UNIVERSITY OF CAMBRIDGE

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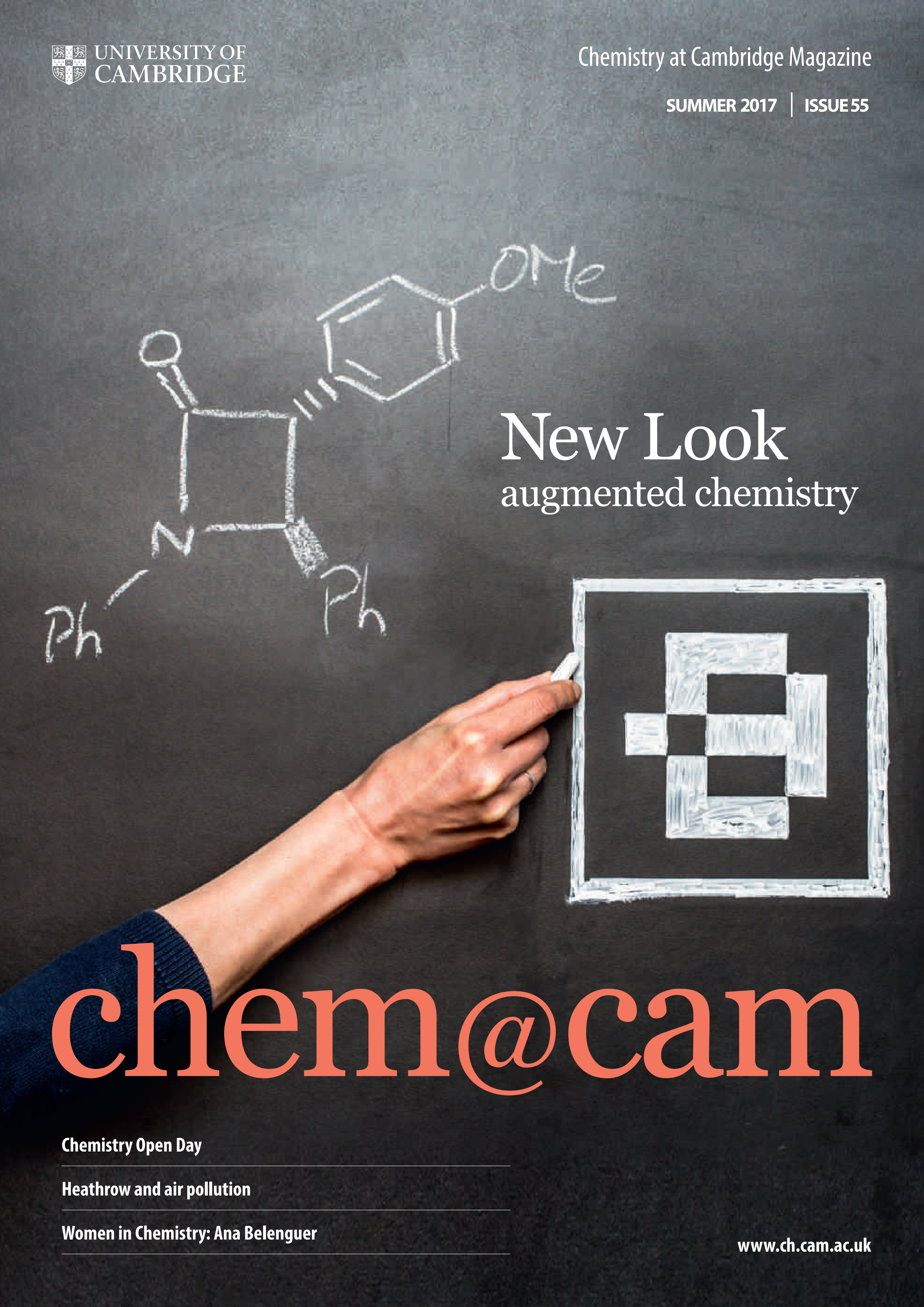


# New Look
## augmented chemistry

# chem@cam

- Chemistry Open Day
- Heathrow and air pollution
- Women in Chemistry: Ana Belenguer

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## WOMEN IN CHEMISTRY



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# Welcome

**The early months of the year are usually extremely busy and this year has been no exception. In March the department pulls together in a great communal effort to support the Cambridge Science Festival. We host the Salters' Festival, promoting chemistry for school children from Year 8 and 9. About 60 children from many schools have the opportunity to spend a day in the department taking part in serious (and fun!) practical chemistry activities. In parallel, we run our enormously successful Chemistry Open Day.**

More than two thousand people, young and old, come through our doors. It's a great opportunity to give people the chance to see some of the amazing work we do here. For many of the young visitors it is their first experience of science and it's wonderful to see the excitement on their faces. I'd like to thank James Keeler, Emma Powney and all the volunteers who prepare and manage the many fascinating demos and workshops that we put on for the public. As ever, Peter Wothers' explosive lecture was one of the highlights, among many.

The Chemistry of Health building is on track for completion in early 2018, further supported by a recent donation of £5 million from R. Derek Finlay towards the cost of the building and to fund research into neurodegenerative diseases. Derek's wife Una suffered from Alzheimer's disease and died in 2016 (page 7). We are enormously grateful for his wonderfully generous donation.

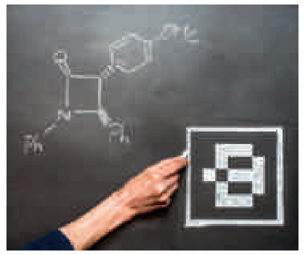
I'm pleased to announce Sir John Sulston as the 2nd recipient of the Department of Chemistry Alumni Medal. The medal recognises services to the community that have brought honour to the University of Cambridge Department of Chemistry. Sir John is a former member of the department and Nobel Laureate. He was a founding director of the Wellcome Trust Sanger Institute and a major influence in the development of gene mapping and DNA sequencing techniques. He is an advocate for open access to genetic information and describes the idea of patenting DNA as immoral and damaging to science. The Medal will be presented at an event mid October 2017.

In a novel initiative of the School of Physical Sciences, nine new interdisciplinary lectureships, the positions to be held jointly in two departments, have recently been created. Chemistry is pleased that three of these lectureships will be associated with us. The lecturers, Drs Hugo Bronstein (Functional Materials, joint with Physics), Robert Jack (Soft Matter, joint with the Department of Applied Mathematics and Theoretical Physics), and Anja Schmidt (Climate Modelling, joint with Geography) will all start in the autumn. I am very excited to see how these appointments develop and enrich our already very diverse research areas. We'll feature their research in future editions of Chem@Cam.

Finally, I hope you enjoy the mix of research items included in this issue (pages 16 – 25). We have articles from the Grey, Lee, Klenerman, Jones, Reisner, Bender and Ley Groups. Plus contributions from emeritus staff Anthony Stone and Sir John Meurig Thomas.

John Pyle
**Head of Department**

On the cover...



Trans-beta-lactam molecule and its corresponding hand-drawn 2D marker (see New Look: augmented chemistry, page 16). **Back cover:** QR code and 2D marker for trans-beta-lactam.

Department of Chemistry
University of Cambridge
Lensfield Road
Cambridge CB2 1EW

T 01223 761479
E news@ch.cam.ac.uk
W www.ch.cam.ac.uk
@ChemCambridge



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CONTRIBUTORS

**Carmen Pryce**
Editor

**Diane Harris**
Contributing editor

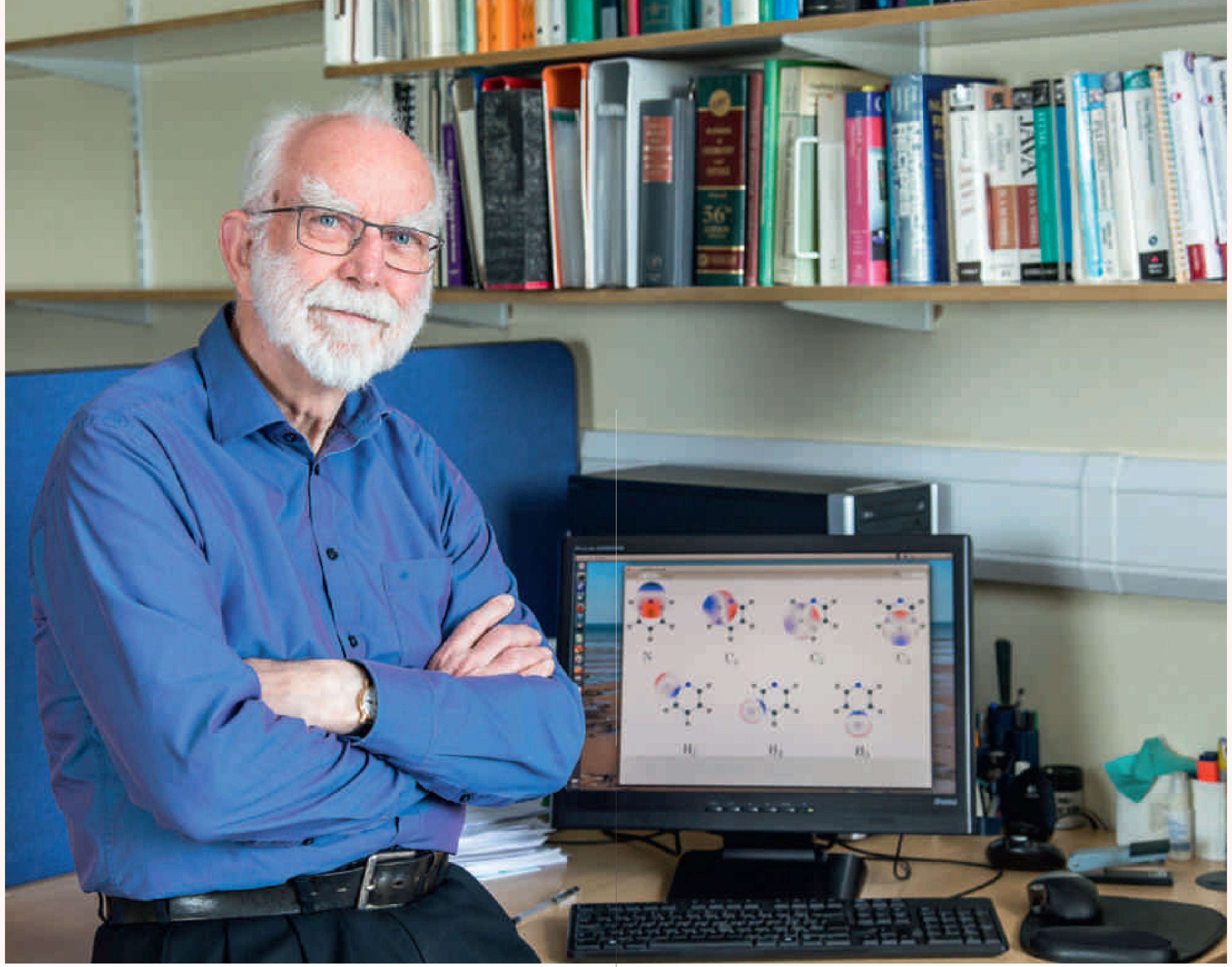
**Nathan Pitt**
Head of Photography and Reprographics

**Gabriella Bocchetti**
Photographer

**Contributing reporters:**
Mike Gaultois, Kent Griffith

Q&A

# Anthony Stone



**Anthony Stone was Professor of Theoretical Chemistry in the department until 2006. And although officially retired you can still find him, in the emeritus staff office, most days of the week. In his recent publication, Anthony argues that the long standing debate around hydrogen bonds is now settled (page 25). Here, Anthony completes the Chem@Cam Q&A.**

**What is your earliest memory?**
The only thing I can really bring to mind is seeing the night sky. I grew up during World War II and in blackouts it was very dark at night, so I got a wonderful view of the stars.

**What makes you happy?**
Being at home with my wife, dancing with my friends.

**Which dead chemist do you most admire?**
Michael Faraday.

**What is the trait you deplore most in chemists?**
People taking credit for their students' work.

**What is the trait you deplore most in yourself?**
Paying too much attention to detail.

**What or who is the greatest love of your life?**
My wife, Sybil. We married in 1967, she was a GP.

**Who would play you in the film of your life?**
Never thought about it. *Bill Nighy?* **- ED**

**What is the worst job you've done?**
A holiday job washing cars.

**What has been your biggest disappointment?**
That the grandchildren are all boys. But you can't say that?

**What was your biggest discovery?**
Making a minor discovery that opened up a new area of research in intermolecular forces. In 1981 I worked out a simple and very efficient method of calculating the electrostatic potential around a molecule, which I called distributed multipole analysis. It allowed us for the first time to describe the electrostatic part of the interaction between molecules simply but accurately. This was important fundamental science. We're dealing with the forces that make molecules stick together and it's important to understand because it has implications for the way molecules behave. If you don't understand how water molecules stick together you can't describe water. If you can't describe how drug molecules attach to proteins, you can't explain how drugs work. So, this really very simple discovery gave an entry into one aspect of intermolecular forces, and led to further research, calculating the other components of intermolecular interactions.

This work was carried out over a number of years in collaboration with Alston Misquitta, now at Queen Mary University of London.

**Reference:** Alston J. Misquitta and Anthony J. Stone: *Ab initio atom–atom potentials using CamCASP: Theory and application to many-body models for the pyridine dimer.* Journal of Chemical Theory and Computation, 2016. DOI: 10.1021/acs.jctc.5b01241

**Speaking of collaborations, what is your reaction to your former PhD and postdoc Sally Price (now Professor of Physical Chemistry at University College London) becoming FRS?**
I'm delighted for her. It's excellent. Of course, she extended the description of the electrostatic interactions between molecules by developing an anisotropic atom-atom description of the repulsive forces, initially to explain the unexpected crystal structure of chlorine ($Cl_2$). And then she has applied it very effectively to the study and prediction of molecular crystal structures, with important applications in pharmacology and molecular materials.

**What inspires you?**
I just have a continuing curiosity and desire to understand.

**What is your blood type?**
A negative – my wife was relieved because she's negative too.

**What type of music do you listen to?**
Classical and country dance music.

**Is there something you constantly lose at home or elsewhere?**
No, my wife is the one who loses things. I'm the one who finds them.

**Have you been pulled over by the police?**
Yes, in the states for crossing the no overtaking double lines. I was driving behind a lorry for a long time and I got a chance to overtake but I just clipped the line. I thought it was quite unfair actually.

# John & Shankar New Year Honours

Professors Shankar Balasubramanian (above) and John Pyle were named in the Queen's New Year Honours List, in recognition of their contributions to society. Shankar has been given a knighthood for services to science and medicine. John has been appointed CBE, for services to atmospheric chemistry and environmental science.

# New electron microscope to streamline research

The department has secured a grant of £1.9 million from the EPSRC to purchase a new transmission electron microscope (TEM).

The EPSRC scheme, for the support of multi-user equipment, offered up to £2 million for instrumentation that appeals to a wide range of users. A TEM was chosen because it will be useful not only in the Department of Chemistry but also to groups from a lot of different departments with varying research interests, and the department's existing transmission electron microscope is approaching the end of its life.

Dr Andrew Wheatley, who headed the department's application said: "We could have bid for an array of items adding up to £2 million but we urgently needed the microscope. We also had support from other departments, including Materials, Chemical Engineering, Biochemistry, the Sainsbury Laboratory and Architecture."

The new instrument will help prevent research bottlenecks. Andrew said: "People often find they can't get rapid access to machines like the one we're going to buy. And that's a problem. Our current TEM is approaching 20-years-old and wasn't designed for the materials portfolio that the department has now. There are high-end microscopes available in the University, which are good for the very detailed analysis of samples but they're in great demand, so only a small number of really good samples are looked at in this way."

On the new TEM, researchers will be able to take a quick look at a lot of samples to determine which are the best options for further study. This will allow people to streamline their research. Andrew added: "We also hope it will be available to people outside the University, in industry as well as other educational establishments. "The microscope is expected to be commissioned by mid 2018 and will be located at Lensfield Road where its running will be overseen by in-house microscopist, Dr. Heather Greer (right).

Professor Sir John Meurig Thomas, who first brought electron microscopes to the department in 1978, said: "I'm delighted to hear that a new microscope is on its way. It is now an indispensable feature of any chemistry department. One cannot study nanoscience without it (see page 23). The power of electron microscopy is essential, especially in the study of catalysts." Sir John went on to say: "I'm also thrilled that Heather is going to be in charge of the TEM; not least because she was supervised in her PhD by my former PhD student Wuzong Zhou, now Prof of Chemistry at St Andrews. So in a sense, Heather is my academic granddaughter."

# New Mass Spectrometer

On the subject of new equipment, a year ago the department purchased a new mass spectrometer, VION, manufactured by Waters. The equipment has now been commissioned and is fully operational. Dijana Matak-Vinkovic (above), senior technician responsible for Mass Spectrometry said: "This new and unique instrument is excellent for measuring accurate masses of various compounds and peptides. It's also able to routinely measure collision cross sections of analysed ions, which gives information about the size of the molecule." Researchers interested in learning how to use the machine can now access training by contacting Dijana.

# Philanthropic support buoys CMD research

Philanthropic donations and seed funding will underpin the next stage of the Chemistry of Health building (CoH), due to open in spring 2018.

Mr R. Derek Finlay has donated £5 million to fund the completion of the department's new Chemistry of Health building, and to support new research into neurodegenerative diseases in the Centre for Misfolding Diseases (CMD), which will be housed in the new building. The CMD's primary focus is to understand the molecular origins of diseases associated with the misfolding and aggregation of proteins, including Parkinson's, Alzheimer's, type II diabetes and amyotrophic lateral sclerosis (ALS), all of which have huge personal and social costs.

Mr Finlay heard Professor Chris Dobson, CMD co-director talk about the research centre at a University event. He was moved to make the gift because his wife, Una Finlay, suffered from Alzheimer's and died of the disease in 2016. He said, "It is my hope that the new Chemistry of Health Building will enable breakthroughs to be made in our understanding of neurodegenerative diseases, bringing us closer to the development of new treatments. My gift to support Cambridge's pioneering work in this area is in memory of my dear late wife, Una."

Professor Dobson said: "We are enormously grateful for this generous benefaction from Derek, and honoured that our laboratories within the building will be named after his late wife Una. Disorders such as Alzheimer's and Parkinson's disease are becoming frighteningly common in the modern world. The Chemistry of Health building will enable us to make a giant step forward in translating recent breakthroughs made in Cambridge into future treatments to combat these rapidly proliferating and truly devastating conditions."

The new building will also house the Chemistry of Health Incubator and the Molecular Production and Characterisation Centre (MPACC).

Nidus Laboratories Limited has agreed to invest £1 million annually in the Incubator and MPACC. The Incubator will nurture spin-out companies from inception through early growth by providing flexible space for adapting basic research into practical applications. MPACC will provide researchers across the department with a wide array of highly specialised instrumentation and will link directly to the department's existing NMR spectroscopy, mass spectrometry, x-ray diffraction and microanalytic services.

**R. Derek Finlay at St John's College**
**© chrisloades.webs.com**

# Jane Clarke becomes 1st female president of Wolfson College

Lucy Cavendish Honorary Fellow, Professor Jane Clarke FRS (above) is the sixth President of Wolfson College and the first female president of the college. She starts her tenure in October 2017. Jane succeeds Professor Sir Richard Evans FBA. Her appointment brings the number of female College Presidents at the University of Cambridge up to 11 out of 31.

Jane is Professor of Molecular Biophysics and Senior Wellcome Trust Research Fellow in the Department of Chemistry. She began her career in science as a teacher in a comprehensive school. Later she moved, with her family, to the USA where she took a master's degree that kick-started her new career in research.

We celebrated Professor Clarke's appointment as Honorary Fellow at Lucy Cavendish College in March 2016, when she gave a lecture as part of the Cambridge Science Festival. She spoke about her work in biophysical and structural studies of protein folding. She also discussed the obstacles she encountered and why she is passionate about ensuring girls and young women have every opportunity to pursue a career in science.

President of Lucy Cavendish College, Jackie Ashley said: "We are thrilled to hear news of this well-deserved appointment, and I look forward to working closely with Professor Clarke in the future."

# Andrew Holmes awarded Companion of the Order of Australia

Andrew (above) was the Director of the Melville Laboratory and brought it into the department from the New Museums site in 2003. His academic career in the department extended over 30 years; he led an incredibly productive group in organic and polymer synthesis. He was involved in setting up Cambridge Display Technology, with Richard Friend in Physics and at one point was one of the most highly cited chemists in the world. He overlapped with many of our current academics including Steve Ley and worked closely with Ian Paterson. A fellow of Clare College he returned to Australia in 2004 on a prestigious Federation Fellowship. Currently he is President of the Australian Academy of Science. The Companion of the Order of Australia is the highest civilian honour granted to only a handful of people every year.

# GYSS 2017

*It's all about the young researchers reports Grey Group member, Dr Michael Gaultois, one of five Cambridge researchers selected to attend the Global Young Scientists Summit (GYSS).*

The Singapore National Research Foundation GYSS is based on the Lindau Nobel Laureate Meetings model - put a few hundred engaged young minds together with great older minds and great things happen. But a deliberate emphasis is placed on the young scientists, rather than on the established scientific giants as explicitly mentioned by the closing speaker, Dr. Jürgen Kluge, Chair of the Lindau Nobel Laureate Meetings Foundation Board.

Researchers from fields across mathematics, sociology, health sciences, chemistry, physics, geology, and computer science provided a rich diversity of experience and knowledge from which to learn in discussions. Outside the planned conference, the GYSS programme allowed lots of free time. "Singapore is incredibly easy to get around and there's so much to see, an ideal environment for a bunch of young people to explore together and begin to form new relationships," says Mike.

The conference programme included a series of field trips designed to showcase Singapore's commitment to research and development as well as its impressive industrial and academic facilities. These included A*STAR, a government-funded business incubator space, CREATE, a research campus and innovation hub that hosts many research centres (such as the Cambridge Centre for Advanced Research and Education), and the Tuaspring desalination plant, among others.

The GYSS model of laying on high-impact shows, brilliant minds, time and space, is undoubtedly a great way to recruit foreign talent. It's no surprise then that the plan is to hold the GYSS annually and that this successful conference model is being used around the world to attract young scientists.

# Clare Grey advises Samsung

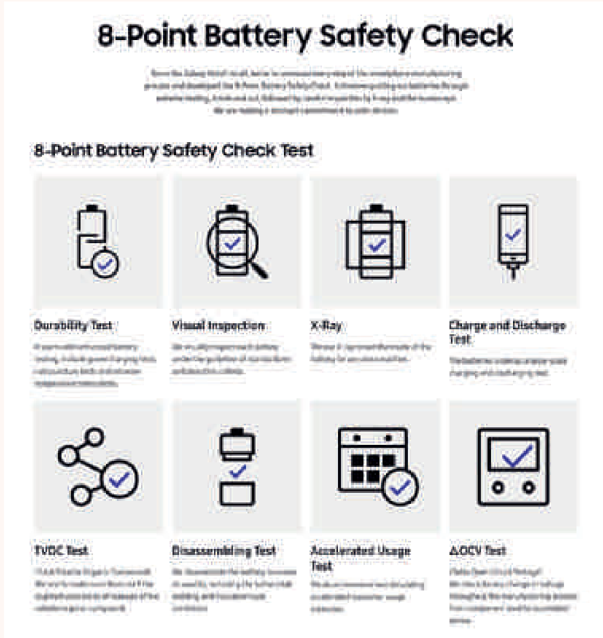
In January 2017, after a number of Galaxy Note7 smartphones over-heated and burst into flames bringing production to a halt, leading to a product recall and a plane ban, Samsung announced the results of its investigation into the cause.

Prof Clare Grey (above right) together with other external advisers, academic and research experts helped Samsung get to the bottom of the problem.

Errors both in design and manufacturing were identified. In some cases the battery was crammed into a corner causing electro deflection, while in others there was not enough insulation between the battery components leading to an internal short circuit.

Clare said: "There are two things going on; one is there is a demand from the electronics industry to have higher energy density, which means the batteries last longer. And then there's a desire to put batteries in increasingly smaller spaces. So inevitably there are risks associated with this drive for increased performance – in the end there is no getting away from the fact that you've got highly oxidised and highly reduced materials in very close proximity."

Following the report Samsung introduced an 8-point battery safety check to catch the problems they identified. However, Clare made the point that battery safety is the responsibility of and a challenge for the industry as a whole and not just Samsung.




Samsung's new 8-point battery safety checklist

# Correspondence

## Write to us

**We are always delighted to receive your emails and letters.**

**Email your comments to:** news@ch.cam.ac.uk
**Post your letters to:** Chem@Cam, Rm142, Department of Chemistry, Lensfield Road, Cambridge CB2 1EW


**Dear Editor**

I normally read most of your magazine and I am usually informed and satisfied by its content. But one item in the Winter 2016 issue concerned me and I wish to comment.

The high level point is that you provided two pages of space to the pro-remain views of Julian Huppert with no counter-balancing position. On the next page the department then appeals for direct funding.

As you know, 52% of the population supported Brexit, so you have potentially alienated half of your possible donors by this editorial choice. I voted to leave for what I considered to be sound reasons. These concerned the lack of democratic accountability, the fiscal irresponsibility and the inappropriate overall direction of the EU. I know there will be winners and losers that result from the leave decision. I understand that academics (and probably farmers) are the two groups that are likely to be most affected, but these are not the dominant interest groups in the country. In the many discussions I have had on this issue, the only truly valid reason I have identified for voting to remain in the EU is if the voter believes that the UK should be part of a federal Europe (full political and monetary union, which is the logical endpoint of "ever closer union"). I don't think this is the right direction for the UK or for the majority of European States.

I understand this is an emotive issue and different people will draw different conclusions even from the same evidence base. I respect that. My view is that the debate and the referendum were necessary and actually well overdue (the UK people were denied a popular vote at the time of the significant Maastricht and Lisbon treaty changes). The referendum was not lightly given, but grudgingly forced from the Westminster politicians, mostly by the democratically applied pressure of UKIP (which, you may recall, was the largest polling party in the UK 2014 European election). I would argue that the Conservative election manifesto promise of an "in-out" referendum was the main reason the Conservative government was returned to power with a majority in the 2015 general election. I note that the referendum bill received widespread support in Parliament in 2015 (544 votes in favour and 53 against).

I think no one can confidently know if the vote to leave the EU will be positive or negative for the UK or for the EU. The future is inherently uncertain and there are upside and downside risks associated with both leaving and remaining outcomes. As I see it, the facts of the matter are that a referendum was held following sustained, democratically applied pressure and 52% of the votes were cast to leave the EU. This is the valid result of a fair, democratic process. It should be accepted and implemented.

In the future kindly either avoid political comment or provide balance.

Yours sincerely

**Dr Tim Fowler** (1977–1983)

*We also received a similarly Brexit focused letter from Malcolm Stebles (Downing 1966–1972), who made the point that, "there is no reason to believe that the underlying funding and research collaboration should not continue more or less the same as it is now, except that it would be by different mechanisms."*

*Now that article 50 has been triggered we shall continue to watch developments here at Chem@Cam.* - **Editor**

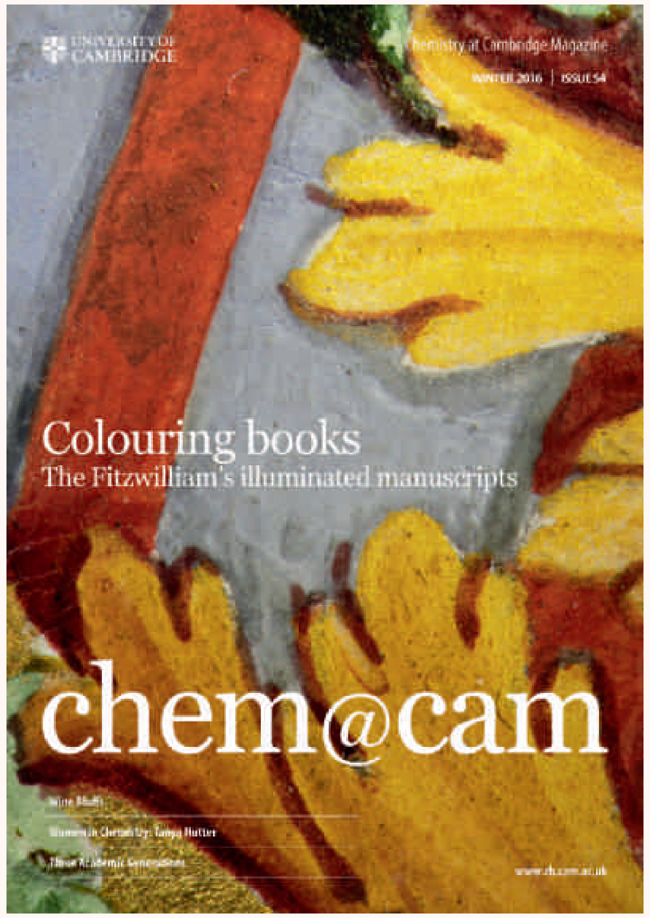
**Dear Editor,**

I really enjoyed reading the latest edition of the magazine, winter 2016.

Adding the chapter on recent research by the department gives this publication a lot more weight and gives an accurate reflection about the real work going on in the department.

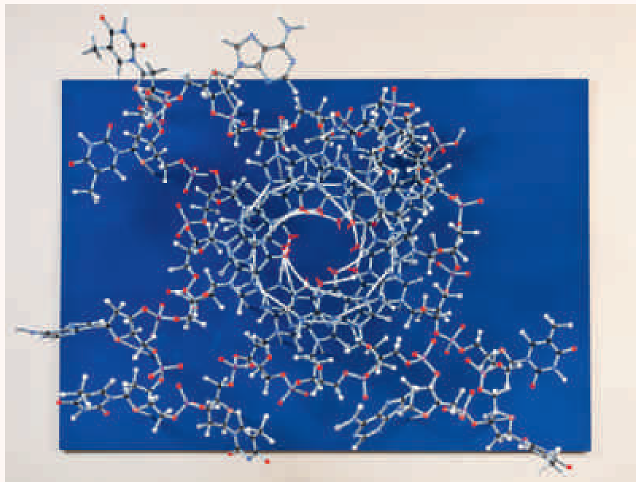
Looking forward to reading more soon!

**Christian Fink** (PhD, 2008)

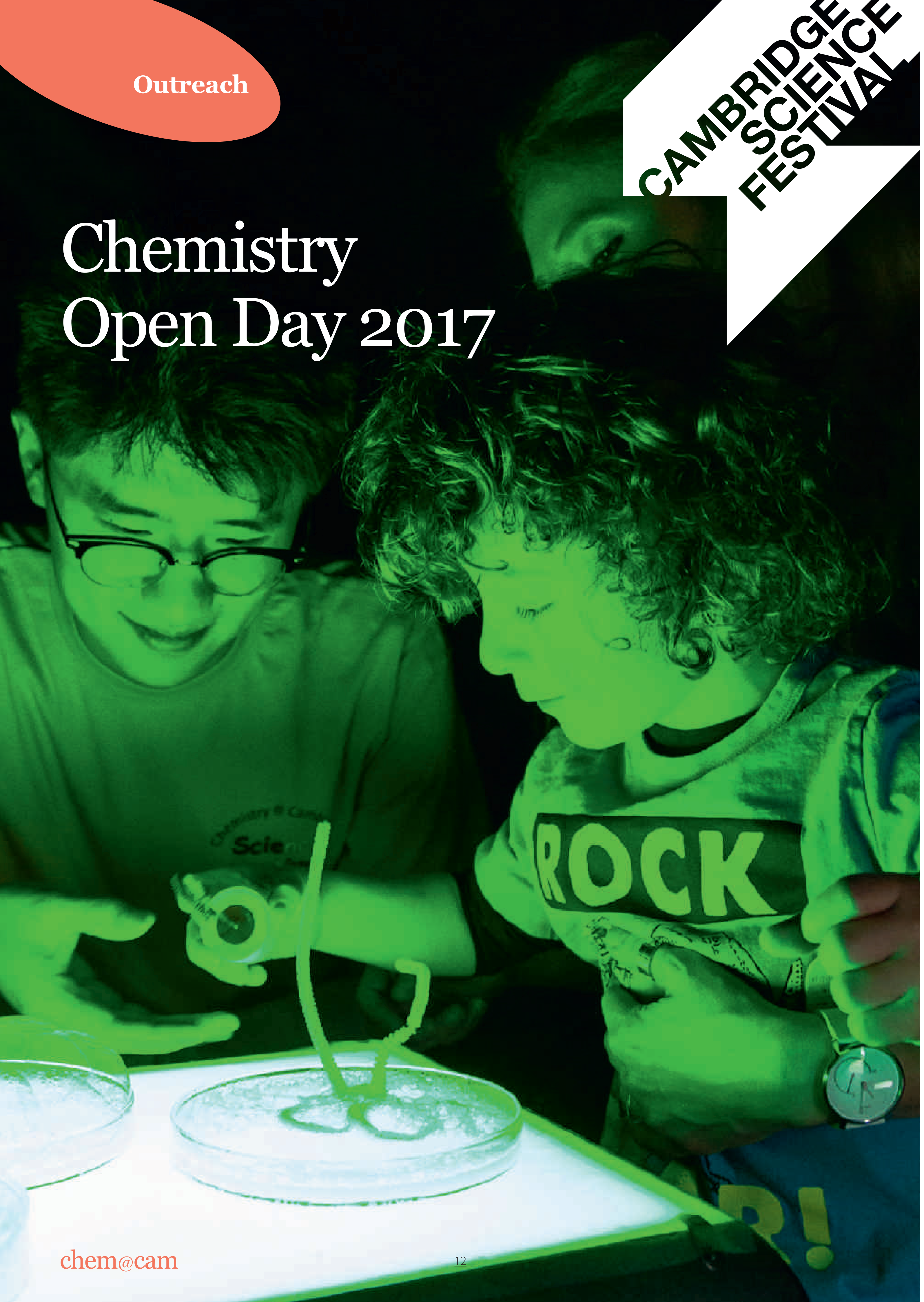



**Correction**

In our research article, '4-stranded DNA helix points to possible new cancer treatments' (page 21, Chem@Cam: issue 54, December 2016), we referred to guanine as an amino acid. Guanine is one of the four main nucleobases found in the nucleic acids DNA and RNA. Thank you to John Anderson (1956-1962) for spotting the error.



# Chemistry Open Day 2017




**The doors of the Department of Chemistry were open once again for the annual Chemistry Open Day on Saturday 18 March. More than 2000 people, many of them children, visited the department and took part in numerous workshops and demonstrations.**

Visitors to the department took the opportunity to don white coats – including a 3-year-old in a lab coat down to his ankles, open mouthed in the battery fruit zone – in wonderment or hunger? It was hard to tell.

Deputy Heads Nick Bampos and James Keeler were handing out safety glasses and directing traffic. Meanwhile, Professor Jonathan Nitschke, whose group researches complex matter through molecular self-assembly, gamely bounced through a vat of cornflower slime. He lingered slightly too long and sank up to his calves in goo, before aptly demonstrating how to get out of quicksand – very, very, very, slooooowly.

There was goo absolutely everywhere. Goo being shaped into rubber balls, goo floating around in newly created lava lamps. Goo in the Cybercafé. Guanglu Wu and Magda Olesinkska showed people how to make supramolecular structures with brightly coloured goo. Thea Precht, Rose Ng, Beth Connolly and Maureen Georges demonstrated edible cold goo, using liquid nitrogen to make ice-cream.

There was also an oasis of quietness in the Todd-Hamied room. People sat for hours in the modelling zone diligently piecing together molecular structures of Menthol, Adenine, Jasmone, Caffeine, DEET, Camphor, Indigo dye – it was beautiful.

One mother said, "I've been coming to this event for 16 years. I brought all four of my girls and it's so exciting and inspiring for them. In fact, one of my girls is now studying theoretical chemistry - sadly at Oxford but hey! Another parent added: "We think this event is so good we bring a group from Camberwell in Southwark, one of the poorest boroughs of London, and they're so bowled over by it. One little boy came last year and he's already saying he wants to study at Cambridge." A third adult remarked: "Sometimes the explanations are brilliant, sometimes not but I've always found the children are questioning and curious and the students engage with the them at the right level."

Over 100 staff members, postdocs, PhDs and undergraduate volunteers helped to make the day go very smoothly. Huge 'Thanks' to everyone who took part. We would also like to thank the Walters Kundert Charitable Trust for its continued transformational support.

## A day of discovery for visitors and host

*Mike Gaultois, a postdoc in the Grey Group, put together a number of demos including magnetism, hydrophobic and hydrophilic materials, and one showing how batteries work. Here he reflects on the Chemistry Open Day.*

Naturally, the kids were most excited, darting quickly between experiments dragging parents around because they want to try the next thing.

One young girl was connecting lemon batteries in series. When she realised that if one lemon gave 1 volt, two gave 2 volts, and three lemons gave 3 volts, then ten lemons should give 10 volts, she began jumping around with unbounded joy.

Everyone expects children to get excited on these days, but it was a surprise, to me, to see the parents and adults becoming as intrigued as their children. They often lingered and continued to ask questions, while their kids pestered, "Come on, I want to make slime!"

I was particularly fortunate to share an experience of discovery with one parent, who confided in me that until our discussion, and despite having a degree, they never really understood why putting metal prongs in a lemon produced a voltage.

The day is a great way to get young, and older, minds excited about science, and to share in the joy of scientific discovery. When we're in the lab every day, it's easy to forget how cool our work is, how lucky we are to be practising scientists and how fortunate we are, as postdocs, to be paid for our endeavours. Open Day is a beautiful way to rekindle our own love of science, and it's rewarding to share that. I think it's our responsibility to bring our science to the public, because by providing this service everyone in our community can reap the rewards.

## Burning Issues Fire and Flame

**"One of my favourite demos is burning a jet of oxygen in an atmosphere of hydrogen, it's a bit risky but it all adds to the fun."** Pete Wothers



# Salters' Festival of Chemistry 2017

**Once again, the Salters' Festival of Chemistry took place in the Department of Chemistry. Children from years 7 and 8 experienced hands-on practical chemistry in the teaching lab. Teams of four, from 20 schools in and around the East of England, competed in two fun challenges, one set by Salters', the other set by the department. The first, Salters' Challenge, "Who is the Prime Suspect?", required analytical chemistry skills to discover who murdered a fictional member of the company. The second, University Challenge, asked the teams to separate food dyes using a chromatography column. Prizes were awarded for both challenges.**

### Salters' Challenge Winners

- 1st Prize Richard Hale School, Hertford
- 2nd Prize Bedford Prep School, Bedford
- 3rd Prize Sandye Place Academy, Sandy

### University Challenge Winners

- 1st Prize St. Faith's School, Cambridge
- 2nd Prize Culford Preparatory School, Bury St Edmunds
- 3rd Prize St. Francis College, Letchworth Garden City

After the prize giving ceremony the participants enjoyed Pete Wothers' Open Day demonstration lecture, 'Burning Issues'.

# New Look: augmented chemistry

## Ley Group

**Postdoc researchers in the Ley Group, inspired by Hollywood movies and gaming, have developed a new web-based molecular viewer, and used it to enhance their most recent publication. The viewer combines three technologies in one: Star Wars-like holographic display, Pokémon Go augmented reality and motion sensing cameras as seen in Minority Report with Tom Cruise. The result is a 2D marker that looks like a very simple QR code. But anyone using a smartphone to look at it will be treated to a 3D version of a trans-3-(4′-methoxyphenyl)-1,4-diphenylazetidin-2-one molecule.**

The web-based molecular viewer accesses an augmented reality (AR) library, displays the images as holograms and allows the user to manipulate the 3D image. This application is expected to become not only a powerful research tool but also a useful educational resource.

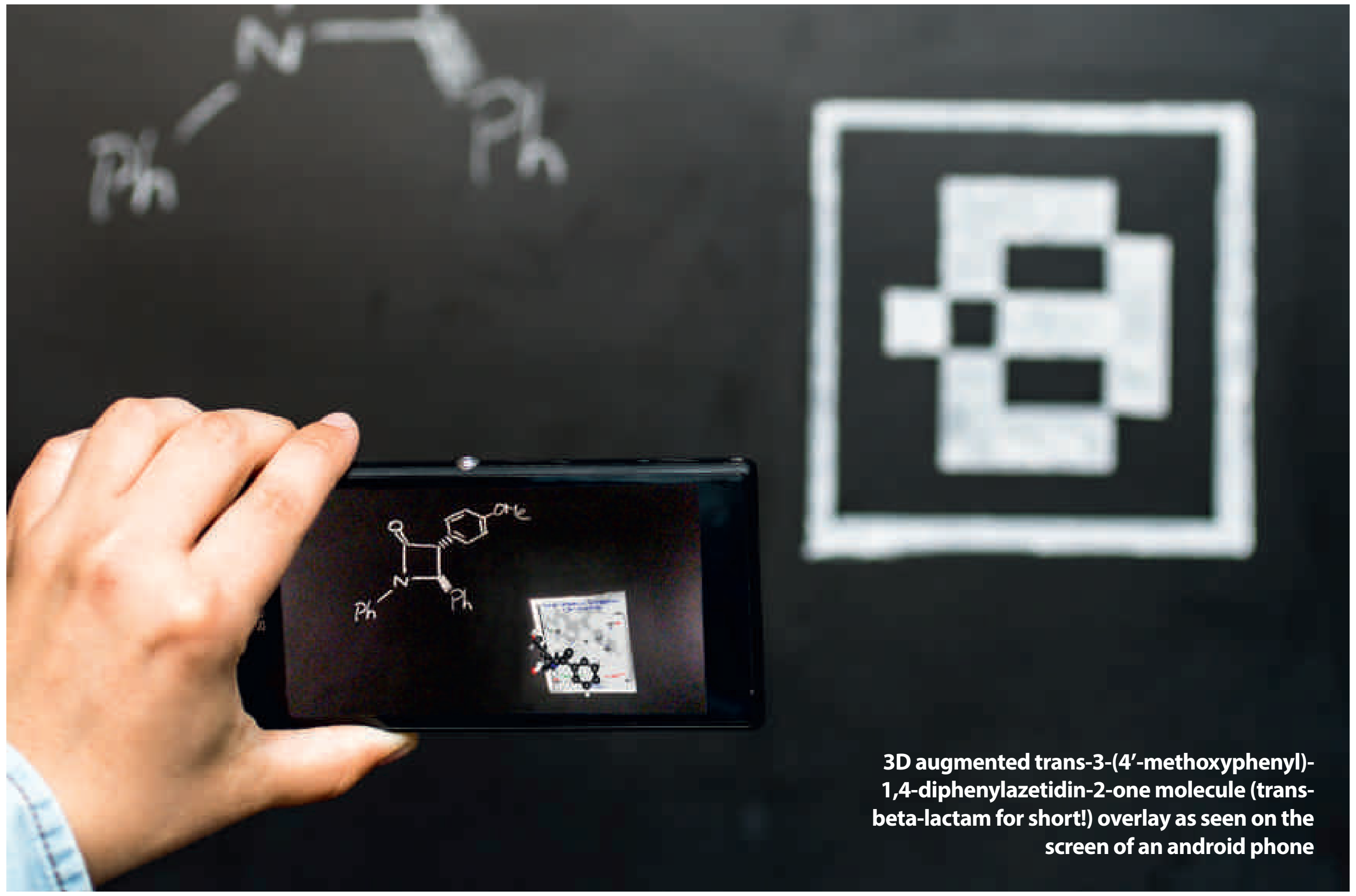
Eric Śliwiński (above 2nd right), who worked on molecular visualisation data representation for the viewer, explains: "This system uses computer vision exactly in the same manner as the recognition of quick read (QR) codes but with fewer dots. Using my phone I can superimpose a model on a sheet of paper. I can then toggle the animation to display the molecules and a cheap motion sensing camera (Leap Motion™) allows me to move it around with my hands."

"You can see the computed reaction pathway for a transformation and within this representation you can see not only the 3D structures of the molecule but also the associated reaction intermediates and the corresponding Gibbs energies. The log files from computational research are automatically processed in this viewer. All of this information can be easily referenced in the publication using one URL or QR code."

Gina Musio (above 2nd left), lead author on the first augmented chemical research communication published with the new 2D marker, says: "This technology helps the synthetic chemists to interpret more easily the computational data. I find it exciting to read an augmented scientific paper with the ability to visualise, on-the-fly, the molecules described and the parameters associated with them; dihedral angles and bond distances – by just scanning a 2D marker and without installing any licensed software!" Gina continues: "The point is, a solid bridge has been built between the computational chemists and synthetic chemists, who routinely collaborate and can now easily communicate."

In the past, synthetic chemists have been very conservative, doing the same experiments





3D augmented trans-3-(4′-methoxyphenyl)-1,4-diphenylazetidin-2-one molecule (trans-beta-lactam for short!) overlay as seen on the screen of an android phone

on the bench that were used 100 or 150 years ago. Mikhail Kabeshov (above right), the computational scientist behind the viewing software, says: "Synthetic organic chemists were not taking advantage of emerging technology. With this system researchers will be able to quickly digitally compare reaction conditions that have been published elsewhere. For example, in the past you wouldn't think about comparing activation energies from ten procedures. But if you have easy access to an application that can produce and display them and the process takes five minutes, why not? You would quickly see that out of five procedures, four are not efficient."

The beauty of the system is that it uses open source technology, it works natively on the web, running JavaScript in a web browser, which is the same tech for all computing devices, from mobile phones to a massive work station, and it's free. The only exception is Apple; it doesn't work on iOS, at the moment, because Apple policy does not allow the free "getUseMedia()" application programme interface (API) to run natively on its devices.

However, the team continues to develop the viewer. Eric says: "So far we have 1024 different markers within the augmented reality library. But the recent release of the JavaScript version of ArToolKit 5 in open source, a state-of-the-art augmented reality library, could allow us to have over 4 million markers (the exact number is 4194304 for 5x5 markers). People will be able to drag and drop their own structures into the webpage, design their own markers and show whatever they want, including videos."

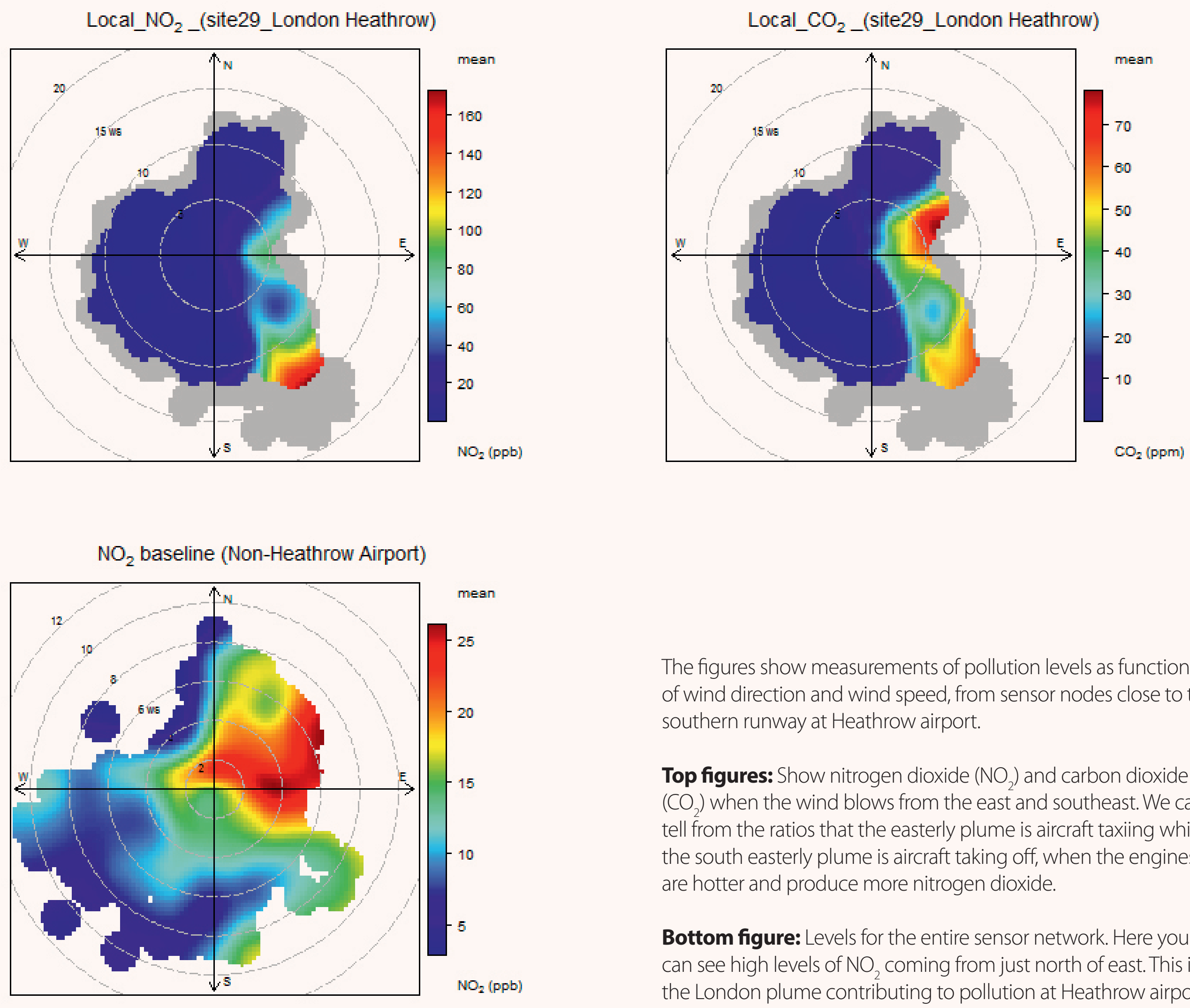
Augmented reality techniques are impacting widely in many other areas of science. Steve Ley and his group believe that these methods have a role to play in visualising chemistry and that the combined use of modern machinery will help transform the practice of molecule synthesis.

**Try it for yourself. This QR code will take you to instructions for using the 3D viewer. Use the image on the back cover to experience the full effect. Alternatively, for instructions go to: http://github.com/es605/HTMoLAR**

**Reference:**
B Musio, F Mariani, EP Śliwiński, MA Kabeshov, H Odajima, SV Ley: *Combination of Enabling Technologies to Improve and Describe the Stereoselectivity of Wolff-Staudinger Cascade Reaction*. Synthesis (Germany) (2016) 48, 3515. DOI: 10.1055/s-0035-1562579


# Heathrow and air pollution

## Jones Group




The figures show measurements of pollution levels as functions of wind direction and wind speed, from sensor nodes close to the southern runway at Heathrow airport.

**Top figures:** Show nitrogen dioxide ($NO_2$) and carbon dioxide ($CO_2$) when the wind blows from the east and southeast. We can tell from the ratios that the easterly plume is aircraft taxiing while the south easterly plume is aircraft taking off, when the engines are hotter and produce more nitrogen dioxide.

**Bottom figure:** Levels for the entire sensor network. Here you can see high levels of $NO_2$ coming from just north of east. This is the London plume contributing to pollution at Heathrow airport.

**Arguments about the environmental impact of expanding Heathrow, the UK's largest airport, have been raging since the government supported the expansion back in 2009. There may be many reasons for not wanting a third runway at Heathrow, but according to independent research done by Rod Jones and his group, nitrogen dioxide ($NO_2$) is probably not one of them.**

**"We've got lots of different ways of fingerprinting air pollution, and what we're doing is separating what an individual sensor does and what the whole network of sensors does, allowing us to unequivocally identify the sources of pollution."**

Professor Rod Jones set the scene: "Up until now, the emissions from Heathrow were estimated on the basis of what is effectively a spreadsheet evaluation of how many aircraft, how many airside vehicles and how much roadside traffic are associated with the airport.

"There was also a single monitoring site, which measures air quality but the data from it, on its own, cannot be used to tell whether those fluctuations are coming from the airport or if it's wafting in from somewhere completely unrelated. What we've done is place a network of 40 air quality sensor nodes across the whole of the Heathrow site, made measurements, and looked for the common patterns."

The sensor network is able to distinguish between pollutants drifting in from the surrounding area and what is emitted from the airport, something that is not possible with just one sensor. Rod clarifies: "When we look at the results we find that a significant part of the pollution (including $NO_2$) is not related to the airport, but is coming from elsewhere, mainly, in this case, from central London.

"We also have $CO_2$ measurements on each sensor node which allow us to determine 'emission indices', for example how much $NO_2$ is produced per unit of fuel burnt. We then put all these results into a computer model, run by David Carruthers at Cambridge Environmental Research Consultants (CERC), which we then use to create maps of air pollution in and around the airport. We can then use the model to predict $NO_2$ levels outside the airport with different third runway configurations and we find that non-airport emissions tend to dominate.

Rod says: "If you allow a third runway, the airport component of pollution will go up, no question. But, taking some indicative numbers, if we imagine the pollution at a point is 100%, only around 10% is coming from the airport activities; leaving around 90% from elsewhere.

"With a third runway, the airport contribution would rise, perhaps to 15%, but at the same time, with anticipated improvements in the traffic fleet, the 90% will drop significantly.

"Even with a third runway there would be a net fall in $NO_2$ pollution levels. So overall you're below the health impact threshold."

Supporters of expansion have seized on this fact with the headline grabbing suggestion that, together with mitigating developments in technology, Heathrow airport could build a new runway without breaking European pollution laws.

However, Rod says when it comes to the question of Heathrow's expansion he is completely 'agnostic'. "But I do think that if you're going to use evidence to make policy decisions, base it on good science rather than opinion."

The research was funded by the Natural Environment Research Council (NERC). The senors were installed at the airport by the department with the help of Heathrow.

Currently researchers from the Jones Group are in Beijing studying the links between air quality and human health.

READ MORE:
www.cam.ac.uk/research/impact/better-sensors-cleaner-air

# Battery safety All Solid State

## Grey Group

**When it comes to battery performance, higher energy density, which means longer lasting batteries, has always been the main emphasis. However, recent events at Samsung have pushed battery safety in phones to the top of the list of requirements. PhD student Kent Griffith (above right) considers the current situation and introduces the idea of a solid-state alternative to today's most successful rechargeable batteries.**

There can be different initiating factors but catastrophic battery failure that results in an explosion or fire is due to combustion of the organic liquid electrolyte inside the cell. Overheating in the cell is obviously the main cause, it may be external, but is often due to an internal short circuit. The most widely used batteries in phones are Lithium-ion. In these cells, lithium can deposit into branch-like structures known as dendrites, which can grow all the way from the negative to the positive electrode. This short-circuit provides a direct pathway for rapid discharge and heat generation, which cause the electrolyte to break down, generates gas and, if the pressure/heat continue to increase, can catch fire or explode.

There are different approaches to improving the safety of current commercial battery technology, including using sensors and thermally responsive polymers that seek to shut down current flow once a certain temperature threshold is detected. However, this approach is still susceptible to manufacturing defects or cell puncture. For this reason, the ultimate goal for battery safety would be to get rid of the flammable liquid electrolyte altogether and replace it with a nonflammable solid electrolyte. This is all-solid-state battery technology, one of the research areas the Grey Group is currently working on.

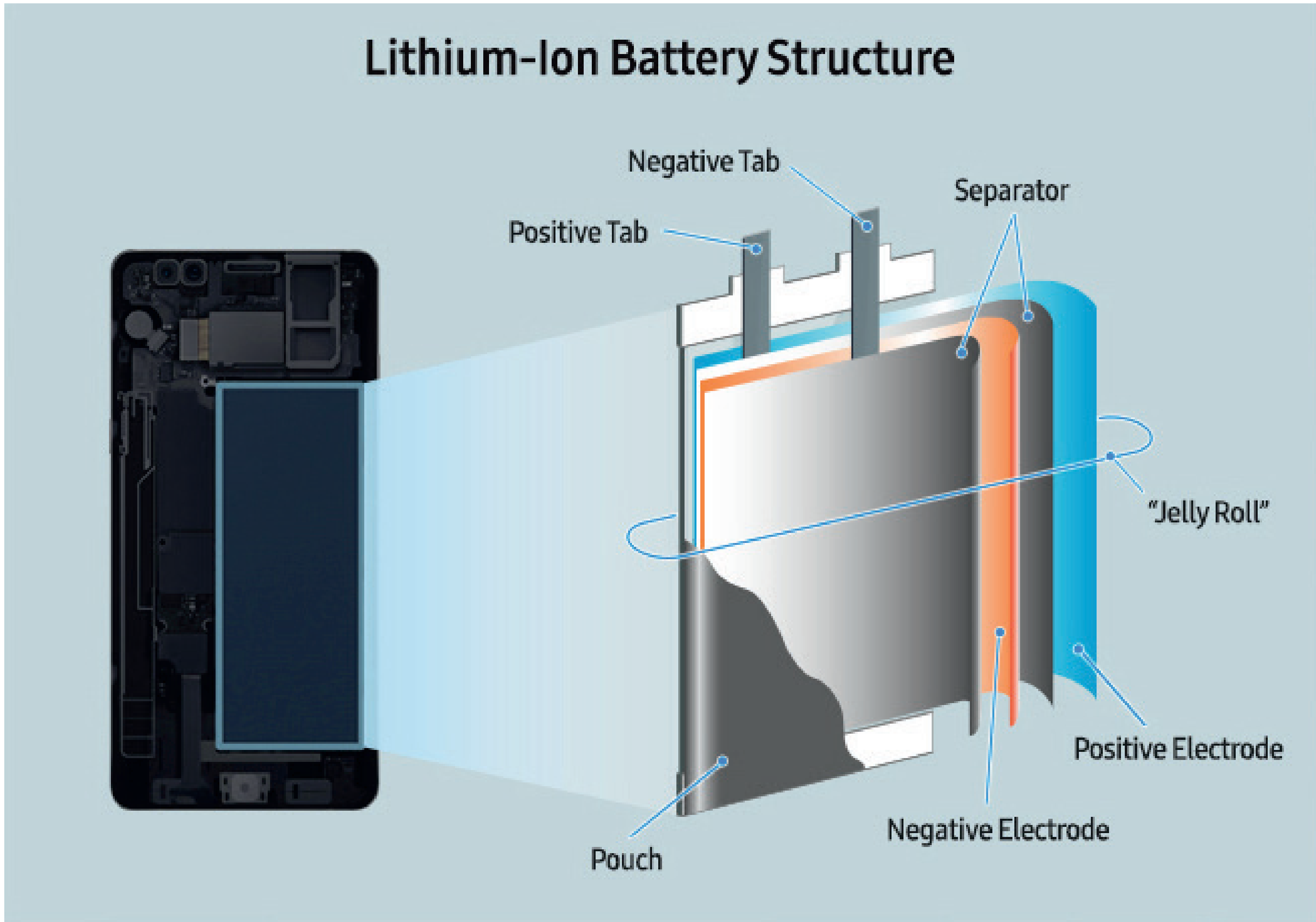
A solid electrolyte, as part of an all-solid-state battery, could allow the transport of lithium ions while physically blocking dendrite growth. In addition to preventing the main cause of overheating, a solid electrolyte also avoids the consequences of a short-circuit or other heat generating events because there is nothing to burn. The solid electrolyte material is typically an oxide, sulfide, or phosphate, which means a fully inorganic battery that could have an operating temperature ranging over several hundred degrees Celsius. This would mean you would not have to worry so much about leaving your phone exposed to the full power of the mid-day sun or cooling down car battery packs.

The issue is that, ultimately, we want batteries that readily interface with the electrodes and have good ionic conductivity; liquid electrolytes do this very efficiently. Unfortunately, at the moment solid electrolyte materials generally have relatively low ionic conductivity, react with air, and do not form a good interface with the electrodes.

Now, usually ions diffuse faster in liquid than they do in solids, but surprisingly, some families of solid structures have been discovered that allow lithium ions ($Li^+$) and sodium ions ($Na^+$) to diffuse or conduct as fast as in conventional liquid electrolytes. Some of the most promising solid electrolytes are synthetic garnets, Na Super Ionic CONductor (NASICON) and related phases, glass-ceramics and argyrodite. In most of these systems, dopant atoms - trace impurity elements - are crucial for stabilising the conducting structure and/or improving conductivity. Our group is using solid-state NMR, density functional theory (DFT), and other structural methods to understand the diffusion mechanisms and dopant chemistry in this area.

When safety is such a major constraint, it is more challenging for industry to put higher energy cathode or anode materials into the battery. High energy density lithium anodes and >5 V high-voltage cathodes have been around for years but they cannot be used with organic liquid electrolytes.

If we can achieve an all-solid-state battery that contains nonflammable components and prevents dendrite formation, battery markets could open up and move into new territory in terms of devices and chemistries. In fact, there are many big industry players looking into this field. Electrification of transportation, longer lasting mobile devices, and increased electrochemical grid storage would all benefit from the advent of the new safer battery technology. The race is hotting up – Germany is pushing for a move away from diesel and towards electric vehicles by 2030 and plans are afoot to locate new gigafactories in Europe. Here in the UK, similar big plans are predicted.



Research

# Big Data harnessed to tackle antibiotic resistance

## Bender Group

**Dr Daniel Mason (above right), a former postdoc in the Bender Group, has developed a machine learning approach that enables the prediction of more effective antibiotic combination treatments, potentially speeding up the search for new ways to fight antibiotic resistant bugs.**

The overuse of antibiotics in livestock, unnecessary prescription in humans and the fact that no new antibiotic classes have been discovered in the past 40 years mean our arsenal of treatments is gradually succumbing to multi-drug resistant organisms.

Daniel, who developed the computer-designed system during his time at the Centre for Molecular Informatics, says: "Being able to predict which compounds are likely to produce a synergistic antimicrobial effect when combined together has the potential to greatly reduce time and resources spent on experimental screening for new treatments."

The work published in the *Journal of Medicinal Chemistry* shows that once trained using a dataset of 153 pairs of antibiotics screened against *E. coli*, the method is able to classify synergistic combinations largely correctly when testing on an unseen dataset. This is very significant in practical terms as pairwise screening a library of just 50 compounds would result in over 1,200 combinations. "The rate of prediction corresponds to a 2.8-fold increase in the discovery of synergistic combinations over that expected by a brute-force screening effort," says Daniel. The research has resulted in a list of 4,950 combinations of 100 compounds of which 691 are now the starting point for designing future antibiotic combination treatments.

The computer-designed approach was developed in collaboration with the research group of Dr Murat Cokol at Sabanci University in Turkey and Harvard University in the United States.

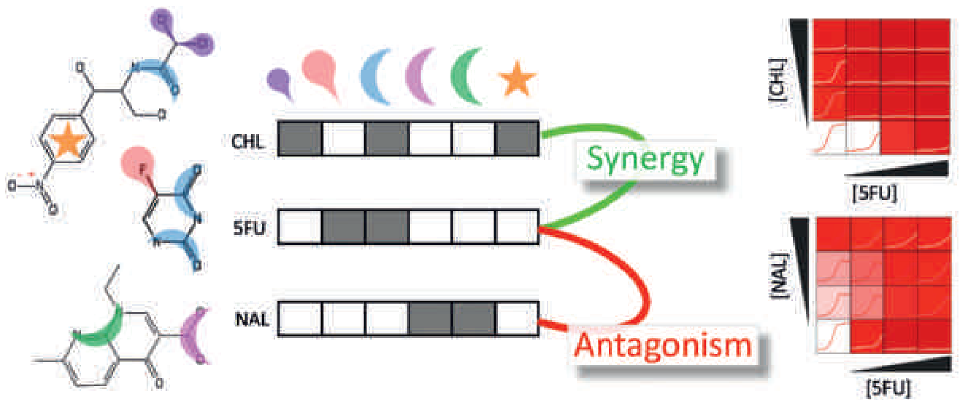



**Figure:** Using the fingerprint features of antibiotics (displayed as different colours and shapes), in this case chloramphenicol, 5-fluorouracil and nalidixic acid, the machine learning approach is able to model and predict synergistic combinations of new antibiotics.

**References:**
Daniel J Mason et.al., *Prediction of antibiotic interactions using descriptors derived from compound molecular structure,* J. Med. Chem., April 6 2017 DOI: 10.1021/acs.jmedchem.7b00204.



# Light makes biomass produce clean hydrogen

## Reisner Group

Researchers in the Reisner Group have developed a way of using solar power to generate a fuel that is both sustainable and relatively cheap to produce.

The technology uses natural light to generate hydrogen from biomass. Group leader Dr Erwin Reisner says: "Our sunlight powered technology is exciting as it enables the production of clean hydrogen from unprocessed biomass under ambient conditions."

The main component of plant biomass is lignocellulose and up to now its conversion into hydrogen has only been achieved through a gasification process, which uses high temperatures to decompose it fully.

Dr Moritz Kuehnel, a postdoc in the Reisner Group and joint lead author on a new research paper published in Nature Energy, says: "Lignocellulose is nature's equivalent to armoured concrete. It consists of strong, highly crystalline cellulose fibres that are interwoven with lignin and hemicellulose, which act as a glue. This rigid structure has evolved to give plants and trees mechanical stability and protect them from degradation, and makes chemical utilisation of lignocellulose so challenging."

The new technology relies on a simple photocatalytic conversion process. Catalytic nanoparticles are added to alkaline water in which the biomass is suspended. This is then placed in front of a light in the lab, which mimics solar light. The solution is ideal for absorbing this light and converting the biomass into gaseous hydrogen, which can then be collected from the headspace. The hydrogen is free of fuel-cell inhibitors, such as carbon monoxide, which allows it to be used for power.

**READ MORE:**
www.cam.ac.uk/research/news/scientists-harness-solar-power-to-produce-clean-hydrogen-from-biomass

**Reference:**
David Wakerley et al: *Solar-driven reforming of lignocellulose to H2 with a CdS/CdOx photocatalyst.* Nature Energy 13 March 2017 DOI: 10.1038/nenergy.2017.21

# Reflections on electron microscopy

## Sir John Meurig Thomas

***In 2016 Professor Sir John Meurig Thomas was awarded a Royal Medal by the Royal Society for his pioneering work in catalytic chemistry, in particular on single-site heterogeneous catalysts, which has had a major impact on green chemistry, clean technology and sustainability. He is one of the best-known electron microscopists in the field. In January 2017, Sir John's overview of what has been achieved through electron microscopy in heterogeneous catalysis appeared in the Royal Society Proceedings A. The abstract of that paper is reproduced here.***

Electron microscopy (EM) is arguably the single most powerful method of characterizing heterogeneous catalysts. Irrespective of whether they are bulk and multiphasic, or monophasic and monocrystalline, or nanocluster and even single-atom and on a support, their structures in atomic detail can be visualized in two or three dimensions, thanks to high resolution instruments, with sub-Ångstrom spatial resolutions. Their topography, tomography, phase-purity, composition, as well as the bonding and valence-states of their constituent atoms and ions and, in favourable circumstances, the short-range and long-range atomic order and dynamics of the catalytically active sites, can all be retrieved by the panoply of variants of modern EM. The latter embrace electron crystallography, rotation and precession electron diffraction, X-ray emission and high-resolution electron energy-loss spectra (EELS).

Aberration-corrected (AC) transmission (TEM) and scanning transmission electron microscopy (STEM) have led to a revolution in structure determination. Environmental EM is already playing an increasing role in catalyst characterization, and new advances, involving special cells for the study of solid catalysts in contact with liquid reactants, have recently been deployed.

**Reference:**
Thomas JM: *Reflections on the value of electron microscopy in the study of heterogeneous catalysts.* Proc. R. Soc. 2017 A 473 DOI: 10.1098/rspa.2016.0714

# Visualising the genome
## Lee & Klenerman Groups

**Scientists in the Lee and Klenerman groups together with colleagues from the Department of Biochemistry, the Wellcome-MRC Stem Cell Institute, and the MRC Laboratory of Molecular Biology, have determined the first 3D structures of intact mammalian genomes from individual cells, showing how the DNA from all the chromosomes intricately folds to fit together inside individual cell nuclei.**

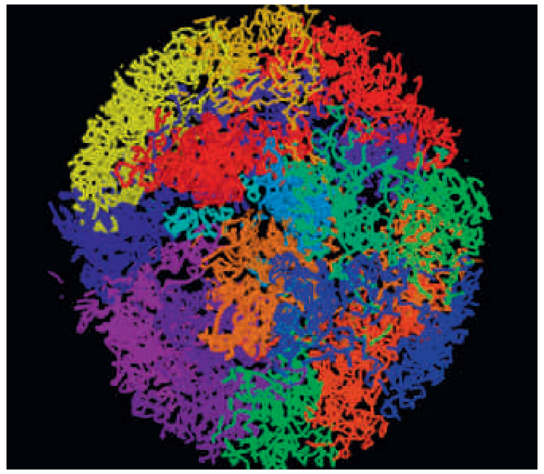
Researchers used a combination of imaging and up to 100,000 measurements of where different parts of the DNA are close to each other to examine the genome in a mouse embryonic stem cell. Stem cells are 'master cells', which can develop – or 'differentiate' – into almost any type of cell within the body.

David Klenerman said: "We used the super-resolution optical microscopes to help find the position of key markers in the nucleus. This gave the bioinformaticians a 'guided map' of how to efficiently assemble these fragments into a coherent structure."

Using their new approach, the researchers have determined the structures of active chromosomes inside the cell, and how they interact with each other to form an intact genome. This is important because knowledge of the way DNA folds inside the cell allows scientists to study how specific genes, and the DNA regions that control them, interact with each other.

The genome's structure controls when and how strongly genes – particular regions of the DNA – are switched 'on' or 'off'. This plays a critical role in the development of organisms and also, when it goes awry, in disease.

Steven Lee said: "Single cell Hi-C represents a new way of determining the three-dimensional organisation of the genome. Rather than looking along the length of a long 'strand' of DNA, this technique looks at which areas of the DNA are in close spatial proximity. Understanding how this organisation of DNA in the nucleus varies from cell-to-cell will be an essential tool in our further understanding of epigenetics."



**3D genome from individual mouse stem cell**
**Credit: University of Cambridge/MRC Laboratory of Molecular Medicine**

The researchers have illustrated the structure in accompanying videos, which show the intact genome from one particular mouse embryonic stem cell.

The research was funded by the Wellcome Trust, the European Union and the Medical Research Council.

READ MORE:
www.cam.ac.uk/research/news/visualising-the-genome-researchers-create-first-3d-structures-of-active-dna

**Reference:**
Stevens, TJ et al: *3D structures of individual mammalian genomes studied by single-cell Hi-C.* Nature; 13 March 2017; DOI: 10.1038/nature21429



# Hydrogen bond debate settled?
## Professor Anthony Stone

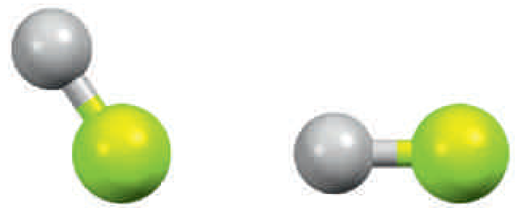
**In 1981 Professor Stone worked out a simple, efficient method for calculating the electrostatic potential around a molecule. The discovery opened up a new area of research in intermolecular forces and led to further research calculating the other components of intermolecular interactions. Over the years, a debate grew up around the nature of hydrogen bonds. Anthony has continued to take the view that hydrogen bonds are more electrostatic than covalent. In his latest publication, he argues that the debate is now settled.**

The debate centres around whether hydrogen bonds are more covalent than electrostatic. One view is that a hydrogen bond is mainly an electrostatic attraction between charge distributions on hydrogen and another, electronegative, atom. The other is that hydrogen bonding involves transfer of electrons, and therefore charge, between atoms, which gives it covalent character. "That issue has never really been resolved, partly because of the results from natural bond orbital (NBO) theory, which appear to support the argument that it's essentially chemical bonding," Anthony explains.

He continues: "I've been concerned about this for some time. But it was only recently that I worked out just what the problem was and it has some importance because it helps to demolish the idea that hydrogen bonding is chemical bonding. It's now clear that all but the very strongest hydrogen bonds are primarily electrostatic."

There is experimental and theoretical evidence that hydrogen bonding involves some charge-transfer – that is incipient chemical bonding - but there is still debate over how much. NBO suggests it dominates, while Anthony and others had noticed that other calculation methods found a much smaller role for charge transfer. The reasons for these differences were unclear.

In a recently published paper, Anthony compared NBO and symmetry-adapted perturbation theory (SAPT) combined with density functional theory (DFT). Using hydrogen bonding between two hydrogen fluoride molecules as an example, he argues that NBO falls foul of 'basis set superposition error'.



**Hydrogen fluoride dimer**

According to Anthony, the problem arises from the way that the natural bond orbitals that give the method its name are constructed. The method distorts the orbitals in a way that makes them less able to describe the individual molecules properly, giving them incorrectly high energies. Starting from this high-energy reference, the NBO calculation of charge-transfer energies combines the individual basis sets of orbitals, and the combined basis set gives a good description of the dimer energy. But the improvement in energy, which the NBO method describes as charge-transfer, includes compensation for the erroneously high energies of the monomers as well as any true charge-transfer energy, and exaggerates the charge-transfer effect by an order of magnitude.

**Reference:**
A Stone: "*Natural Bond Orbitals and the Nature of the Hydrogen Bond*". Journal of Physical Chemistry A, 2017. DOI: 10.1021/acs.jpca.6b12930

# Ana Belenguer

## Women in Chemistry

**Dr Ana Belenguer is a postdoctoral research associate who has been working with Prof Jeremy Sanders on various projects funded by EPSRC grants since 2002. She has been pioneering in the field of solid state dynamic covalent chemistry (DCC) by ball mill grinding. Since 2014 she has been based in the Hunter Group. Ana discusses her life in chemistry with Carmen Pryce.**

## Tell me about your job, what do you do?

I am an expert in high performance liquid chromatography (HPLC) and liquid chromatography mass spectrometry (LCMS) and a good deal of my time is taken up helping colleagues and students with separation problems. But the rest of the time, I am working on the synthesis of organic reactions in the solid state using ball mill grinding. This is a very new area of science, which is poorly understood. We have a multidisciplinary project, led by Jeremy, and collaborating with Giulio Lampronti, a crystallographer from the Department of Earth Sciences at the University and Aurora Cruz Cabeza, an expert in crystal lattice calculations from the Chemical Engineering & Analytical Science department at the University of Manchester. We are a very enthusiastic team sharing our interest in understanding the fundamentals of this new field of science. I'm combining my preference for organic synthesis with my expertise in analytical chemistry.

## How did you get into chemistry?

My father was a chemist specialising in physical chemistry. He built an industry in Spain manufacturing laboratory equipment. His circle of friends were all either professors in chemistry at the University of Madrid or academics in research facilities in Madrid. My father expected me to follow a scientific career. I attended the German School in Madrid, my mother is German, and although I became fluent in German, mathematics was very poorly taught at the school. So, I chose chemistry rather than physics, which of course is applied mathematics.

After finishing my degree, specialising in organic chemistry, I started to work in the quality control department in the pharmaceutical industry in Madrid. I knew from the beginning that this was a mistake as I was not financially driven. I was curious about science. I moved from Spain to Germany and on to England in that industry, learning chromatography, a new technique to me, on the way. I took a risk and left a permanent job to do six months' research in the chemistry department at City University in London. But, luckily for me, the research job was extended and I obtained my PhD. I must confess that I did not know what to do on completion of my PhD, so I went back to the pharmaceutical industry but this time to a research and development facility, hoping it would be similar to working in academia. Unfortunately this was not the case but I progressed. I became leader of a chromatography group with SmithKline Beecham and later an analytical manager in PowderJect Technologies, a start-up company.

Finally, I spotted a research job, here, advertised in New Scientist. And now I am very happy and settled working in this research environment.

## What's the most rewarding thing about your life in chemistry?

I like research and I enjoy working in a research environment where students, postdocs and research leaders are motivated by science. I specially enjoy working with Prof Jeremy Sanders because he is motivated to discover the fundamentals of the research topic we are working on. My research discussions with Jeremy normally revolve around his scheme on the different progressive stages of research:

**"Data --> Information --> Knowledge --> Wisdom"**

We obtain data, which when processed becomes information; leading to knowledge and, if we're lucky moves on to wisdom. I feel very strongly that nothing is beyond a good explanation. I enjoy expanding my mind and feel privileged, and spoiled in the department; I have the opportunity to attend so many talks about the latest discoveries in a variety of fields, not necessarily my own.

## Do you think being a woman in the department has helped or hindered your career?

No, I honestly think that gender was not even a consideration in my suitability for the jobs I've had or even in the day-to-day work with my colleagues. However, I had one experience of gender discrimination. My English husband had a computing job in Nuremberg, we were living there, so naturally I applied for a position at the University of Erlangen – I thought I could do my PhD there. I was told by a very old fashioned male professor that women should be at home cleaning the house. I took that comment to mean the poor professor had lost his mind!

In my opinion, success depends on the attitude, determination and research skills of the individual. I think the lack of balance between male and female group leaders in the department has to do with the fact that, for whatever reason, women are more reluctant to apply for key academic positions even though their skill sets are the same as the male applicants. I think unless the academic system can persuade females to apply for these positions the gender imbalance in the department will not be resolved.

## What would you say to postdocs starting out on a career in the department?

I think Postdocs and PhD students need to consider how best to progress their careers. In the past, there was very little advice and people were totally confused. For example, most people didn't realise that there is a time limit on applying for fellowships after you've completed your PhD. Postdocs are contract workers without links to colleges, unless they studied in Cambridge as undergraduate or postgraduate. In the past, there was no infrastructure to advise postdocs where to apply and what to do to progress their academic career. So, particularly for women, if they want to have a family, they must be aware and develop a strategy for moving ahead with their careers.

# As I see it...

## Oliver Pecher

**Dr Oliver Pecher specialises in the application of solid-state nuclear magnetic resonance (NMR) spectroscopy. He's particularly interested in the design of new *in situ* NMR techniques to study battery materials. Until very recently, February 2017, he was a postdoctoral research associate and Marie Skłodowska-Curie Fellow in the Materials Chemistry group of Professor Clare Grey. Now, based back home in Germany, he uses his expertise to help others prepare and develop their research experiments using NMR. Oliver talks us through what he did in the department and what he plans to do in the near future.**

> "We realised others would want and could benefit from a working relationship that bridges the gap between research and industry."

I am a solid-state chemist and joined the Grey Group to study the properties and performances of battery materials for lithium and sodium-ion technologies. I specialise in a technique called NMR spectroscopy, which is comparable to magnetic resonance imaging (MRI) body scanners in hospitals, where strong magnetic fields are involved.

This method produces information about what the sample material is made of and what keeps it together. My particular interest is real-time investigations of the batteries. I try to understand why something is happening while the device is working rather than after the process has ended. Applying *in situ* NMR on batteries doesn't come without its challenges and hardware modifications are required – and that's where I come in. I focus on the design and development of new hardware and equipment to make these experiments actually happen.

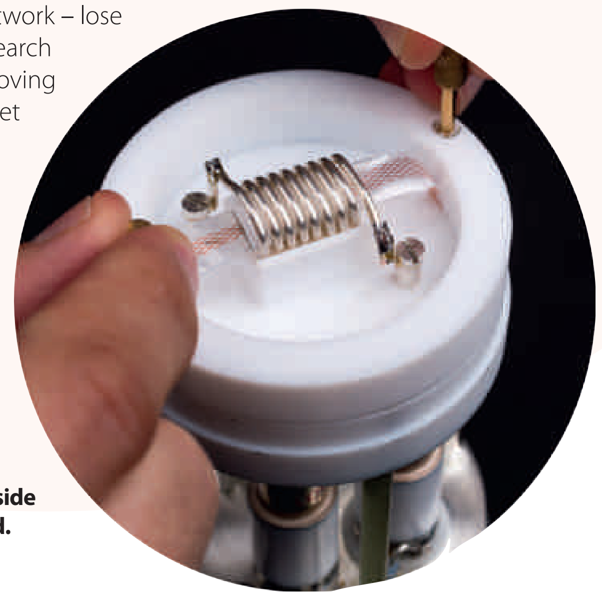
Until relatively recently, it wasn't possible to do *in situ* NMR investigations with high efficiency. Putting a 'real' battery (we actually use model systems that are as close to reality as possible) into one of the NMR machines and looking at how it functions while it's operating requires new methods. What we've developed is a specially designed *in situ* NMR probehead. It's basically a very expensive radio that can automatically tune to different frequencies, be recalibrated if needed, and is also highly shielded to prevent interferences between the circuits of the battery (the electrochemistry) and one of the NMR measurements.

This new tool allows us to put a sample – a battery – into the magnetic field, capture and measure what's going on. We also built a robot attachment for the probeheads, which automates some of the processes, and allows us to set-up, run, and monitor long experiments without the need for manual checking.

Now, I'm joining NMR Service GmbH (Erfurt, Germany; nmr-service.de), a company that offers customer specific solutions for NMR spectroscopy using probeheads, spectrometers, complete setups, as well as equipment for *in situ* NMR and automation in solid-state NMR spectroscopy. I've been made the Vice President of the company and I'll work as an application scientist and account manager. I will help customers to define their, often very complex, problems or challenges. I will work with researchers and industry to find the right experiments and then design and develop those experiments. It's basically a new position within the company that came about after we worked together on various projects for the Grey Group. We realised others would want and could benefit from a working relationship that bridges the gap between research and industry.

I always thought I would go down the pure research path. I absolutely enjoyed my time in the Grey Group, working with so many great postdoc colleagues and students on different approaches to problems – theoretical, experimental – the synergy of combining complementary information to learn something new about the materials. I thought I would go back to Germany, join a lab, apply for a huge grant, hopefully get it and go on to become a professor. I thought, if I join a company I would lose this great network – lose the connection to this amazing research world and I didn't want that. But moving to work in Germany now means I get to see something of industry but I also stay very close to research – and I get to see my wife – so it's beneficial for all sides.

And I still have a connection to the Grey Group through GREY MATTER Enterprises – but that's another story.



**Right:**
**An electrochemical cell (battery) inside the coil of an *in situ* NMR probehead.**

# Noticeboard

## Recognitions and awards

**Professor Clare Grey**
Elected Foreign member of the American Academy of Arts & Science

### Royal Society of Chemistry Prizes & Awards

**Professor Melinda Duer**
Interdisciplinary Prize

**Professor Stephen Elliott**
John B Goodenough Award

**Professor Tuomas Knowles**
Corday-Morgan Prize

**Dr Steve Lee**
Marlow Award

### Scholarships awarded for 2017 entry

**Peter Bolgar, PhD**
Herchel Smith

**Tegan Stockdale, PhD**
Herchel Smith

**Akhila Denduluri, PhD**
Gates Cambridge

**Sandile Mtetwa, MPhil**
Gates Cambridge

**Grant Simpson, MPhil**
Gates Cambridge

**Jessica Waters, PhD**
Walters Kundert

**David Izuogu, PhD**
Cambridge Africa Scholarship

**Bang Huynh, PhD**
Cambridge International

**Oded Rimon, PhD**
Cambridge International

**Eric Zhao, PhD**
Cambridge International

**Benjamin Williams, PhD**
Vice-Chancellor's Award

**Jessica Day, PhD**
Vice-Chancellor's Award

**Abigail Hanby, PhD**
Vice-Chancellor's Award

**Alasdair Keith, PhD**
Vice-Chancellor's Award

**Antanas Radzevicius, PhD**
Vice-Chancellor's Award

**Daniel Sharpe, PhD**
Vice-Chancellor's Award

**Julian Vigil, MPhil**
Churchill Scholar

**Anthony Tabet, MPhil**
Churchill Scholar

**Rosie Bell, MPhil**
Newton College Masters

**Karen Stroobants and George Trenins**
PhD students selected to represent the department at the Lindau Nobel Laureate Meetings 2017

## Appointments and promotions

**Professor Jane Clarke**
Elected the 6th President of Wolfson College. She takes up the post in October 2017

### Interdisciplinary Lectureships, autumn 2017

**Dr Hugo Bronstein,**
Functional Materials, joint with Physics

**Dr Robert Jack**,
Soft Matter, joint with Applied Maths

**Dr Anja Schmidt**,
Climate Modelling, joint with Geography

(further details in future issues of Chem@Cam).

## Upcoming events

**Professor Jean-Marie Lehn Lecture**
22 June 2017

**Sutton Trust Summer School**
14 – 18 August 2017

**Protein Folding, Evolution and Interaction Symposium**
03 – 05 September 2017

**Call My Bluff wine tasting**
22 September (further details to be announced)

**Chemistry Showcase Week**
25 – 29 September 2017

**Department of Chemistry Alumni Medal presentation**
19 October 2017

**Graduate Admissions Open Day**
20 October 2017



# How you can contribute

## Be a part of the future with a gift in your Will

A gift in your Will is a wonderful way to help the department flourish far into the future, and for you to be able to make a significant and lasting contribution. Such a gift can open up a world of opportunity for future students, researchers and academics, helping to provide the environment and tools they need to continue to achieve great things.

For further information about the impact of a legacy, and guidance on how to leave a gift to the Department of Chemistry in your Will, please contact Head of Department Professor John Pyle at **chemhod@hermes.ch.cam.ac.uk**

Scan
to discover

https://es605.bitbucket.io/Staudinger/

To access the animated 3D structure of trans-beta-lactam, first, scan the QR code (top image) – recommended browser Firefox Mozilla. (Instructions are provided by clicking on the question mark in the left-hand corner of the webpage.)

If you then click on the augmented reality button and accept the camera request, you may then scan the 2D marker (bottom image) to see the 3D augmented structure overlay on your device screen.