.

## COMPENSATORY MUTATIONS

'The hypothesis is that if one of a pair of close amino acids mutates, the protein might not fold or function properly,' Lucy says. 'But this might be "rescued" by a compensatory mutation at the second site. These two sites could be far apart in the sequence yet close in the 3D structure because of the way it folds up. This correlation of sequence residues allows us to predict which amino acids will be close in the 3D structure.'

Reasonable 3D structures can be predicted from a large set of sequences in this way. 'There are caveats – you need hundreds of sequences, and the performance of our method varies across different proteins,' she says. 'But it does allow us to make predictions for proteins where experimental information is not available, and these predictions may also provide an insight into how the protein functions.'

It remains impossible to take a single protein sequence and predict the folded structure. But by extracting information from evolutionary sequence variation between different proteins, she can gain insights into which variations in amino acid residues are allowed, and which

**Born:** London, where she went to school

**Education:** A Cambridge maths degree was followed by a PhD with Michael Brenner at Harvard.

**Career:** After a further 10 months at Harvard as a postdoc, she was awarded an EPSRC fellowship and spent time at the MRC-LMB, Cambridge applied maths, Harvard and, most recently, the Institute for Advanced Study, Princeton, NJ. She was appointed as a lecturer in chemistry this summer.

**Interests:** Rock climbing and other outdoor pursuits such as skiing and hiking – in her undergraduate days the flatness of the terrain around Cambridge meant regular treks to North Wales! She also enjoys reading and escaping to spend time near the sea.

**Did you know?** At Harvard Lucy helped undergraduates learn to cook, which involved putting out a number of small fires... she hopes Cambridge will be exciting in a very different way!

Lucy Colwell  
CV



aren't, if the structure is to fold correctly. By inferring the constraints on the model that generated the data, they can predict which pairs of amino acids are close in the 3D structure.

### STRUCTURAL INFORMATION

It's increasingly clear that a large amount of information about the properties of proteins can be extracted from the sequences, not just the 3D structure. These include quaternary structures such as oligomer formation or protein-protein interaction partners. 'We're essentially working backwards, a little like a Bayesian

inference problem – we have the data, and we want to be able to infer the parameters for the model that created those data,' she says.

There's still a long way to go. 'It's like any experimental technique – you have to learn how to optimise the conditions,' she explains. 'You can imagine that, in an evolutionary sense, the residues that are important for the active site of the protein or a ligand binding site are more constrained than other residues. We are seeing these constraints in our statistical analysis.'

Lucy's instinctive feeling is that the data problem is going to get bigger with the rapid

increase in the amount of sequence data that is now available. This statistical tool could provide the answer to making sense of these data much more widely.

'It could be applied to genome sequences to give a better insight into the genetic causes of disease,' she says. 'Some diseases, such as sickle cell anaemia, are clearly down to single mutations, but many genetic diseases are more complicated, with many genes and mutations that could contribute. But with sufficient data, it might be possible to pinpoint correlated gene mutations in patients with a disease.'

## Stretching chiral surfaces

Chiral molecules – ones that exist in left-handed (LH) and right-handed (RH) mirror-image forms – are familiar. But surfaces can also be chiral, and chiral surfaces can be created by making a cut at an asymmetric angle to a crystal that is otherwise achiral. This observation has led to a lot of interest in whether chiral molecules selectively adsorb to LH or RH surfaces.

Steve Jenkins, in collaboration with experimentalist Roger Bennett (and former Cambridge chemist Georg Held) at Reading, has been looking at a surface created in this way from a hexagonal close packed rhenium crystal. 'The surface is unusual in that it is, in a way, racemic,' Steve explains. 'If you cut it at one point, it creates a LH surface, but if you then strip a single layer of atoms off, the surface left behind would be RH, and so on.'

This means that on a real-world surface that is not completely flat, there are little terraces differing in height by one atom, and alternating in chirality. 'The work done at Reading involved using low energy electron diffraction to study



the surface, and scanning tunnelling microscopy to look at the surface's overall morphology,' he says. And, sure enough, as expected there are patches of LH and RH surface.

Steve carried out density functional theory calculations that backed up the experimental findings, but in addition he went a step further and calculated the surface stress. 'Any time you take a bulk

material that is not itself under stress, it can be cut to create a surface that will be under stress,' he says. 'This can make it susceptible to reconstruction or otherwise changing in some way, in particular if you deliberately strain the material. As each terrace is chiral, the surface stress pattern on LH surfaces is the mirror image of that at RH surfaces – they don't line up with each other.'

This means that if the crystal is mechanically stretched in an asymmetric direction, one terrace should be favoured over the other. In principle, it should be possible to cause the RH terraces to grow at the expense of the LH terraces, and vice versa. 'This has not yet been done experimentally, but theoretically it should work. One could then imagine depositing racemic molecules onto the racemic surface, and if you were lucky with your choice of molecule, all the LH molecules might adsorb onto the LH terrace, and the RH molecules onto the RH terrace. If the surface were then mechanically stretched and the LH terraces, say, suddenly vanished, all the LH molecules would pop off the surface. This could be a great way of separating them.'

**Phys. Chem. Chem. Phys.**  
2013, **48**, 20773

## Supersaturated protein problems

Diseases such as Alzheimer's, Parkinson's and Huntington's are believed to arise when proteins misfold, aggregate and become toxic. It had been thought that only a handful of misfolded proteins were involved in any given disease, such as amyloid- $\beta$  and tau in Alzheimer's. However, under the right conditions, most proteins can misfold, and these conditions can arise in the cell for many different proteins. But why do some proteins misfold and aggregate in disease states while others do not?

'We wondered whether this widespread aggregation process could be predicted from chemical principles,' says Prajwal Ciryam, a PhD student working with Michele Vendruscolo and Chris Dobson. Proteins have physical chemical properties that predispose them to aggregation, in particular their solubility. If their concentration in a cell exceeds their solubility and they become supersaturated, then aggregation becomes more likely.

'We made predictions about the solubility of proteins, and identified those which have a tendency to become supersaturated,' he says. 'We found that those proteins known to aggregate in Alzheimer's and Parkinson's, and also in the nematode worm *C. elegans* as it ages, were all ones that we predicted could become supersaturated. The classic amyloid proteins were particularly supersaturated.'

Indeed, the most supersaturated proteins from their predictions are very highly enriched in the complex disease pathways for Alzheimer's, Parkinson's and Huntington's – and were very specific to these diseases. But do they have anything to do with the functions or dysfunctions that are seen in the disease? Surprisingly, it appears they might.

'Large portions of these disease pathways, such as mitochondrial dysfunction, are not obviously populated with aggregating proteins. But their involvement in disease can often be

explained simply by asking chemical questions, and it appears that the many diverse pathways can be simplified down to this principle of supersaturation,' Prajwal says.

He hopes this might make discerning the causes of multifactorial diseases a little easier. 'It might not be that a lot of different things are all going wrong at once,' he says. 'It could well be that there's just a few, but these propagate in many ways.'

In future, they hope to be able to understand how this supersaturation process is regulated, and whether the cell itself develops some kind of response to supersaturated proteins when it's under stress. 'We also want to see if we could use information about supersaturation in disease and non-disease states to make long-term predictions about the risk and severity of disease. We may also be able to take some of these computational and bioinformatics predictions, and understand what the best experiments will be to validate our observations, and then expand them to answer broader clinical questions.'

**Cell Reports**, 2013, **5**, 781

## Tuning guest affinity

Supramolecular chemistry has already given a good deal of insight into the way complex natural signalling systems operate. While great strides have been made in creating synthetic receptor mimics, in practice there is a long way to go in tuning affinities in the host molecules to the guests.

One way this might be done is being explored by Will Ramsay, a second year PhD student in Jonathan Nitschke's group. 'Jonathan asked me to create a supramolecular cubic structure based on a "paddle wheel" motif that's fairly common in metal-organic frameworks,' he says. 'We wanted to use the binding sites on the molybdenum atoms on each face of the cube to bind guests. This would give six independent binding sites within the framework.' Most supramolecular structures have just one or two binding sites in one cavity, so only a single guest molecule can be bound. Constructing the host framework in this way allowed him to start looking at complementary tandem binding of guests.

Will looked at a variety of small molecule guests that might bind within the cube, and discovered it's possible to increase the binding affinity of a guest if the size and shape of another guest, already bound within the cavity, is complementary to the added guest. If, however, the two guests sterically hinder the other's binding or electrostatically repel each other, a second binding event would be disfavoured.

'If the host cube were pre-loaded with one guest in solution and a second guest added, would the guests competitively inhibit one another, or would they cooperatively enhance each other's binding affinity?' he says. This is analogous to the way that enzymes regulate binding affinity.

Will's current goal is to try and develop an allosteric system, where a binding event somewhere on the outside of the cube could influence the binding inside it. There are already organic examples of allosteric receptors, but very few metal-organic supramolecular structures are able to do this.

'Ultimately, we would like to be able to work in aqueous solution and develop a more biologically compatible system,' he says. 'One might even imagine that this idea could have potential in drug delivery, a key area of unrealised promise in host-guest systems.'

*Angew. Chem. Intl. Ed.*, 2013, **52**, 1349

## From seed pods to proteins

It's not unusual for materials to become frustrated if something attached to the material inhibits relaxation into the normal ground state. These materials include the protein assemblies in amyloid fibres, and if a large cytochrome protein is attached to a fibre-forming protein, such as SH3, to form a fusion protein, then the amyloid loses its normal twisted shape, instead becoming a spiral ribbon. Intriguingly, changing the conformation of the attached cytochrome after fibre formation allows adjustment of the overall morphology.

A very similar morphological transition happens with the well-known seed pods from Bauhinia flowering plants. Chris Forman, a postdoc in David Wales' group, wondered whether the change in morphology of the amyloid was more to do with the fact that, like the seed pod, amyloid is layered, thus offering an explanation for experiments previously conducted in Paul Barker's group.

'We created a coarse grain computer model with internal degrees of freedom to recreate the morphology of various amyloid fibres, and try to understand how frustration of the amyloid structure could be causing the observed changes in morphology,' he says. 'By changing the internal angles between coarse grain units representing the fibre-forming domain, a locked pair of coarse-grained building blocks can assemble into fibres with many distinct morphologies.'

By using David's basin hopping software and exploring minimal energy arrangements of the locked pair at a variety of internal angles, they found that the bilayers formed in the cytochrome-SH3 fibres may have far more in common with a frustrated bilayer than a standard amyloid fibre.

'People usually think that morphology is a consequence of the details of



the underlying amino-acid sequence, but that's not necessarily true – the frustration of the bilayer may be driving the shape,' he says. 'We have shown that adding external factors to the system, thereby disrupting the normal arrangement, may allow control over the morphology independently of the amino acid sequence.'

Their next step is to take a protein that forms amyloid fibres in its native state, make predictions about its morphology, and work out how to design frustration into the system to tune this morphology. 'We want to work from both ends – design the protein using normal genetic engineering techniques, and also work backwards from a specified target *in silico*,' Chris says.

'Hopefully, we would get the same morphology in both theory and experiment, which would show whether or not we have complete control over its shape. This could be really useful in the future design of materials, for example.'

*J. Phys. Chem. B*, 2013, **117**, 7918

## Quadruplexes in RNA

Shankar Balasubramanian's group has found evidence for the presence of G-quadruplex structures in RNA within the cytoplasm of human cells. The four-stranded G-quadruplex structures are well characterised in isolated DNA, and earlier this year the group showed they exist in the nucleus of human cells, too. However, until now, it was not known whether the analogous four-stranded RNA structures – also well known *in vitro* – existed in cells, too.

A similar approach was taken to the one they used with DNA. A G-quadruplex structure-specific antibody was used to visualise the RNA structures within the cytoplasm of human cells.

They also created a new synthetic molecule, designed to be selective for RNA quadruplexes over DNA quadruplexes. 'Because we can now visualise both the DNA structures in the nucleus and the RNA structures in the cytoplasm and

distinguish between them, we could prove that the molecule specifically trapped RNA in the cytoplasm, without doing anything to the DNA structures in the nucleus,' Shankar says. 'This is an important step towards potential chemical intervention studies.'

However, while they have shown that RNA quadruplexes exist within cells, what they do remains unknown. 'In 2007 we published a paper showing that outside the environment of the cell they could modulate, or even regulate, the translation of RNA into protein,' he says. 'But their function within cells remains unclear.'

Importantly, they have already shown via computational experiments that the motifs within the RNA that would be expected to fold into quadruplexes occur in the interesting regulatory parts of RNA transcripts. 'We hypothesised that if they exist in RNA, they may be important for regulating key processes,' he says. 'Now we've got to first base – we've shown

they do exist – and our next task is to figure out what they are doing, and whether we can manipulate them.'

The computational mapping studies showed that the motifs cluster in numerous cancer-causing genes. 'In the past we've speculated that if you target the DNA, you may be able to find ways of modulating cancer-causing genes,' Shankar says. 'Of course, a lot of these motifs in DNA will also exist in the corresponding RNA if it's transcribed. This gives the opportunity to explore whether targeting these structures in RNA can interfere at the level of RNA function, including being translated into proteins.'

The ERC grant Shankar was awarded earlier this year will enable the group to explore the whole area in much greater depth. 'There are also a lot of non-coding RNA functions to investigate,' he says. 'It will keep us busy for the next decade!'

Nature Chemistry doi: 10.1038/nchem1805

## Electric dreams

While electric cars are gaining in popularity, they remain expensive, and their range is somewhat limited. A Nissan Leaf will cover about 100 miles before the battery goes flat, while a (significantly more expensive) Tesla might make it a couple of hundred miles. The battery is by far the most costly part of the car, and if cheaper batteries with high energy densities were available, then prices would come down, the cars would be able to drive further between charges, and market penetration would surely rise.

The key will be in developing rechargeable batteries with high energy densities. However, for all the promising high-energy density batteries, such as Li-air and Li-S, degradation makes the capacity retention very poor. This is not commercially viable. One focus of the science in Clare Grey's group is to work out the mechanism for this degradation, in the hope that tactics can be applied to minimise it.

'Batteries are very simple, comprising two

electrodes and a separator filled with electrolyte in between them,' explains postdoc Yan-Yan Hu. Degradation mainly happens at the interface between electrodes and electrolytes. It is very difficult to use routine techniques such as x-ray diffraction/absorption or microscopy to study what's going on as the battery degrades as the structure formed is amorphous and complex.

'NMR is good at determining short-range local structures and identifying chemical composition, so it's ideal for investigating of battery degradation and the formation of solid-electrolyte-interphases, or SEI. We're developing a systematic characterisation protocol to identify all the chemical species formed and their relative location, at what stage the electrolyte decomposes, and what it decomposes to.'

Yan-Yan used the protocol to study a model ruthenium oxide-based Li ion battery system. Batteries based on transition metal fluorides and oxides have much higher energy density than commercially available batteries and, surprisingly, their energy capacities are much higher than what is predicted to be theoretically

possible. The reason for this was unclear. By using a combination of multidimensional high-resolution  $^1\text{H}$ ,  $^7\text{Li}/^6\text{Li}$  and  $^{17}\text{O}$  NMR, she's gained an insight into the decomposition process, and identified the pathway by which the additional capacity arises.

'This extra capacity is a very general phenomenon with transition metal oxide and fluoride battery systems,' Yan-Yan says. 'It was discovered more than a decade ago, and people assumed the extra charge was stored at the interface between two chemical phases. Our NMR studies proved that, in fact, the additional capacity arises from the reversible SEI formation.'

This NMR protocol can be applied to study the degradation mechanism and SEI formation in many battery systems. Degradation contributes enormously to the cost of the battery, and being able to study exactly what's going on will have a real impact in the design of cheaper, higher energy density batteries with good capacity retention that should greatly reduce the cost and increase the range of electric cars.

Nature Materials doi: 10.1038/NMAT3784

## Colourful catalysts

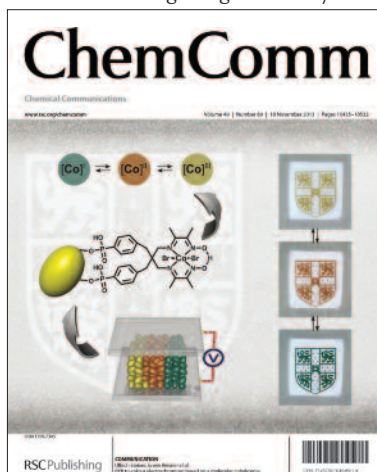
Modern colour displays typically use solid state materials to generate the colour. A serendipitous discovery in Erwin Reisner's lab might provide an alternative means – a molecular chromophore integrated in a nanostructured electrode material that changes colour when different electric potentials are applied to it.

Erwin's work focuses on catalyst systems that mimic photosynthesis, with the aim of developing better ways of creating solar power. 'We have been working on cobalt compounds that are catalysts for the evolution of hydrogen,' he says. 'When Nicoleta Muresan, a postdoc in my group, started immobilising these coordination compounds on nanostructured indium tin oxide electrodes, to our surprise we found it had a very strong electrochromic effect, with dramatic coloration.'

Unusually, it does not just create two colours when the potential is changed, as is fairly common – it can change in a step-wise manner between three different colours, blue, red and yellow, as the oxidation state of cobalt moves from I to II to III. This piqued Erwin's interest, and he got in touch with Ulli Steiner in the Cavendish, who's an expert in building electrochromic devices. His interest was also piqued, and his PhD student Maik Scherer built a prototype electrochromic device using the immobilised cobalt complex.

While Erwin's main research focus remains in the energy field, this observation is too interesting to ignore. 'Very little work has been done on this sort of functional immobilisation chemistry,' he says. And because the single molecule can create all three colours required for electronic displays, one day displays comprising many pixel-sized electrodes with immobilised molecules could be possible.

Chem. Commun., 2013, 49, 10453



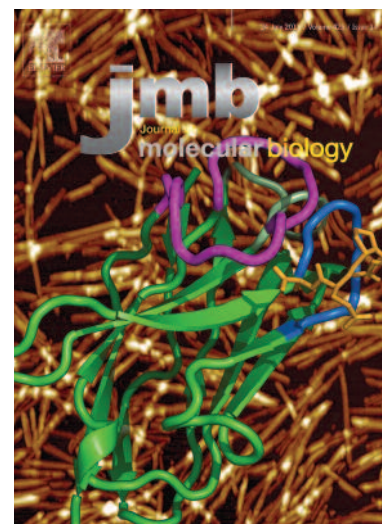
## Probing fibril maturation

The protein  $\alpha$ -synuclein is involved in Parkinson's disease; its pathological misfolding into amyloid fibrils causes the progressive loss of dopaminergic neurons in the substantia nigra of the brain, leading to dementia and, eventually, death. Erwin De Genst, a postdoc in Chris Dobson's group, is looking how nanobodies, which are antibody fragments derived from camels and llamas, can give insights into the way the protein misfolds into its toxic conformation.

Pathological misfolding of  $\alpha$ -synuclein results in the formation of fibrillar structures. However, little is known about how these fibrils change after their formation, a process called fibril maturation. 'We have generated several nanobodies against alpha-synuclein that bind to a well-defined region at the C-terminal end of the protein,' he says. 'These nanobodies are helping us study what happens as the fibrils mature – something that is difficult to follow and quantify using conventional techniques.'

His colleague, PhD student Tim Guillems, has been using isothermal calorimetry and nanobody binding to study this process. By measuring the thermodynamics of the binding of the nanobodies to the fibrils at different maturation stages, structural changes occurring in this process can be detected.

'It's really very difficult to get detailed structural information on these protein species as they are very heterogeneous,' Erwin says. 'Most methods only give average and low resolution structural information, making it extremely hard to detect subtle differences, such as those that occur in this fibril maturation process.' The antibodies bind specifically and with high affinity, thus enabling



these subtle differences to be detected and studied.

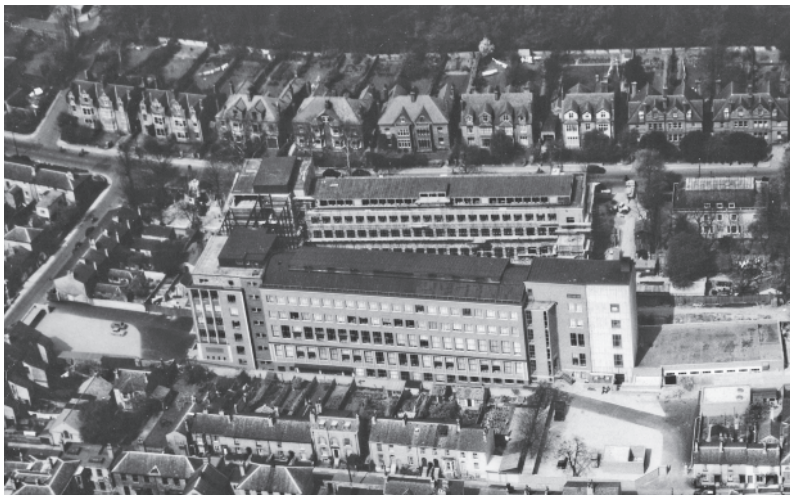
These, and other nanobodies that are being developed, will also allow them to look at different species that appear before the fibrils start to form, such as the toxic  $\alpha$ -synuclein oligomers they are now studying. 'As these single domain antibodies are very small and easy to handle, in contrast to full-length antibodies, they are easy to use in biophysical techniques like this,' he says.

Nanobodies are also emerging as alternative therapeutic molecules to monoclonal antibodies, which constitute a huge market in biopharma today. Nanobodies are much smaller than full-length antibodies, making them much easier to produce. Erwin now hops to develop more of these nanobodies as diagnostic tools and, potentially, therapeutic leads for Parkinson's disease.

J. Mol. Biol., 2013, 14, 2397

# Memories of Lensfield Road

Chemistry's not what it used to be... JA Green recalls the explosive days in Lensfield Road in the late 1950s



The Lensfield Road building in 1957 – its footprint has changed somewhat since then!

I was one of the 56'ers who started my career in Pembroke Street and moved to Lensfield Road in the summer of 1957. Apart from the gas lamps, another disturbing feature of Pembroke Street was the high ceilings in the labs. These were covered with a generous layer of soot from decades of exposure to Bunsen burners. Over the soot was a tangled mass of spiders' webs. It was not unusual to find one of its inhabitants crawling down the back of your neck – much to the consternation of the (very few) girl students (and most of the men).

My first visit to Lensfield Road was in the Long Vac 'Course' of 1957. 'Scientists' were required (voluntarily) to give up their summer holiday and do six weeks of lab work to catch up with the overcrowded syllabus. The staff went to great lengths to make it interesting. One exercise was to make a nitrosamine of some sort. Purple crystals – orange solution – a nasty habit of suddenly becoming a sticky black mess – you know the one I mean. It was my first experience of explosions in Lensfield Road, but more of that later.

We were all assigned places at the shiny new benches. The lab had clearly been used for the practical exams at the end of the spring term and the names of the candidates were still stuck on labels on the shelves over the bench. Mine read 'White'. Almost as soon as we settled in the door at the end of the lab swung open and in surged Professor Todd and a small entourage, including a bemused looking chap in a brown suit. Terrifyingly they made straight for me. 'Now, Mr White,' said Todd, sternly. 'Tell the Minister what you think of the new lab.'

'I'm not White, I'm Green,' I said,

overwhelmed by panic. Todd lowered his eyebrows 'Laddie, the Minister doesn't care what colour you are, tell him if you like the new lab. I think I managed to mutter something complimentary, but it did not adequately express the real pleasure of moving to such a fine place.

I mentioned explosions earlier and my recollection is that in the early days at Lensfield Road we (in Phys Chem) managed quite a few. I think the most spectacular was the exploding shock tube. The tube was located on the second floor in a lab above Professor Norrish's office. Fifteen feet or so long, it was a Pyrex tube about three inches in diameter, with half-inch thick walls. The 'driver' was a steel cylinder separated from the tube by a thin metal diaphragm. The driver was charged to some awfully high pressure with hydrogen, and then the diaphragm was ruptured by poking it with a steel pin. Nice shock wave zips down tube.

Lateish one evening on a Sunday, I think, the chap in charge decided to do the definitive experiment at an unusually high pressure. The tube disintegrated along its whole length and this shock wave tore out the windows along the length of the room above Lensfield Road. Homegoing churchgoers were showered with glass.

In the lab, the Pyrex tube itself had been reduced to the consistency of sand. This had blasted everything that it hit. Varnish had been stripped from tables and paint from gas cylinders. And the perpetrator? It was said that the explosion bypassed him completely and he had escaped unscathed. We never got the chance to ask him. He was rumoured to

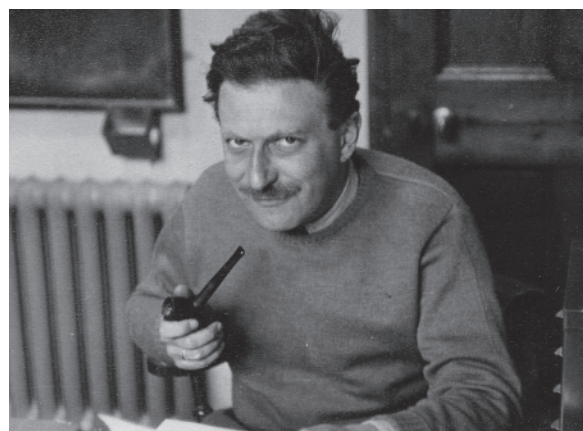
have been on the first train out of Cambridge the following morning.

Some nice explosions were caused by my lab-mate Bob Tufnell. He shared a lab with Mike Osborne and me. It was on the second floor opposite the glass-blowers' workshop inhabited by Fred Webber and Cyril Smith. Bob and Mike worked in Norrish's group on flash photolysis, and I was in Morris Sugden's flame chemistry group. It was necessary for Bob to make quantities of ozone for his experiments. He would painstakingly set up his generator and, very slowly and very carefully, condense the ozone into a collecting tube. If things went well, he would eventually ask us to take cover and very, very delicately lower the vacuum flask to reveal half an inch of solid ozone in his tube. The colour of solid ozone is unforgettable. An unworldly misty purple like looking into a summer sunset.

When things did not go well (not very often, fortunately) there would be a heart-stopping bang and a vacuum flask case blown out into a near perfect sphere would roll lazily off the bench and across the floor. Bob's face, well protected as always, would appear from behind a collapsing wall of shattered apparatus. 'B\*\*\*\*r it, I'll have to start again!'

No reminiscence of Lensfield Road could be complete without reference to the Spread Eagle. Several members of Morris Sugden's group including, quite often, Morris himself, would adjourn there each evening to nurse half a pint of bitter and play bar billiards. Kingsley Amis, who also liked a half-pint and was fascinated by all things 'scientific', occasionally came in. He claimed that he intended to write science fiction and was collecting material. He was greatly impressed by the new lab, but always turned down our invitations to come and look round. He said he didn't want to see scientists blowing themselves up!

Morris Sugden, whose flame chemistry group didn't supply all the explosions!



## A plea to readers...

Once more, the Chem@Cam reminiscences cupboard is bare. Do you have memories or photos of your time in Cambridge Chemistry? We'd love to hear from you!

## Poetry corner



Leanne Moden lives an interesting double life – secretary to Shankar Balasubramanian by day, performance poet by night. ‘I’ve been writing poetry for the past eight years, and performing and doing workshops since 2010,’ she says. And in March of this year, she was made Fenland Poet Laureate for 2013.

Each year, the Atelier East organisation runs a poetry competition, in partnership with Arts Development in East Cambridgeshire (ADeC). Entrants have to write a poem about, related to or inspired by the fens, and the winner is crowned Fenland Poet Laureate, to represent poetry in the area for the year. This year, Leanne won – and is now coming to the end of her term as Laureate.

‘I’ve had a great year,’ she says. ‘I’ve been working on various local poetry projects. For example, we’ve just started monthly open mic nights in Ely and Wisbech so poets can meet like-minded individuals and read their work. I’ve also written poems for local museums, such

as one about fen skating in Wisbech, and one in Chatteris museum about its 19th century fen cottage display. I’m also hoping to write on about the workhouse display in Whittlesea museum.’ She’s also been running poetry workshops with community groups, from schoolchildren to the elderly.

‘I will be sad to relinquish the title, but it will be great to let someone else have the opportunity to have all the fantastic experiences I’ve had this year,’ she says. The hunt for the next Laureate is now on. The competition is open to anyone who lives, studies or works in the fens – so if you write poetry, why not enter and see if we can keep the title in the department? You can find out more at [www.adec.org.uk](http://www.adec.org.uk).

This poem was written for the Flock Together community arts project at the Welney Wildfowl and Wetlands Trust. It references ancient European mythology surrounding swans.

### Mythology

I am the Child of Lir – Apollo’s light –  
A tireless traveller, gliding through the night.

I am St Hugh’s lieutenant, Lincoln-born.  
My duffel coat of feathers keeps me warm.

Heraldic pilgrim; knight from days of old.  
I am sweet Leda’s lover, bathed in gold.

I am no ugly ducking. Sleek and keen:  
My loyalty is always to the Queen.

I am the maiden drinking from the well.  
I am the secret lost. I will not tell.

Blank pages here, unwritten on my wing.  
I will stay Mute, until it’s time to sing.

## A fishy tale...



Alan Battersby sent along this photo of him showing off a rather fine catch. He says... ‘David Grayson, a young Irish chemist, joined my group in 1971 for postdoctoral experience. He became a professor at Trinity College Dublin and, later, head of school. He’s also a skilled

and experienced fly fisherman. So over the past 20 years, he and I have regularly fished the Irish loughs and rivers.

‘One lough, Lough Sheelin, is world-renowned for the size and power of its wild brown trout, but it is a difficult lough, and we’d spent several days there over the years failing to catch anything. However, in October I boated the superb 4lb brown trout shown in the photo, which also gives a feeling for the wildness of the lough and of the weather!

‘For the fly fishermen among readers, it took a Black Chenille. I’d tied this myself from feathers and chenille on the fly-tying table that was my retirement present from the department in 1992. It had been constructed by Harry Naylor and David Coleman, carpenters on the assistant staff at that time (who will be fondly remembered by many readers) using wood from the lovely old teak tops of the original benches that had been stripped off when a lot of the benches were modernised.’

## A trio of farewells



Photo: Gaby Bocchetti

Safety officer Mags Glendenning (above) left the department in August after nine years here in chemistry. She hasn’t left us completely, though – she’s now got a new role as the university’s fire safety compliance officer, so there’s a good chance she’ll be back in the department from time to time checking up on us!



Photo: Caroline Hancox

Teaching lab technician Pat Chapman (above) retired in July after more than 20 years in the department. She celebrated in style, with afternoon tea and cake!

Also leaving us recently was Tina Jost (below), who was secretary to Clare Grey and David Klenerman. Tina’s a keen artist, and is now concentrating on her painting.



Photo: Gaby Bocchetti

# Party in the garden

Nathan Pitt took his camera to the assistant staff summer garden party, held in Peterhouse College in July. For once, the weather was kind, and they didn't have to decamp indoors to avoid the rain!



Clockwise from above right: Nic Davies and Ryan Bentley with Sophie Jackson and her rather bouncy dog Lulu; Mike Todd-Jones and Gaby Bocchetti; Richard Preston and Dan Ayling; David Plumb and John Offley; Matthew Brooker, Bill Jones and Chris Chalk; John Offley, Pat Chapman, Ray Freshwater and Rod Jones; and a fine spread was laid out in the sunshine!



## Last issue's solutions

### Killer ChemDoku

David Thompson's chemical take on the killer version of chemdoku garnered much praise from readers, many of whom said how satisfying it was to solve. And we had a fair few entries.

Correct ones came from Diana Sandford, Diana Isherwood, Paul (who failed to include his surname, but a combination of his email address and Chem@Cam's psychic skills suggests it might be Littlewood), Richard Brown, Bill Collier (who says that, as usual, his coffee mug bearing a periodic table was invaluable), John Wilkins, Godfrey Chinchin (who says he was prodded to crack the puzzles as soon as the magazine arrived in response to my comment about not having so many entries as usual last time, and hoped this didn't result in catastrophic errors – fear not, Godfrey, it didn't!), Tim O'Donoghue, Alison Griffin (who says the puzzles whiled away an hour of a rainy Sunday afternoon), Richard Butler, Jimmy Chung, R.E. Moss, Steve Sunderland, Morgan Morgan, Donald Stedman, Tom Banfield (who describes the puzzle as elegant – and that he hopes David Thompson will be pleased that a fellow Old Novocastrian solved it – they both attended the Royal Grammar School in Newcastle!), Patrick Barrie, John Billingsley, David Wilson, Audrey

Herbert, Noel Waite (who accompanied his first-ever Puzzle Corner entry with a note, saying he spent his career as a chemistry teacher until his retirement in 1996, but keeps in touch with chemistry and very much appreciates receiving Chem@Cam) and Kevin Harrison.

As, for once, Chem@Cam is putting the pages together in a small corner of the department, not her usual abode these days of the 'other' Cambridge 3000 miles away, she's separated from the normal winner-picking skills of her feline office assistant. So – tragedy! – she's been forced to resort to old-fashioned random picking out of a hat (OK, cardboard box, as her rather lovely hat isn't big enough). And the winner is... drumroll... Patrick Barrie. The prize will be winging its way over the road to you in Chem Eng.

### All but one

Also attracting many entries and much praise was David Wilson's elementary puzzle.

Correct entries came in from Diana Isherwood, Tom Sullivan (a 13-year-old from Cornwall), John Wilkins (who adds that this was the ideal puzzle for the meticulous, and he admires the setter's dedication!), Paul (again, I assume, Littlewood, who says it's an excellent way to revise the periodic table), Richard Brown, Godfrey Chinchin, Alison Griffin,

Richard Butler, Jimmy Chung, R.E. Moss, Steve Sunderland, Kim Whittaker, Pete Walker (who says he's finally managed to complete one of our quizzes, and therefore it must be a particularly good one – or maybe a particularly easy one!), Patrick Barrie, Julian Langston and Audrey Herbert.

And the first out of the box-shaped hat this time was the entry from Tom Sullivan. Congratulations!

If anyone was bamboozled by the puzzle, here's the answers...

Noble gases: 2He; 10Ne + 18Ar + 36Kr + 54Xe + 86Rn = 204

Elements whose names have five or fewer letters: 18Ar; 5B + 10Ne + 26Fe + 30Zn + 50Sn + 54Xe + 79Au + 82Pb + 86Rn = 422

Elements whose symbol is a single letter: 92U; 1H + 5B + 6C + 7N + 8O + 9F + 15P + 16S + 19K + 23V + 39Y + 53I + 74W = 275

Elements whose names begin with 'T': 65Tb; 22Ti + 43Tc + 50Sn + 52Te + 69Tm + 73Ta + 74W + 81Tl + 90Th = 554

Elements whose symbol does not begin with the same letter as its name: 47Ag; 11Na + 19K + 26Fe + 50Sn + 51Sb + 74W + 79Au + 80Hg + 82Pb = 472

Transition elements Sc–Zn inclusive: 23V; 21Sc + 22Ti + 24Cr + 25Mn + 26Fe + 27Co + 28Ni + 29Cu + 30Zn = 232.

## This issue's puzzles

### An abundance of elements

Buoyed by the success of his last puzzle, David Wilson sends along this little teaser which should get the brain cells working. He says...

Mathematicians have devised the idea of perfect numbers, that is, numbers which also happen to be the sum of their factors such as  $28 = 14 + 7 + 4 + 2 + 1$ . If the sum of factors is greater than the original number, then that number is said to be abundant and, conversely, if the sum is lower, then it is deficient. It is high time that this principle was extended to chemistry!

Define the atomic value (AV) of an element as the product of the positions of the letters in the alphabet that make up its symbol, and its abundance as the difference of that product from the atomic number.

Thus, as 'M' is the 13th letter of the alphabet and 'g' the 7th, the AV of Mg is  $91$  and its abundance is  $91 - 12 = 79$ . Similarly, Rb has an AV of  $18 \times 2 = 36$  and a deficiency of  $36 - 37 = -1$ .

Elements with single letter symbols obviously have a 'second letter' value of zero, and the AV of such elements is thus zero. It follows that all these elements have a deficiency equal to their atomic number e.g. F, AV =  $6 \times 0 = 0$ ; deficiency =  $0 - 9 = -9$ .

The molecular value (MV) of compounds is found by adding the abundances/deficiencies for the constituent elements, weighted for the number of

atoms in the formula. Thus the MV for  $\text{CaCl}_2$  is  $-17 + 2 \times 19 = 21$ .

Readers are invited to find (a) the only perfect element, and (b) the compounds with the greatest positive and negative MV.

Only compounds described in the chemical literature are allowed (no technetium astatide!); no polymers or carbon chains (too easy!) and no transuranic elements. A quick search revealed examples of MVs of  $+533$  and  $-413$ , but I'm sure readers of Chem@Cam can do better.

### Who's who?

This rather shorter puzzle was sent in by Tom Banfield. 'It has no chemical content whatsoever, but at least it's local,' he says.

One day Davina, from Churchill, parks next to three other members of the department in Lensfield Road. They all study different areas of chemistry, are fellows of different colleges and drive differently coloured cars:

Alan drives the red car.  
The biotechnologist (who is not Alan) is a fellow of Jesus.

The fellow of Pembroke owns the black car.

The silver car is driven by the quantum chemist.

Caroline works on catalysts.

Brian owns the white car.

What colour car does the fellow of King's drive, and what is the name of the protein chemist?

### ChemDoku Plus

And finally... another slightly modified take on the glorious ChemDoku (you saw it here first – accept no imitations!), this time from Keith Parsons.

The rules are the same as for ChemDoku, with the additional rule that no element is repeated along either of the two main diagonals. In this puzzle, you'll notice that only eight elements are already mentioned in the grid – but the puzzle can still be solved. Which is the missing element, and why?

Don't worry if you have no idea – we'll accept otherwise correct answers, as long as you come up with some imaginative rationalisation for your element!!

Email entries to [jsh49@cam.ac.uk](mailto:jsh49@cam.ac.uk) or send them by snail mail to Chem@Cam at the address on p3 Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW

O		Sc	Li	Ac			
							B
Ac						Sc	
He	Cs			Se			
	B			Cs			Se
Sc				O			
Li		Ac					
B							Li
							He



Maybe this is one wavefunction we should throw away?



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

Printed by Callimedia, Colchester