Monitoring ocean ecoystems p.4

Chemistry in the Botanic Gardens p.16

Green chemistry revolution p.28

Periodic

Magazine of the
Department of Chemistry

UNIVERSITY OF OXFORD

Issue 10
2022 – 23

From the Head of Department
Professor Mark Brouard

I am pleased to introduce the latest edition of *Periodic*, now in its tenth year. I hope you will like its new look and enjoy reading about some of the exciting news and research from the Department in the forthcoming pages.

2022 has been a year of many achievements, both individual and collective. The results of the Research Excellence Framework were announced in May and demonstrated the Department's continuing strength as a research powerhouse. 66% of our submission was judged to be 4*, the highest score available, for research quality that is world-leading in terms of originality, significance, and rigour.

There were also some outstanding individual achievements including Peter Hore's election to Fellowship of the Royal Society and many awards and prizes from the learned societies. Professors Iain McCulloch and Charlotte Williams were awarded prizes by the Royal Society, and Professor Dame Carol Robinson received the 2022 Benjamin Franklin Medal in Chemistry. I congratulate my colleagues on their very well-deserved recognition and success.

Five new academic colleagues join us this year as Associate Professors and Tutorial Fellows: Robert Hoye, Adam Kirrander, Michael Neidig, Yujia Qing, and Alice Thorneywork. I am delighted to welcome them to the Department. To the Chemistry Management Board we welcome John McGrady, who became Head of Inorganic Chemistry in September. John takes over from Simon Clarke to whom we are very grateful for his leadership and dedication throughout his term of office.

We are delighted to say that the new Waynflete Professor of Chemistry is Véronique Gouverneur. A renowned fluorine chemist, Véronique joins an illustrious list of distinguished chemists to hold this most prestigious position.

Over the past year, as the pandemic receded, our lives and work have settled into a more normal pattern. We have been pleased to resume a wide range of activities in person, from school outreach visits to events for Chemistry alumni. At our September alumni meeting Iain McCulloch gave an excellent talk about organic semiconductors and the exciting possibilities they offer, one of which is to help reduce our dependence on fossil fuels. This kind of chemistry, which helps us work towards sustainability and net zero, is one of our key research challenge

areas and you can read more about some of the work going on in the Department on pages 28–29.

I look forward to seeing old friends and new again at our next alumni gathering. Meanwhile I would like to thank all our alumni for their continuing support for the Department's work in general, and particularly for their support for our DPhil students. The DPhil provides the formative experience that enables so many Oxford chemists to go on to make exceptional contributions to science and society, and we will continue to make the support of the best and brightest young scientists a top priority. ■

Contents

News and achievements

For more news throughout the year head to www.chem.ox.ac.uk/news

Professor Peter Hore has been elected as a Fellow of the Royal Society. Professor Hore is elected for his pioneering work on the biophysical chemistry of electron and nuclear spins and their effects on chemical reactivity. Using specifically developed spin dynamics simulation methods and sensitive spectroscopic techniques, he has made major contributions to our understanding of how migratory songbirds sense the Earth's magnetic field as an aid to orientation and navigation. Peter has been an outstanding researcher, teacher, and colleague in the Department for many years, and we congratulate him on this very well-deserved success.

Professor Véronique Gouverneur has been elected as a member of the American Academy of Arts & Sciences as an International Honorary Member. Membership in the Academy is a singular distinction, recognising people from a wide range of disciplines who are making extraordinary contributions to society.

Within the Department, Professor Gouverneur has also been appointed as the new Waynflete Professor of Chemistry. First awarded in 1859, the Waynflete Chair has previously been held by organic chemists including William Henry Perkin Jr., Sir Robert Robinson, Sir Jack Baldwin and, most recently, Steve Davies.

The work of Oxford chemists was recognised by both team and individual Royal Society of Chemistry Awards, which celebrate outstanding work and achievements in advancing the chemical sciences.

Professor Emily Flashman was named winner of the Norman Heatley Award for the elucidation of molecular mechanisms of oxygen-sensing enzymes in plants and animals.

Professor Volker Deringer received the Harrison-Meldola Memorial Prize for innovative contributions to the modelling and understanding of amorphous materials.

Professor Tim Donohoe received the Tilden Prize for innovative development of catalytic methods that activate organic molecules by redox processes.

The collaborative and interdisciplinary Molecular Flow Sensor Team, led by Professors Gus Hancock and Grant Ritchie and including Electronics Workshop Supervisor Kevin Valentine was awarded the RSC's Analytical Division Horizon Prize: Sir George Stokes Award. The team developed a non-invasive breath analyser to provide measurements of respiratory disease and cardiac output.

Laura Bickerton (Langton group, DPhil student) was selected as a 2022 CAS Future leader by the American Chemical Society. The programme awards early-career scientists leadership training and a trip to the ACS National Meeting.

DPhil students Katharina Eisenhardt and Michael Howlett were selected to participate in the 71^{st} Lindau Nobel Laureate Meeting, held to facilitate exchange between generations, disciplines and cultures.

Professor Dame Carol Robinson was awarded the 2022 Benjamin Franklin Medal in Chemistry. The award recognises Professor Robinson's work developing techniques for analyzing the interactions of biological molecules such as proteins and lipids, which helps understand their biological functions and aids pharmaceutical discoveries.

Two members of the Department of Chemistry were among the winners of this year's Royal Society Prizes.

Professor Charlotte Williams received the Leverhulme Medal for her pioneering work developing and understanding high performance carbon dioxide utilization catalysts.

Professor Iain McCulloch received the Royal Society Armourers and Brasiers Company Prize for making fundamental contributions to the application of materials chemistry to organic electronic applications, with an applied, results-oriented focus, demonstrating translational impact and commercial potential.

New research

Karen Heathcote reports on some of the latest stories from the Department.

Compton group

Monitoring ocean ecosystems

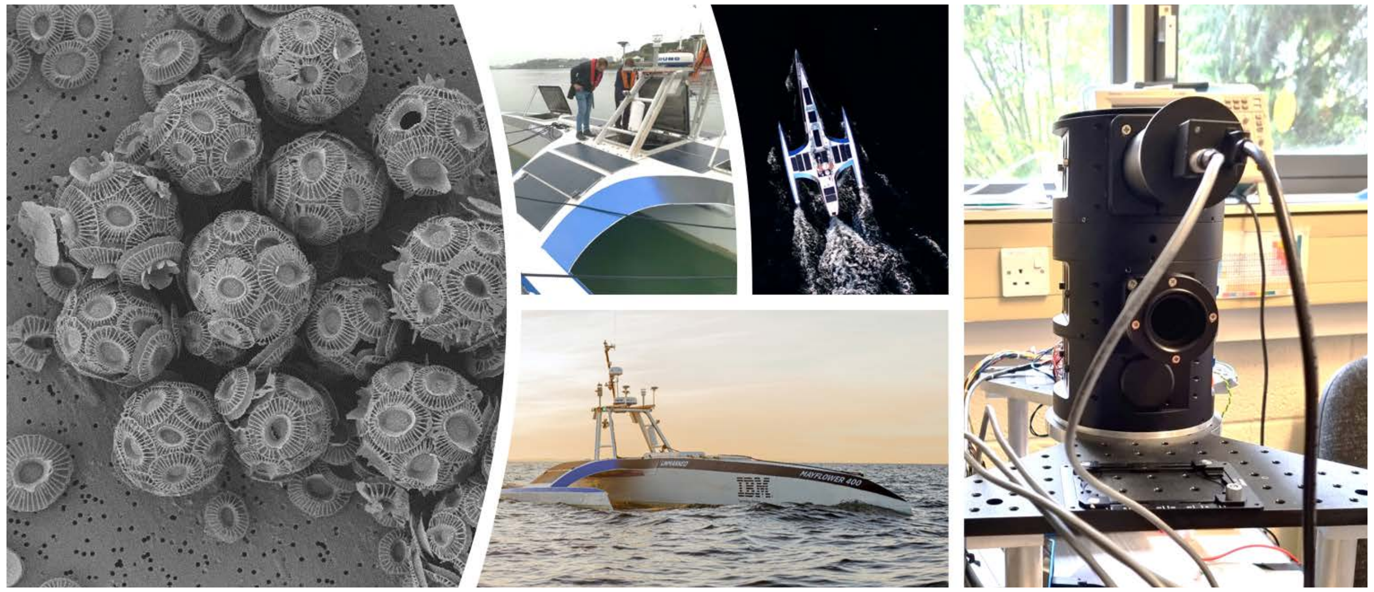
Using electrochemistry to count and identify phytoplankton.

Phytoplankton are microorganisms that live in open surface water. There are thousands of different species of phytoplankton, spanning twelve different taxonomic divisions and ranging in size from 1 to 100 micrometres. These microscopic organisms are responsible for approximately half of all photosynthesis occurring on Earth and play a critical role in the ocean carbon cycle. As phytoplankton are not farmed or fished, changes in their abundance or diversity are a direct indication of environmental pressures such as ocean acidification or rising temperatures. Presently, however, there is no good way to monitor them.

The Compton group has developed a new way to count and, importantly, identify these phytoplankton using electrochemistry and fluorescence microscopy.

All phytoplankton contain chlorophyll-a for photosynthesis, which is fluorescent. In 2019 the Compton group, with Heather Bouman and Ros Rickaby in Earth Sciences, showed how to distinguish between different species of phytoplankton by electrochemically oxidising their seawater environment and monitoring their chlorophyll-a fluorescence. Phytoplankton were placed in a 'fluoro-electrochemical cell', containing a working electrode, to which a strong oxidising potential was applied.

This electrochemically generated radicals in situ, which killed the fluorescence of the phytoplankton at a rate characteristic of the plankton species and reflecting the physical and chemical properties of the phytoplankton's shell and outer membrane. These measurements, together with control of the identity and quantity of the oxidising chemical species formed (via the electrode potential), allows the plankton to be identified at the individual level.



Left to right: scanning electron microscope image of phytoplankton; three images of the Mayflower Autonomous Ship (IBM's AI powered marine research vessel); ocean-going sensor prototype.

The continuing collaboration is supported via an Oxford Martin School project: "Monitoring Ocean Ecosystems". Most recently the team has measured the degree of calcification of individual phytoplankton, using electrogenerated acid to dissolve the calcium carbonate shell, with optical microscopy giving the calcite content of single plankton. Phytoplankton with these calcium carbonate shells are known as coccolithophores and are estimated to sequester more than 10^{15} grams of CO_2 per year. The rate of biomineralization by phytoplankton is key to global carbon dioxide fixation and is crucial data for modelling climate change. A patent application has been filed via Oxford University Innovation (OUI).

To translate the novel chemistry into ocean-going sensors – with participation booked on IBM's AI powered marine research vessel, the Mayflower Autonomous Ship – Jake Yang and Chris Batchelor-McAuley are currently working on a prototype comparable in size to a microwave oven.

Richard Compton says: "Understanding and responding to climate change requires new measurements and bespoke sensors. The latter pose urgent challenges to analytical chemists. Our team has started early in the field and now has two distinct methodologies – one to count and identify plankton, the other to quantify CO_2 biomineralization rates. For maximum and rapid impact we next need to commercialise electrochemical ocean monitoring and are seeking sponsors and investors." ■

Probert group

Maternal microbiome

Links to anxiety in mouse offspring

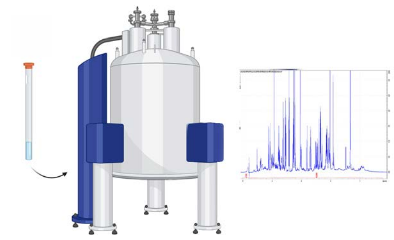
In 2021, one in six children in England were thought to have at least one mental health problem. Studies over the last decade have shown that behavioural issues in children are more likely to occur after exposure to maternal obesity *in utero* and early life.

The microorganisms that live in the digestive tract (gut microbiome) can modify brain chemistry and influence behaviour. So, researchers in Chemistry, Psychiatry, and Pharmacology (Probert, Burnet and Anthony) have been investigating the link between a diet-induced disruption of the maternal microbiota in mice and abnormal behaviour of their offspring.

This study compared the effect of feeding mice a high fat or control diet, and treating those mice with either a probiotic or a control during pregnancy and lactation. The probiotic contained 14 strains of live bacteria, and was predicted to modify the maternal microbiome. Researchers were able to confirm that maternal obesity induces long-lasting negative effects in the offspring, which perinatal probiotic treatment was able to protect against.

Nuclear magnetic resonance (NMR) was used to analyse the levels of small molecules (metabolites) in the gut and brain of mice. One of the most significant findings was increased levels of lactate in the mothers' milk and offspring's brains after probiotic treatment. Lactate has been shown by others to have antidepressant-like effects in mice. In this study, higher levels of brain lactate were linked to reduced anxiety-like behaviour.

Daniel Radford-Smith, the first author on the paper published in *PNAS*, says: 'We were very surprised at how maternal probiotic treatment could instil such enduring brain metabolism and behaviour changes in the offspring. We don't know to what extent these results may translate to humans; however, our study suggests that the maternal gut microbiota and associated metabolites should be considered ... as potentially having an enduring effect on the health trajectory of the offspring.' ■



Samples were taken from mice and maternal milk for metabolomic analysis by NMR spectroscopy. Lactate levels were increased in the mother's milk during nursing, as well as in brain, gut, and liver of the offspring after perinatal probiotic treatment.

Hayward group

The future of lithium-ion batteries

Towards more sustainable cathode materials in Li-ion cells

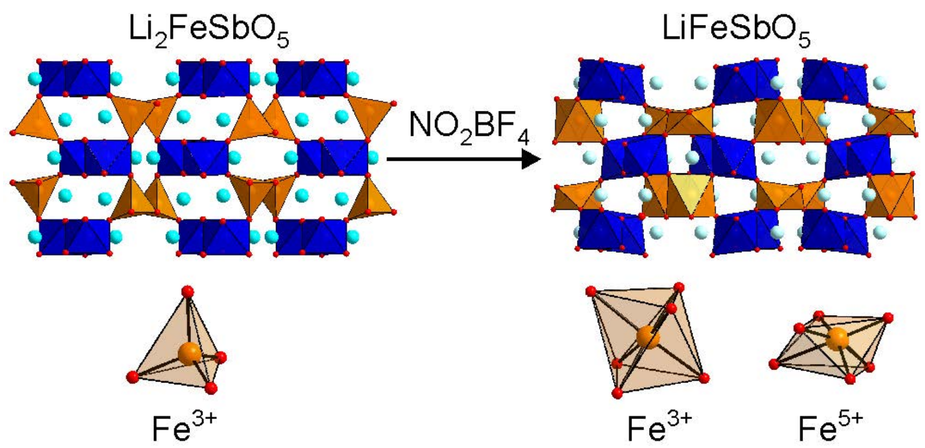
In 2019, Professor John Goodenough was one of the recipients of the Nobel Prize in Chemistry for his research into lithium-ion batteries while Head of the Inorganic Chemistry Lab at the University of Oxford (see p.25). The most common cathode material in rechargeable lithium-ion batteries is $LiCoO_2$ (lithium cobalt oxide). However, there is a need to develop new cathode materials as cobalt is both expensive and toxic. An attractive alternative metal to use is iron (Fe) as it is cheaper, more abundant and much less toxic.

Developing new cathode materials containing iron is challenging for a number of reasons, including: iron cation movement during charging/discharging; structural changes; and unwanted oxidation of oxygen anions.

The Hayward group has been investigating making lithium iron oxide cathode materials using an additional metal as a 'scaffold'. In this paper the metal used is antimony (Sb), to make $Li_{2-x}FeSbO_5$.

Researchers were able to make Li_2FeSbO_5 by first making Na_2FeSbO_5, then performing lithium-sodium cation exchange. This method is useful as it allows unusual lithium structures to be accessed, providing flexibility for cathode materials. A key achievement in this study was extracting lithium from Li_2FeSbO_5 to make $LiFeSbO_5$ without oxidising the oxygen atoms. Instead the iron was oxidised from Fe^{3+} to a mix of Fe^{3+} and Fe^{5+}. Unfortunately, this did lead to a structural change in the material, preventing electrochemical cycling. This project has enabled the Hayward group to identify key issues in production of Fe-containing cathode materials that can be addressed when investigating future alternative cathode materials. ■

Figure top of p.6



Hayward group research: Deintercalation of lithium ions from Li_2FeSbO_5 cathode leads to oxidation of iron, but is accompanied by a structural change that prevents electrochemical cycling. Li = light blue, Fe = orange, Sb = dark blue, O = red.

Williams group

Chemical recycling of polymers

Reforming monomers from plastics to improve industrial sustainability

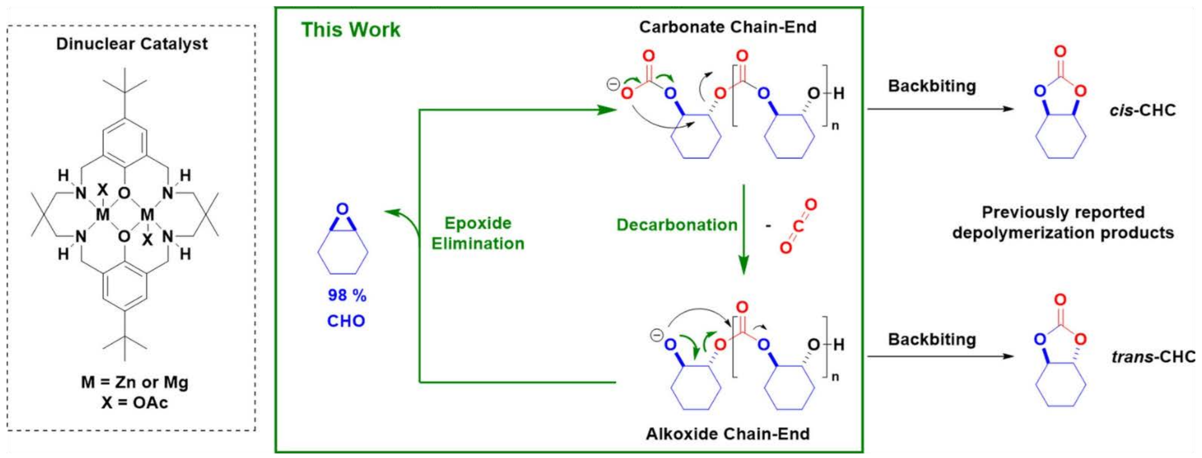
Since entering production in the 20th century plastics have become an essential part of our lives. The UN estimates that approximately 400 million tonnes of plastic are now produced globally each year. One option to help improve the sustainability of the plastics industry is to develop methods of recycling plastic polymers to re-form their constituent monomers.

This is known as 'chemical recycling' and is difficult to achieve. It is not well understood how to catalyse the 'back reaction' in polymer chemistry. Although all polymers have a 'ceiling temperature', above which depolymerization is theoretically possible, very few can be chemically recycled. Chemical recycling is preferable to mechanical recycling, in which plastic is crushed and melted down in order to make new plastic products. Mechanical recycling weakens plastic, whereas polymer properties are uncompromised after re-polymerisation of monomers produced by chemical recycling.

In a recent paper the Williams group, together with the Buchard group at the University of Bath, published the first method of chemically recycling a widely investigated polymer, poly(cyclohexene carbonate), PCHC. The class of catalysts described in this paper are particularly interesting as they are fast in both the forward and back reactions.

Two binuclear catalysts were trialled in this paper; one containing zinc and one magnesium. Both were able to catalyse the depolymerisation reaction, producing the epoxide monomer cyclohexene oxide (CHO) and CO_2. Better selectivity was observed with the binuclear magnesium catalyst than with the binuclear zinc catalyst. The CHO and CO_2 produced could be used in future polymer production. The Williams group had previously shown that the binuclear zinc and magnesium catalysts can be used to catalyse the copolymerisation of CHO and CO_2.

Researchers involved in this project hope that discovery of this new method will inspire investigation of other di- and multi-nuclear catalysts in depolymerisation reactions. ■



Known depolymerisations of poly(cyclohexene carbonate), PCHC, to cyclic carbonates, CHCs. The green box shows the depolymerisation reported by the Williams group, where PCHC is converted to cyclohexene oxide, CHO, and carbon dioxide, CO_2 using binuclear (or dinuclear) zinc or magnesium catalyst.

Explore Chemistry, Ask a Chemist, Virtual Autumn Chemistry Conference, Covid-19 Chiral Chemistry workshop, Plastic Fantastic?, remote interview workshops, ChemA*stery, Poison Puzzle, Lab Lurker, Thiking 3D, Small yet Mighty!, Chemistry Taster Days, Destination STEMM - Chemical Sciences, Target Oxbridge, RSC Women in Chemistry, Power UP!, Women in Science, MPLS Science Together, Chemistry at Home, Primary Science Days, UNIQ, Secondary School Teachers and Technicians Conference, OxBox, ChemBox, Marie Curious Days, Plastic from Another Perspective, Colourful Chemistry, Chemistry in the Gardens, DPhil Outreach Ambassadors...

Outreach update

Interacting face-to-face with nearly 1500 people during one week in July means it is strange to reflect that in-person outreach didn't really begin again until March 2022. Educational Outreach Officer Saskia O'Sullivan reflects on the highlights of the Department of Chemistry's work with schools and the local community over the last 12 months.

Michaelmas 2021 remained very much online, with the continuation of our Explore Chemistry series of career and research talks featuring Q&A sessions with our enthusiastic body of DPhil students. Alongside this we continued to run our Ask a Chemist Q&A sessions, featuring current researchers and alumni.

Our second Virtual Autumn Chemistry Conference focused on 16 to 19-year-olds, attracting a global audience, whilst our online interactive Covid-19 Chiral Chemistry workshop continued to be popular with sixth formers. We piloted a brand-new primary workshop, Plastic Fantastic?, with materials sent to the school in advance, and the session co-led by members of the Department online with the class teacher in school. We also took the opportunity to record our lecture demonstration on All Hallows' Eve and Bonfire Night, co-delivered with the University of Bristol.

November saw the return of remote interview workshops for virtually all undergraduate courses. It is good news that this valuable programme, pioneered by Chemistry, has now been fully adopted by the central university for 2022.

Aware of the challenges the pandemic has brought to students in secondary education, the Department ran a nine-week online programme called ChemA*stery, focusing on the most challenging topics of the A-level syllabus. This pilot programme of small group support for offer holders with their academic pre-university course is the first of its kind amongst departments and faculties across the University, and participants reported a growth in academic confidence and sense of belonging during the Hilary term.

Last year we developed three workshops destined for colleges: Poison Puzzle, Lab Lurker and Thinking 3D, and these highly enjoyable and interactive workshops have been much in demand since the return to in-person outreach in Hilary, reaching nearly 700 young people. Feedback from colleges, teachers, and students taking part has been stellar.

A successful application to the PER Seed Fund allowed the development of a workshop for 14 to 16-year-olds focused on research into artificial enzymes. The aptly named Small, yet Mighty! workshop considers the role of enzyme fuel cells as potential solutions to climate change and the energy crisis.

The number of Chemistry Taster Days for Year 12 increased with Trinity College and St John's joining Balliol in hosting. These provide excellent opportunities for

Clockwise from above: Master Glassblower Terri Adams gives a demonstration at the Secondary School Teachers' and Technicians' Conference; celebrating success at our Poison Puzzle activity; students consider the role of enzymes as catalysts.

University Chancellor, Lord Patten, visits the Chemistry Teaching Laboratories and meets UNIQ summer school students.

Plant practicals, quizzes, chilli tasting, and talks with Q&A at the Oxford Botanic Gardens' 400th Anniversary celebrations.

participants to engage with tutors as well as current students, hearing talks, touring the college, taking part in interactive workshops and Q&As, as well as finding out more about admissions. A partnership with the RSC and Windsor Fellowship ensured young people on the Destination STEMM – Chemical Sciences programme joined us for a similar day at Hertford, whilst Target Oxbridge participants enjoyed a short-form presentation in August.

We continue to promote diversity in the chemical sciences through our thriving RSC Women in Chemistry project, hosting three multi-institution online events featuring women at different points of their careers. Meanwhile, our Girl Guide adaptation of the Oxford part of this project, Power UP!, received a thumbs-up from a local Oxfordshire patrol who kindly piloted this for us.

Recognising the interdisciplinary nature of research, the department played an important role in the Wadham-Jesus-Trinity Colleges Women in Science day in June, kickstarting the event with the keynote address, as well as providing speakers and an interactive workshop. This interdisciplinary awareness also saw us facilitating an MPLS Science Together project involving the Oxfordshire Play Association and researchers from both the University and Oxford Brookes, resulting in the production of a wide-ranging report on the value of play for Oxfordshire communities.

To support and promote high quality engagement between parents and young children, the department has produced a series of Chemistry at Home resources. Additionally, the department led on the organisation of two MPLS Primary Science Days, partnering with Trinity College and the Oxford Hub to offer places to over 200 students from disadvantaged backgrounds. The days consisted of practical workshops focusing on Chemistry, Physics, Earth Sciences, Materials, and Nanotechnology, before students enjoyed a tour of Trinity College and an engaging lecture demonstration highlighting current research in the department.

In addition to the return to live lecture-demonstrations delivered at schools, in the Inorganic Chemistry Laboratory, and colleges, in-person outreach meant we were able to have students back into the Chemistry Teaching Laboratory (CTL), undertaking laboratory days at Easter and in Trinity term. The CTL also hosted our UNIQ programme, the University of Oxford's access programme for state school students, which prioritises places for students with good grades from backgrounds that are under-represented at Oxford and other universities. Having had few practical opportunities during the pandemic, the students relished the opportunity to get hands-on with the kit, as well as greatly enjoying the small group tutorials, whilst lectures and a panel event rounded off the programme. We were delighted to host the University Chancellor, Lord Patten, which gave him a chance to see the fantastic facilities on offer for both current and prospective undergraduates.

The CTL hosted the inaugural Secondary School Teachers' and Technicians' Conference in July 2022, alongside St. Anne's. Fitting for the UN International Year of Glass, delegates enjoyed an absorbing lecture demonstration on the importance of glassblowing. The conference included talks linking cutting edge research to the curriculum, a consideration of effective explanations, and a series of workshops focused on practical resources for teaching chemistry. It wasn't just experienced teachers who benefited from support, with the Oxford PGCE Science cohort joining us on a separate occasion. Feedback to the Department of Education indicated this had been one of their very best experiences of the year!

Away from the CTL, support for teachers and teaching assistants in primary schools remains the focus of our OxBox project. The ChemBOX trial is complete and there are three sets available for the ten schools in our pilot area in Gloucester. The Departments of Earth Sciences and Physics joined the Chemistry team in July to trial activities for an EarthBOX, and a PhizzBOX, which we hope will be ready for piloting in late Michaelmas 2022. Our collaboration with the Department of Physics continued with the provision of enjoyable workshops for two Marie Curious Days, targeting girls aged 11 to 14.

Beyond Oxford, we visited schools and colleges, including a roadshow to Derbyshire in May, working with Teddy Hall to identify the most appropriate schools in their link region. Our Plastics from Another Perspective workshop, which focuses on sustainability, as well as instrumental techniques, allows students the welcome opportunity to interact with the researchers, whilst our newly developed A-level practical lessons, Colourful Chemistry, focus on supporting the practical requirement, yet provide an interesting context and application for students to boost engagement.

July continued to be a busy month with a week of events in the Botanic Gardens, in celebration of their 400th anniversary. Visitors found out more about chemistry and the research in the department through interactive demonstrations, short talks, a molecular treasure hunt, as well as plant quizzes, and highly enjoyable hands-on practical challenges in our Chemistry in the Gardens tent.

The Department's outreach continues to grow from strength to strength due to the commitment and support of so many members. A challenge for the team is how to sustain our programmes and continue to ensure they are relevant to young people and their supporters. To that end, a new scheme offering DPhils the opportunity to have greater responsibility for programmes is being launched in November 2022. Through a grant extension, DPhil Outreach Ambassadors will be able to devote some time in their second year to managing and developing the outreach programmes.

We would be incredibly grateful for any financial support for our outreach programmes, including the involvement of DPhils. ■

A gift to Oxford Chemistry Outreach will help bring chemistry to life and make a chemistry degree or career a reality for students from every background.

You can make a donation at oxgive.info/3QwhG4T or contact Jane Rice, Senior Development Manager, for information.

jane.rice@chem.ox.ac.uk

Physical and Theoretical Chemistry Laboratory,
South Parks Road,
Oxford OX1 3QZ

The power of a DPhil in the lab and beyond

Val Rahmani finished a DPhil in 1981 with Professor Graham Richards CBE FRS and in collaboration with ICI. She sat down with current DPhil student, Heike Kuhn, to share how her DPhil helped shape her career.

Val began her Oxford journey after her physics teacher took her on a tour, trying to encourage the bright student to apply for an undergraduate degree. Whilst Val ended up choosing chemistry over physics, she heeded her teacher's advice and gained a place at Somerville for her undergraduate degree.

When it came time to choose a supervisor for her Part II, she hesitated to approach Professor Graham Richards for a spot in his lab, given that she was slightly intimidated by her smart and fast-thinking quantum mechanics lecturer. "I thought that he was so smart and it's so complicated and there's no way I'll ever get to do that."

> *A DPhil certainly gave me … the ability to thrive when you're thrown in at the deep end. That's perfect because after that you get this sense of 'give me a problem and I'll work on it and solve it'*

Val Rahmani and her former supervisor, Graham Richards.

However, a visit to his lab convinced her that computational chemistry and developing computational models was the right focus for her. "My advice is don't be scared of stuff. There I went [to his lab] and I knew immediately that's what I wanted to do."

People might not always realise how diverse chemistry can be, but Oxford Chemistry truly exemplifies the breadth of the subject, and how different a day of research can look to different people. Whilst the wet lab might still be the 'classic' image of chemistry, Val's time was spent in the computing lab.

"That was what I really enjoyed doing. It was in the very early days of computing and I managed to get access to the Gaussian software program and access to the computing centre, so I spent significantly more time during my DPhil doing computer work than I ever did doing what you would traditionally call 'chemistry'."

Time management played a key role during her time at Oxford. For her, this meant spending nights running computing jobs when things were less busy there. This had the additional advantage of freeing up time for her passions, such as ballroom dancing. "It worked really well for me because it meant you had time when you wanted it to do other things. So, a key skill you gain during your DPhil is how to manage your own time and work in a way that suits you, which might be very different from what suits someone else."

Val's extracurricular activities proved to be a truly valuable addition to her academic experience. "I was running the ballroom dance club and we took it from nothing to being the university champions of the time. We built ourselves a team, we got a teacher, we got costumes, we hired halls. So that taught me a lot about areas like selling, because you had to be raising money and getting people to join and pay their fees and persuading teams to come together. I think that was really huge for me."

Throughout her studies, Val gained valuable confidence in her problem-solving abilities. "I think the other thing a DPhil certainly gave me, and I suspect gives everybody, is the ability to thrive when you're thrown in at the deep end. That's perfect, because after that you get this sense of 'give me a problem and I'll work on it'. And it doesn't really matter what you apply that to, but once you've learned how to do that, you realise that you could probably do it in any environment."

Val has an immense respect for the work of her former supervisor Professor Graham Richards, with whom she is still in touch. She credits him as a driving force in helping her realise the potential of connecting research with commercialisation and industry. "He is very commercially-minded, and a really good scientist as well. He taught me how to think and how to sell."

Today, there is a big platform for the commercialisation of research within the University of Oxford and students are encouraged to think about potential patents and spinouts from the start of their research careers. University subsidiaries, such as Oxford University Innovation, which specialise in technology transfer and consulting, are there to help students and researchers commercialise their research. "Graham was a real instigator of that. He wrote books on it, he gave talks on it and worked really, really hard to start making that come to life, because years back it just wasn't there."

The Department of Chemistry maintains strong relationships with industry partners through collaborative research and programmes such as the Oxford Inorganic Chemistry for Future Manufacturing Centre for Doctoral Training. Val reflects fondly on her collaboration with industry partner ICI during her DPhil. "ICI were wonderful at helping me with research and with some of the production of my DPhil. Not only did they do the physical experiments, which was critical because the whole idea was to compare my computation with their real-life findings, but they were also a great sounding board. I spent a lot of time with them because what they were doing was really interesting to me, and I think they were also very interested in what we were doing."

An IBM recruitment event became the catalyst for the future of her career in technology. "I ended up going into IBM as a systems engineer, but with every intention of becoming a salesman as soon as they would let me. I don't think I would ever have thought of doing that if it hadn't been for the commercial approach that we took in the lab. And that sounds strange because we clearly were a lab, but there was always a consideration of what our work could do commercially, which I had never thought about until then."

Her advice for the next generation of students is something that will hopefully resonate with many others as well. "If a great opportunity comes up and it sounds interesting and it moves you forward in some direction, any direction – have a go at it. You should take whatever opportunity intrigues you because everything you learn is going to move you forward – it really doesn't matter what it is."

She clearly took her own advice, not having been set on a postgraduate degree and having taken the opportunity when it presented itself. "I'm just so pleased I joined Graham's group. It wasn't what I had thought about doing. I hadn't thought about a DPhil at all and then when I did, I don't think I thought about doing it in something that was essentially computational chemistry. As it turns out, that set the whole path for everything I've done since."

Whilst it is essential to be excited about your DPhil project, not everyone needs to have a clear vision of their future career to pursue graduate studies. Students use their DPhil experience for a wide range of opportunities, in academia, industry and in many other sectors.

"A DPhil is a pretty awesome thing to do, actually. And I truly do think it can take you in any direction because you're learning how to do all these things and, most importantly, how to trust yourself." ■

Since completing her DPhil in 1981, Val Rahmani has had an impressive career in the technology industry and is currently a non-executive director for a range of companies, including the London Stock Exchange and RenaissanceRe. She spent the majority of her career at IBM, where she had roles including General Manager of: IBM Internet Security Systems; a $2.7 billion Global Technology Services business; a $3.5 billion UNIX server business; and IBM's Mobile business. Val left IBM after 28 years, and has since been CEO of Damballa, Inc. and part-time CEO of the Innovation Panel of Standard Life Aberdeen plc. When she's not working Val flies aerobatics, dances street jazz and is attempting to surf.

Heike Kuhn is a fourth year DPhil student in Professor Paul Beer's group. She is interested in supramolecular chemistry and her current project in the Beer group involves the synthesis and study of dynamic, halogen bonding interlocked structures for anion recognition and sensing.

Would you like to share your DPhil story?

Please get in touch with Jane Rice, Chemistry's Senior Development Manager, if you'd like to share your experiences and advice with a current DPhil student. We hope to publish future interviews on our website.

jane.rice@chem.ox.ac.uk
Physical & Theoretical Chemistry Laboratory,
South Parks Road,
Oxford OX1 3QZ

Out of the lab...

DPhil internships

Tristan Johnston-Wood and Stamatia Zavitsanou, DPhil students in Fernanda Duarte's research group, both work on computational methods to predict the outcomes of organic reactions using machine learning. Periodic caught up with them about the exciting placements they've recently completed alongside their studies.

Why did you decide to do an internship? How did you apply to and get the post?

Tristan I was interested in an internship at the Government Office for Science to see how decisions and policies in science affect our lives. The UKRI Policy Internship Scheme allows UKRI funded postgraduate students to take three months out of their studies to do an internship in policy.

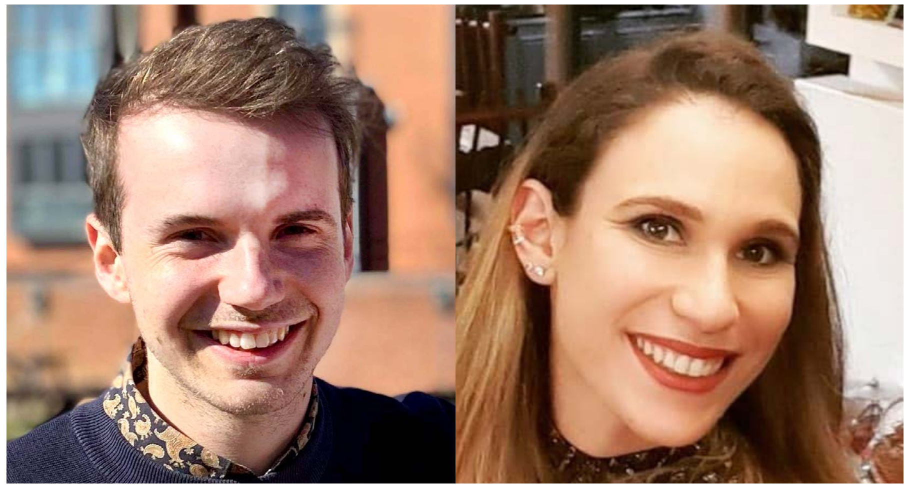
Stamatia My supervisor shared an advert with our research group for a research scientist position at IBM, applying machine learning to carbon capture technologies. The project was very interesting, and relevant to what I was doing in my DPhil – I soon realised I would have the chance to learn from the best.

Can you tell us about a typical day on the job?

Tristan I was placed in the Science, Systems & Capability team, looking at how research funding is allocated across public sector research establishments and also at the Government's current focus on AI. The internship was for three months in 2021, and I was working remotely. A typical day working from home involved a mixture of Teams meetings, reading government policy papers, and writing new policy.

Writing was a long process, deliberating between ourselves as well as talking to experts from outside government. Part of my work also involved coding, and I got the chance to produce data analysis that was presented to the Chief Scientific Adviser, Sir Patrick Vallance.

Stamatia My internship was for a whole year, but because of the pandemic my work was also done from home. The days started slowly catching up on emails and preparing for meetings – I met my supervisor twice weekly to discuss progress, ideas, and problems very informally. After our meeting I'd implement what we'd discussed, perhaps writing code or running calculations. Once a week I'd also meet the rest of the team, discussing progress and priorities.



Tristan Johnston-Wood (left) completed an internship at the UK Government Office for Science, and Stamatia Zavitsanou (right) at IBM.

What lessons did you take away from the experience, and how does it relate to your studies in Chemistry?

Tristan I found it particularly interesting to see how science impacts society from the other side, compared to my day to day DPhil research. The decisions we made would reach many people, but progress was often slow making these decisions. It opened my eyes to the importance of the allocation of money for research, as well as the complex application processes scientists have to complete to get this funding.

Stamatia Actually, the project I was working on was highly relevant in itself to my studies. I had the chance to learn about new machine learning implementations, improve my coding skills, and produce science that I can now use back in my own DPhil studies.

Do you have any advice for young chemists looking to work, or do internships, in similar areas?

Tristan I'd highly recommend applying to the UKRI Policy Internship Scheme to any PhD students interested in science policy. It gives you the opportunity to try policy work without the full commitment of applying to a graduate job, and an opportunity to tackle problems from the top-down, as opposed to research which can feel bottom-up.

Stamatia My advice would be to go for it! I had a great time, learnt a lot, and it was even relaxing sometimes compared to a DPhil – plus I had the chance to work with many people who are experts in the field.

Before the internship I was considering doing postdoctoral research, but IBM offered me a permanent position and so I agreed to return after I finish my studies – on top of this, the last part of my DPhil will now be in collaboration with IBM.

Any final comments?

Tristan Although I didn't get a chance to work at the London office, we did meet up as a team later on – talking to each other on Teams made me assume that everyone was the same height, but after we got the chance to meet up in person we all laughed about how different in height we all were, especially one of the Oxford rowers on the team!

Stamatia Like Tristan, I was mainly interacting with my team over video meetings, and I must mention how friendly and supportive everyone was at IBM. They made me feel part of the team from day one, listened to and valued my opinions, and they were happy to mentor me every day.

Something I am very proud of is that in one year I contributed to three papers as well as a patent, and I can't wait to see them published. ■

Professor Wasielewski's research focuses on light-driven processes in molecules and materials, covering areas from artificial photosynthesis and molecular electronics to quantum information science, ultrafast optical spectroscopy, and time-resolved electron paramagnetic resonance (EPR) spectroscopy.

Generously sponsored by Refeyn Ltd., the title of Professor Wasielewski's series of six lectures was *Exploring and exploiting quantum coherence in molecular systems for solar energy conversion and quantum information science.*

Named for Sir Cyril Hinshelwood, a Nobel Prize-winning chemist who was Dr Lee's Professor of Chemistry at Oxford in the early part of the 20th century, this was the first time the lectures took place in person since 2019 because of the Covid-19 pandemic.

Covering singlet fission and charge separation in solar cells, artificial photosynthetic systems, and spin dynamics of quantum information systems, Professor Wasielewski gave an enlightening tour of his recent research, which throughout his career has resulted in over 750 publications.

Professor Wasielewski is a member of the National Academy of Sciences and the American Academy of Arts and Sciences, and in 2022 he won the Faraday Division Lectureship Prize. ■

Professor Michael R. Wasielewski

The **science** of **baking** to **perfection**

Dr Katarina Cermelj (Balliol, 2012) is a baker, recipe developer, food writer and photographer. After moving to Oxford from Slovenia ten years ago, Kat completed her MChem in 2016 and went on to do a DPhil in the O'Hare group, which she completed in 2020. Along the way, she also founded a successful baking blog and published an award-winning book of gluten-free recipes, Baked to Perfection. Kat talks to Periodic about her extraordinary achievement and her two loves: baking and chemistry.

Which came first for you, chemistry or baking?

Both! Science and baking were always my interests. When I was little I had lots of discussions with my dad about science and used to ask him all kinds of questions. My mum is an amazing baker, and I always used to help in the kitchen, so those two things were always there. By the last year of my high school in Slovenia though, I decided that I really loved chemistry and I imagined then that chemistry and research would be my career.

You started your hugely successful blog, The Loopy Whisk, when you were still a student. Can you tell us about that?

I started the blog between my undergraduate and DPhil. I had always followed food blogs and wanted to start one, but I had never had time as undergraduate years were very busy. Then during the summer before starting my DPhil I thought: if I'm ever going to start a blog I should do it now.

Also, I was experimenting more and more with gluten- and dairy-free recipes, because at the time I had had to eliminate both of those things for health reasons. I started incorporating more of my science background into my recipes, and that's when I realised I could enjoy doing both science and baking together.

How did you come to write a book?

Actually, it was a complete coincidence. I was thinking about starting my DPhil thesis, so I would never have thought of starting a book at the same time. But I received an email – which I almost deleted thinking it might be spam – from someone at a literary agency in London (who later became my agent) saying: "Would you consider writing a book?"

I started talking to her and that's how the book eventually came about. I thought if I didn't say yes, I would always regret it. I knew I wanted to do a book about gluten-free baking and I thought if I could somehow incorporate science into it that would be perfect. So we began writing the proposal, sending out to publishers, and so on – it was nerve-racking but very exciting.

How did you manage to write a book, maintain a blog and do a DPhil all at the same time?

I spent all my weekdays in the lab, and evenings and weekends were for the book and the blog. My sleep schedule suffered a bit! But I enjoyed everything, which made it much easier. I loved going to the lab and I loved baking and shooting photos, so it was all worth it. And it was good to be able to bring in the results of my baking for the O'Hare group to sample and give their feedback!

How did your scientific training help with your baking and writing?

People often imagine that the way in which the science would help most would be in understanding the reactions that occur in baking, but I think it is more important in my approach to developing recipes – that is the crucial thing. Knowing how to set up an experiment – even if it is a baking experiment – is what helps. Being able to change individual variables is important, especially with 'free from' baking.

The science also helps with knowing how to think about the ingredients. For example, right now I am working on egg-free swiss rolls, which is tricky. But when you look at the ingredients and see that egg yolks provide fat and moisture, and egg whites provide lift and structure, and start thinking about their properties and alternatives, like you would in a chemistry experiment, you realise that it is easier than you might first imagine.

Do you find that people are surprised to realise there is such a strong connection between science and baking?

I think people are starting to make the connection, and some of the connections are obvious; baking soda is basic and will react with an acid, and so on. I was surprised when I was researching for the book that although there are quite a few scientific general cookbooks, there wasn't much specifically on baking. And baking is quite a quite a precise and scientific thing, especially 'free from' baking, where you do need to understand what is going on if you want things to work.

Your book has lots of helpful scientific explanations and illustrations. What made you decide to take that approach?

I know from the comments I get on my blog that people are always tempted to tweak things, and if they don't understand how a particular recipe is designed to work, things can fail. And if things do go wrong it is helpful to understand why. I think that having lots of notes and explanations is super-useful for the reader, it's not just for my inner nerd!

Your book has been through quite a few reprints now and won awards from Fortnum and Mason and the Guild of Food Writers, as well as being a finalist in the IACP Cookbook Awards 2022. Congratulations! How do you feel about your success, and what is next for you?

It has been amazing, and I'm so thrilled that one of the things people love most about the book is precisely the science aspect. As for the near future, I am continuing to work on the blog, and am currently enjoying getting to grips with TikTok, because everybody wants to see videos of recipes.

I'm also slowly building up an even larger and more extensive arsenal of 'free from' recipes: vegan, gluten-free, egg-free and so on. I like being creative and doing so many different things; I feel like I am still doing science, and I am also doing photography and so many other things – I'm really just enjoying the whole process.

Do you have any advice for aspiring young scientists considering a degree in chemistry?

I think that regardless of where you end up career wise, a degree in chemistry or in science in general gives you everything you need to succeed in pretty much any career.

Fellow students from my undergraduate year have gone on to so many different careers, and it is not so much the chemistry knowledge that's important – I speak from personal experience that some of that gets forgotten! But I think a chemistry degree equips you with a certain intuition and the ability to approach any problem in a systematic manner, which makes it much easier to understand what you are doing and solve problems. And that can help you in all aspects of your life and career.

Also, chemistry teaches you critical thinking. In the current age of so much information online, knowing how to find reliable information is really important. I would say that if you come to Oxford for a chemistry degree, regardless of where you end up, you'll be very thankful for it – I certainly am. ■

Katarina's book, Baked to Perfection, is published by Bloomsbury Publishing (ISBN 1526613484).

The delicious recipe below is reprinted by kind permission of Katarina and her publishers.

Gluten-Free Lemon Drizzle Cake

Serves 10 | Prep time 30 min | Bake time 1 hour | Storage 3–4 days in a closed container

Absolutely loaded with lemon zest, this cake couldn't be more lemony if it tried. It also boasts the most perfect, moist, delicate crumb that pairs wonderfully with the lemon icing – especially when the icing dries into a crackly, refreshing, sugary goodness. The cake isn't overwhelmingly sweet. Instead, it is fragrant, aromatic and impossible to resist.

Loaf cake

200g plain gluten-free flour
*65g almond flour **
200g caster sugar
3 tsps baking powder
½ tsp xanthan gum
¼ tsp salt
225g unsalted butter, softened
zest of 3 unwaxed lemons
4 medium eggs, at room temp.
120g whole milk, at room temp.
6 tbsps lemon juice
1 tsp vanilla paste

Lemon icing

120g icing sugar, sifted
7-8 tsps lemon juice

Loaf cake

Adjust the oven shelf to the middle position, pre-heat the oven to 180°C and line a 900g loaf baking tin (23 x 13 x 7.5cm) with baking paper.

In a large bowl, sift together the gluten-free flour, almond flour,* sugar, baking powder, xanthan gum and salt.

Add the butter and, using a stand mixer with the paddle attachment or a hand mixer fitted with the double beaters, work the butter into the dry ingredients until the texture resembles coarse breadcrumbs.** Add the lemon zest and mix well.

In a separate bowl, mix together the eggs, milk, lemon juice and vanilla paste. Add the wet ingredients to the flour mixture in two or three batches, mixing well after each addition, until you get a smooth cake batter with no flour clumps.

Transfer the batter into the prepared loaf tin, smooth out the top, and bake for about 1 hour or until risen, golden brown on top and an inserted toothpick comes out clean. If it starts browning too quickly, cover with aluminium foil (shiny side up) and continue baking until done.

Allow the cake to cool in the loaf tin for about 10 minutes, then remove from the tin and transfer to a wire rack to cool completely.

Lemon icing

Whisk the icing sugar and 6 teaspoons of the lemon juice together until you get a thick mixture. Add a further 1-2 teaspoons of lemon juice, mixing well, until you get a runny icing consistency that coats the back of a spoon.

Drizzle the lemon icing on top of the cooled cake, spreading it evenly with the back of a spoon and letting it drip down the sides.

Notes

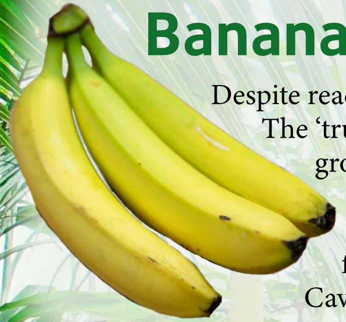
*Almond flour keeps the cake moist for days (see p.35 of *Baked to Perfection* for more details). You can substitute it with an equal weight of gluten-free flour if you like, but the cake will dry out faster.

**The reverse creaming method (see pp.38-39 of *Baked to Perfection*) gives the cake a smooth, velvety crumb.

Chemistry in the garden

A team from the Department of Chemistry has been working with Oxford Botanic Gardens to develop a virtual and digital tour as part of the gardens' 400th anniversary celebrations. The tour details the interesting science of selected plants, and their connection to research happening in the Department.

The tour, which will be available online with 360-degree images of the gardens, will unveil the hidden chemical world of dozens of plants around the gardens. Each plant is explored in five sections, covering the appearance, scientific background, everyday use, history, and research connections of the plants. Periodic had a sneak preview at one of the entries prior to the tour's publication...



Banana *Musa acuminata*

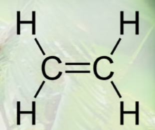
Despite reaching heights of around nine metres, banana plants are in fact herbs rather than trees! The 'trunk' is not woody but is instead formed of the stalks of the large arched leaves which grow from an underground plant stem called a corm. Mature trees are able to produce a single large purple flower, known as a banana heart, from the end of each stem and it is from this flower that the clusters of fruit develop. Bananas are technically classified as berries and around seventy species have been identified including the familiar Cavendish banana, the wild pink banana, and the inedible scarlet banana.

Look around...

Bananas are the fourth most cultivated crop globally and are of huge significance in cuisines across the world. Whilst in the UK bananas are generally enjoyed as a sweet fruit, the term banana actually applies to any fruit produced by a species from the *Musa* genus and includes plantains and many other seeded varieties. Plaintain (or cooking banana) is much starchier than the familiar dessert banana and is a staple food in many tropical regions, featuring particularly heavily in South Asian cuisine. The large fleshy flowers are also sometimes consumed as a vegetable and have a similar flavour to artichoke.

Look deeper...

Have you ever noticed that fruit ripens more quickly if it's next to a banana? This is because bananas release a gas called ethylene, a plant hormone which regulates processes such as growth and aging by temporarily switching specific genes on or off. For bananas, ethylene triggers the production of an enzyme called amylase which breaks down starch into sugar and gives the fruit a sweeter flavour and softer texture. The amount of ethylene released by bananas is actually relatively small, but other popular fruits such as apples and pears are so extremely sensitive to this plant hormone that the ripening effect is much more significant!


ethylene

Look back...

The modern dessert banana was first introduced to South America by Portuguese colonists who began plantations in Brazil and the Atlantic Islands in the 16th century. However, it wasn't until the mid-19th century that consumption of this fruit spread to North America and began to gain popularity. American corporations sought to capitalise on this, opening new plantations across Central America. These companies focused on profits through exports and contributed very little to the local economy, often manipulating local politics to support their business interests. This gave rise to the term Banana Republic, and although fair trade practices have reduced the exploitation of these countries by larger economies, the working people still face many challenges.

Look forward...

Ethylene is not only important as a plant hormone, it's also the major component in common plastic. Plastics are polymers, meaning that they are large molecules produced by the reaction of many identical small molecules. Polyethylenes (also known as polythenes) are the polymers produced from the reaction of ethylene and may be broadly categorised into three groups: high density, low density, and linear low density, each with different properties depending on how the individual molecules of ethylene are connected. The O'Hare group has recently developed a new catalytic system for the polymerisation of ethylene, carefully designing the catalysts to enable them to subtly control the properties of the plastic produced.

Enjoyed our preview? Look out for news on the full tour, coming soon at www.chem.ox.ac.uk and the Department of Chemistry's social media pages!

Bringing science & ventures together

Dr Alan Roth, Royal Society Entrepreneur in Residence and Visiting Lecturer in the Department, talks to Periodic about his work to help academic scientists succeed in the world of innovation.

You did a chemistry degree and PhD in the United States, then came to Oxford to do postdoctoral work with the late Professor Sir Jack Baldwin before moving into the business world. Can you tell us about your career?

I enjoyed my postdoctoral work and then took up an academic position in chemistry. During that time I was asked to do some consulting work for (global management company) McKinsey and Co., and although I was initially unsure about it, I ended up working there for around three years after my academic appointment.

The experience was formidable and a very steep learning curve for an academic scientist, but I got to learn about innovation and business very quickly. I decided to continue to combine science and business and then worked with Commerzbank, a major financial institution that hired specialists like me to look at companies – primarily pharma and biotech companies – to analyse their pipeline and plans to develop new molecules and predict how well they were going to work.

> *"By teaching science students and academics about business, you can optimize the results, interaction, and dynamic between the two sides*

I headed up a team that looked into pharma and biotech, medical devices, and the chemical industry. At that time there was a great flourishing of biotech around the world with very many companies being created and needing funds, so it was very exciting. Being an investment researcher was a very interesting situation to be in because you could really help to optimize how new medicines and products got developed.

My next move came after a conference in China at which I met a former academic colleague who was at Stanford. He was setting up a company based around his work in chiral chemistry, my particular area of expertise, and wanted some advice. We had a series of meetings during which we concluded that we could definitely make a successful company, and that led to the formation of Chiral Quest.

Coincidentally, during that time, Barry Sharpless was awarded the Nobel Prize for his work in chiral chemistry, so it was an exciting time to be working in that field and to be able to combine all I had learned in business with my experience in chiral chemistry. We were fortunate that Barry subsequently joined us as Head of our Scientific Advisory Board! I obtained funding, built up the business and took the company public as CEO in the United States.

It was a dream job in many ways, but it didn't come without challenges – the investment landscape for early-stage companies in New York is tough – but we succeeded, and now Chiral Quest employs over 300 people, we can run complex ton-scale chiral reactions with over 99% ee (enantiomeric excess) and serve around 15 of the top pharma and biotech companies with chiral intermediates for well-known drugs.

After that I set up another firm called Fitzroy Partners which helped to develop early-stage enterprises, as well as more mature biotech companies wanting to develop their business and pipelines.

Today, back in academia in the Department, I am able to share the story of all my experience with my students. They are fascinated to learn about the world of science-based entrepreneurship and the challenges of being on the sharp edge of translating laboratory innovation into real world benefits.

You returned to Oxford a few years ago with an idea to share your expertise in the world of science-based entrepreneurship with students and academics. What did you do?

I conceived and built a course I named 'Scientific Entrepreneurship'. Initially I ran it as a pilot with chemistry and biochemistry students to see if it would fly; I was convinced that no one would sign up!

I had spent over a year preparing all the material which contains textbook academic information together with experiences from my own investment and entrepreneurial work, and it quickly became apparent that people liked it. So for the second cohort we took it to a new level and opened it to a wider range of students.

Now I have students from across

Dr Alan Roth

all the sciences and from medicine, engineering and social sciences. This year 138 people from across all departments signed up for the course, which gives us a balance across different groups and creates a good atmosphere.

Could you tell us more about the course and the kind of people it is aimed at?

It is a modular year-long, three-term course open to postgraduate students, postdoctoral researchers, and academics across the sciences, medicine and engineering. The first term covers theoretical work – a rigorous study of the foundations plus cases – and the second part consists of simulations and special topics. In the third term we offer an entrepreneurial project where students come up with an entrepreneurial idea and develop it.

The course attracts a wide range of students – some people take it because they are just interested in knowing more about the world of business, some want to learn how best to collaborate with industry during their academic careers, and others because they would like to explore how to have both an academic career and develop a spinout company, which is increasingly common nowadays.

What we seek to do is to elevate the level of understanding and effectiveness in the relationship between scientists and business people. The course makes scientists aware of the mindset, concepts and objectives of the business world so that when they do come into contact with that world – either in an industry collaboration, beginning a spinout or a startup, or even if they want to join industry as a career – they feel much more comfortable and have greater impact. Ultimately, the objective of the course is for society to benefit from science-originated entrepreneurship. By teaching science students and academics about business, you can optimize the results, the interaction and the dynamic between the two sides.

How has the course been received?

The feedback has been overwhelmingly positive, and the course is now oversubscribed every year. Almost 40% of students on the course are women, the students come from a wide range of nationalities and academic backgrounds, and we have already created 16 spinout and startup ventures from the course.

I find teaching so interesting – seeing scientists like me coming out from their labs to learn how to think differently. Scientists do this very well if they are given the right tools – and we are solving innovation-related Harvard Business School cases after only a few weeks! It is fascinating to see science people discovering how the entrepreneurial world works.

You are also CEO of Oxford Drug Design, the biotechnology company created by former Chairman of Chemistry Professor Graham Richards. How do you combine your role as a busy CEO with teaching?

It works beautifully well. I learned from my undergraduate supervisor (the Nobel Laureate Roald Hoffmann) that there should be a positive tension between research and teaching and I feel that positive tension now. Oxford Drug Design is a cutting-edge research company that is further developing the fundamental work of Graham Richards to discover novel therapeutics. I am grateful to be able to play a part in that, and believe that to practise what one teaches is really the optimal way.

Of course, there is always a managerial challenge, and one can never be organised enough, but it is very enjoyable. And the symbiosis of Oxford Drug Design being a spinout from the department in which I am lecturing is very satisfying. It is good to be working in a company that came out of Oxford as well as teaching the next generation of scientists who have an entrepreneurial interest.

What are your plans for the future?

From the teaching perspective, the Scientific Entrepreneurship course is open to people from all departments, so in general what's next is to extend the reach of the course participants and to have more in-person activities which have been restricted over the past two years.

We have a visiting lecturer every term, and it is a real highlight for the students to meet and talk with high-profile entrepreneurs who also are or have been practising scientists. This will have its full impact as things go back to normal. And for their future, all of my cohorts have been joining a LinkedIn networking group for Oxford Scientific Entrepreneurship, which is creating a helpful and supportive international community where people can exchange information, opportunities and ideas.

There is also a research angle. I am interested in the way we scientists think at the interface between pure science, innovation and entrepreneurship. From discussions with Harvard I understand that the course I teach is unique. So it gives us a unique opportunity to investigate how we scientists operate differently (or not) to those in or in other areas. It would be fascinating to answer some of those questions and I am first trying to formulate the right questions! That is what research is all about. ■

The new Biochemistry research facility in Oxford was renamed the Dorothy Crowfoot Hodgkin Building this year in honour of the Nobel prize-winning chemist and crystallographer. Here David Dale (Wadham, 1959) remembers his time spent as her research student.

Memories of Dorothy Hodgkin

From 1959 to 1962 I was very privileged to work for Professor Dorothy (Crowfoot) Hodgkin in Oxford's Chemistry Department in South Parks Road. My work was for a DPhil using X-ray diffraction studies, and Dorothy had kindly helped me obtain a place at Wadham College, not far away in Parks Road.

The fact that the King's Arms Hotel, claimed to be the oldest pub in Oxford, was next to the college was a fortunate accident... Both the King's Arms and Wadham were opened a few years into the 1600s, and coming from Southern Rhodesia (now Zimbabwe), where all the buildings were 20th century, I was enthralled by Oxford's antiquity. I was on my first overseas visit away from home, and Oxford was not far from my English roots in Stratford-upon-Avon.

Dorothy's office was on the south-eastern corner of the Chemistry building, overlooking South Parks Road. Across the road were Rhodes House, the University's Computing Laboratory (aka Atlas) and the Commonwealth Services Club, the last two of which I got to know well during my time in Oxford. A long corridor ran down the Chemistry building from Dorothy's office, with laboratories, offices and workshops on both sides. I was pleased to discover that the lane passing near the building's main entrance now bears her name.

At any one time the Hodgkin group was studying the structures of a wide array of molecules, ranging from complex biological to simple inorganic. Members of the group came from around the world: I remember researchers from Australia, Canada, India, Italy, New Zealand, Sweden, and the USA. Other countries may have been represented, and I think that Dorothy was pleased to host such a wide range of nationalities. Certainly, her visitors were very widely drawn. One of the 'local' researchers was a Welsh Rugby Union scrum-half, which impressed me greatly as a sports lover.

Dorothy was a well-known peace activist. She was an active member and, at one time President, of the Pugwash Conference on Science and World Affairs. That group's mission is to "bring scientific insight and reason to bear on the catastrophic threat posed to humanity by nuclear and other weapons of mass destruction."

For many years Dorothy refused to go to the USA because it had banned Dr Thomas Hodgkin, her husband, an eminent historian. He was an expert on Ghana and other West African countries and had very left-wing views. Ghana had recently gained independence from the United Kingdom, and other countries in the region were pressing for independence from the UK or France.

Some Hodgkin group researchers, including myself and Dr K Venkatesan (Ven) from Madras, now Chennai, often used the University's computer Atlas at night. It was only a two minute walk away across South Parks Road and occupied the whole bottom floor of the computer building, including banks of humming cabinets filled with electronics.

It was a prototype, a 'supercomputer' of its time; the most powerful computer in Great Britain. It used discrete germanium transistors, and is now referred to as a second generation computer. Atlas implies power but the computer had much, much less power than today's computers! Even the simplest modern computer would take only a few seconds to do a calculation that would have taken Atlas 24 hours.

Apart from being slow and low-powered, Atlas was run using punched paper tapes for both input and output. The printer could, and often did, punch double perforations alarmingly and without warning, meaning you had lost the results of any calculations. The machine also had the world's first 'virtual' memory, but it could go out of sync, losing all the machine's calculations and work. So, if you were a user doing long calculations, the challenge was when to dump results. You would hope that the tape punch had behaved correctly, and if it had then you could feed in the output punched tape as new tape and restart the calculations.

Another option was to risk things and run the machine for as long as you dared, a gamble not unlike a visit to the roulette wheel. One night Ven and I worked with Atlas from 8pm to 8am on the night shift, not 'dumping' the data at any stage. Unfortunately, at 7:50am Atlas did the dirty on us, whirring out of sync and losing all our results!

If Dorothy found out that a student was short of funds she tried hard to find a source to help them out, despite her own department rarely being well financed. She certainly helped me, and was extremely good to her staff and students.

She also turned a blind eye to departmental 'activities' at times. Once, Ted Maslen, from Perth, Australia, and I were playing miniature cricket in a laboratory, using a long ruler and wooden spheres from a molecular model. Dorothy opened the door and looked in, perhaps just as Ted was hitting a blue nitrogen 'atom' for six onto the far wall. She quietly closed the door and went on down the corridor – Ted and I continued our match.

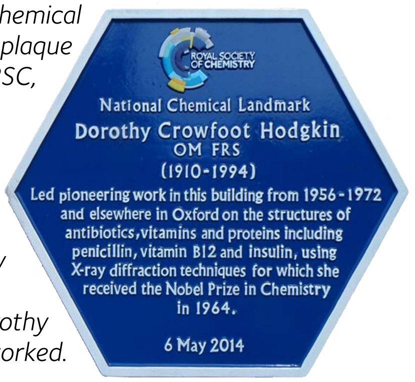
Dorothy had an interesting domestic situation. She and one of her two younger (Crowfoot) sisters lived in adjacent houses in North Oxford, not far from Somerville College where Dorothy was a student and later a tutor. Her sister looked after both households while Dorothy worked at the University. Her husband, Thomas, had been a Classics Scholar at Balliol College and I understand that he spent considerable time at home looking after the three Hodgkin children but also travelling, especially to Ghana.

Dorothy was a pioneering X-ray crystallographer. She was, however, famously afflicted by bad arthritis, particularly in her knuckles. By the time I met her the job of mounting a very small crystal onto a diffractometer would usually be done by whomever she was doing crystallographic research work with. The front cover of the 2021 issue of *Periodic* nicely illustrates a small crystal ready for bombardment by X-rays.

The fast-growing complexity of the molecular structures that Dorothy and colleagues elucidated reflects the great gains in X-ray diffraction and computing power made during her career. She led the field, and among the important crystal structures she successively determined over many years were cholesterol, penicillin, vitamin B_{12} and insulin. Those four important biochemical substances have 27, 16, 63 and 257 carbon atoms in one molecule respectively, underlining the increasing complexity of problems she could unravel.

Awarded the Nobel Prize in Chemistry in 1964 "for her determinations by X-ray techniques of the structures of important biochemical substances," the only time I saw her after I left Oxford was when she visited Melbourne, Australia in 1971. I was working in the Chemistry Department at La Trobe University and she insisted that I accompany her around the city as she visited various luminaries. The world's only living female Nobel Laureate in Chemistry was, of course, the main star, and it is highly appropriate that Oxford's new Biochemistry Building in South Parks Road has been renamed the Dorothy Crowfoot Hodgkin Building in her honour.

Dorothy was a very determined, remarkable and special person. She died in the village of Ilmington, about nine miles south of Stratford-upon-Avon, Warwickshire, in 1994. It is fitting that the Pugwash Conference on Science and World Affairs, of which she was an ex-President, was jointly awarded the Nobel Peace Prize one year later. ■



National Chemical Landmark plaque from the RSC, which can be found on the Inorganic Chemistry Laboratory in Oxford where Dorothy Hodgkin worked.

The newly opened Dorothy Crowfoot Hodgkin Building, named for the Nobel Prize-winning scientist in 2022, houses research in Biochemistry, Nanoscience, Genomics and Medicine, including researchers from the Department of Chemistry.

Schrödinger in Oxford

Periodic talks to theoretical quantum chemist Sir David Clary, who has written a new biography of theoretical quantum physicist Erwin Schrödinger.

Sir David Clary

President of Magdalen College from 2005 to 2020 and Emeritus Professor of the Department of Chemistry, Clary has spent almost two decades drawing together archival materials and interviews covering Schrödinger's time as a fellow at Magdalen in the 1930s.

This little-explored chapter of his life is developed in detail in *Schrödinger in Oxford*, published in March 2022 by World Scientific. *Periodic* caught up with Sir David to discuss his own, and Schrödinger's, lives and careers.

What drew you to Schrödinger?

I first heard about Schrödinger at school – I went to a state grammar school and in the A-Level my teacher wrote Schrödinger's equation on the board. Nobody had a clue what it was all about. It wasn't until I was an undergraduate at Sussex University that I got a good grounding in quantum mechanics. I went on to do my PhD in Cambridge, where I was focused on solving Schrödinger's equation very accurately to find the energies of atoms and molecules.

At the time, in the 1970s, we didn't have particularly good computer facilities to solve anything beyond small diatomic molecules. Nowadays people still use the accurate methods we were developing then, but for much larger systems.

Were the full implications of Schrödinger's equation realised in his time?

Every single observable that you can measure and study in the lab can be calculated by Schrödinger's equation, and nowadays more and more accurate and useful results are possible. When it all started in 1926 you couldn't do these calculations easily at all.

People like Linus Pauling who liked to use Schrödinger's idea of the orbital realised you could overlap orbitals and use their topology to explain molecular properties: the stability of benzene, hybridized orbitals in methane, and so on. This, very quickly, got into the minds of all chemists. People knew it was a big breakthrough, but didn't realise that one day the mathematics would be solvable.

Most of my research in the last 30 years has been on chemical reactions. For chemical reactions there's an energy barrier to go from reactants to products. You can write down the Schrödinger equation for that motion, solve it, and calculate reaction rates.

You did your PhD in Cambridge, went to London, and arrived at Oxford in the early 2000s where you quickly became President of Magdalen College. Would Schrödinger's time in Oxford have looked anything like yours?

Yes! He was a fellow at Magdalen, and all these quaint traditions in Oxford existed then as now. In the book I talk about him coming to dessert after high table, where he was the junior fellow and had to pour the wine.

While Schrödinger was here he gave research lectures, but they were at too high a level and hardly attended. He did almost all of his work on his own – he didn't have a research group, and didn't have much impact in the short time he was here.

But the idea of entanglement, which is now at the heart of quantum computing, was in fact suggested by Schrödinger in Oxford. People don't always know this because it was too early.

Schrödinger's original work on entanglement may lead to quantum computers, which could solve quantum problems even faster than current methods – how realistic is that prospect?

Developing an actual functioning quantum computer experimentally is a huge challenge. Some of the big tech companies are working on it, and every year you see reports of progress – but, like harnessing nuclear fusion, I just hope it's not always "30 years away".

As well as quantum computing, many companies like Google have introduced artificial intelligence. Linking AI with something like density functional theory has become very powerful, and allows more and more accurate calculations to be done on complex systems.

How did Schrödinger's career develop after Oxford?

Schrödinger's later work focused on life, and the physical processes that make it possible.

He was always interested in philosophy – when he was younger he wanted to have a joint chair between physics and philosophy. Even at Magdalen he started talking to biologists. Oxford was very strong in medical sciences, physiology and so on, and that stuck in his mind.

Later in life he lived in Ireland and was very good at public lectures. Talking about the origins of life was natural to him.

It seems obvious to us now that, in order to explain a lot of biology, you need to get into molecules, even if they're complicated ones like DNA and proteins. But at the time the function of DNA wasn't known, and the base pairs were only starting to be understood.

Have you always had an interest in historical research?

When I arrived at Magdalen as President in 2005 one of the things that had attracted me was knowing that Schrödinger had been a fellow there. I realised he had a daughter and managed to track her down. I just wrote to her out of the blue and she wrote back saying she hadn't been to Oxford since she was a baby. So I invited her, and that was the start of the idea for this book.

Schrödinger's life has its controversies, including a string of affairs and accusations of sexual abuse. How did you deal with this side of his life in your research?

Schrödinger's life is certainly very interesting, but I wouldn't say he's a good role model. His wife stuck with him for his whole career – she used to do the accounts, immigration, travel, and he found it very difficult to exist without her. But he had many affairs, which she knew about.

You can have someone who's so influential on the world, like Schrödinger, and yet these aspects of their personal life can come to dominate in the public view. It's a difficult argument. His private life was not perfect – in the book what I've tried to do is focus on evidence, and when there is evidence, I've stated it. In my own research I found no evidence of sexual abuse.

How did you come to write the book?

I retired from being President of Magdalen nearly two years ago, and then the pandemic came along, and I realised I had all this archival material.

My book is mainly about Schrödinger's life, how he moved from place to place and interacted with people in Oxford. There's a lot about the tragedies of the 1930s and 1940s – he was very friendly with many Jewish scientists who had to flee the Nazi regime and came to Britain, America and elsewhere.

Because of Schrödinger's personal life, he wasn't very popular with other scientists. In fact Schrödinger's cat is his most famous aspect, and that's just because it's such a weird idea.

Outside of academia, you were Chief Scientific Advisor at the Foreign Office from 2009–2013. What is that job like?

Nowadays everyone knows about roles like this because of the pandemic. It was a fascinating job – I interacted regularly with other Chief Scientists like Sir Chris Whitty.

I travelled a lot over the world, doing scientific diplomacy and promoting British science. At the time we were particularly trying to promote EU programs, and found that many people in government did not know that the EU was spending vast amounts on scientific research. We've benefitted a lot from it in Oxford – I've had EU finding in my own group ever since the 1980s. It's brought lots and lots of students, postdocs, and faculty to the UK, and to Oxford, and I'm afraid Brexit hasn't been great for science in this country.

We also did a lot of work around climate change. Like nanochemistry and materials chemistry, climate chemistry should be a very prominent area of teaching, and sadly it doesn't always get taught.

What's next for you?

I've enjoyed this project so much that I have started doing more writing. The key to biographies is that you've got to have good archives. You're often working with half a correspondence, trying to work out what the other person said.

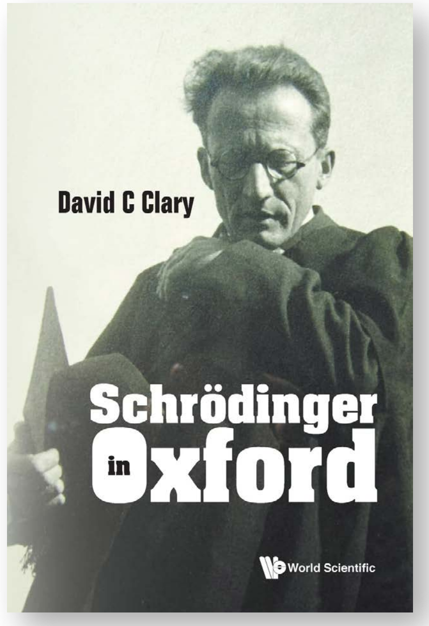
I was so lucky in the pandemic that archivists sent me stuff, it was a big advantage for me that I could correspond with archives around the world.

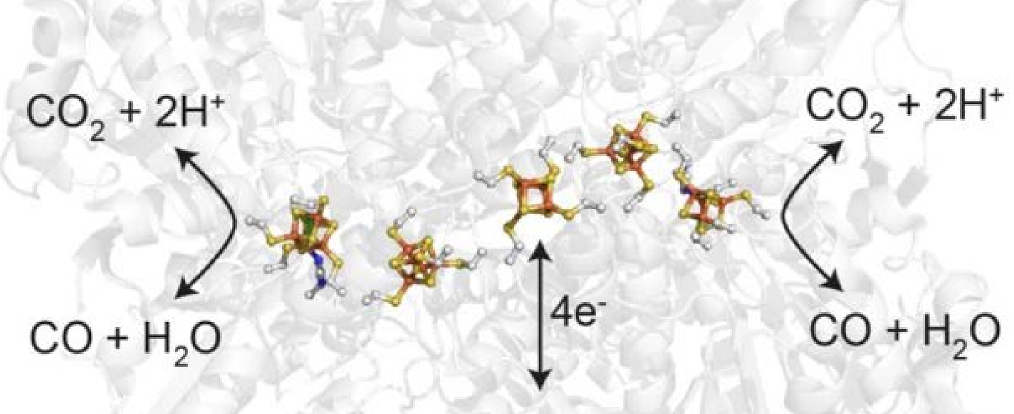
How has engaging with Schrödinger's whole career made you reflect on your own career?

I've always been in what I would call theoretical chemistry, and I never realised until relatively recently how important Schrödinger's equation is to that whole field. Highly correlated systems, polymers, magnetic resonance – it all comes back to wave mechanics.

It's hard to find another scientist who had such a big impact on modern science. ■

Sir David's book, Schrödinger in Oxford, is published by World Scientific (ISBN 9811251002).





Researcher profile

Patricia Rodríguez-Maciá

Dr Patricia Rodríguez-Maciá is a Glasstone Research Fellow in the Department of Chemistry, hosted within Kylie Vincent's research group. She is also a Lecturer in Inorganic Chemistry at Magdalen College, and holds an EPA Cephalosporin JRF at Linacre College. She sat down with Periodic to discuss her research and career.

How would you describe your research?

My research consists of the study of metalloenzymes in nature that catalyse energy conversion reactions. So, for example: the conversion of hydrogen to protons and electrons; the reduction of carbon dioxide; the reduction of nitrogen to ammonia. Basically, small molecule activation.

My group uses a combination of spectroscopic and analytical techniques to investigate the active sites of these enzymes and how the rest of the protein matrix 'tunes' the active site. The goal is to understand exactly what makes these enzymes so efficient, and then to use this understanding to develop artificial catalysts and catalytic materials for these reactions.

What catalysts do you make?

We make artificial, or semi-synthetic enzymes. We synthesise a metallo-organic active site mimic in the lab and use it to reconstitute a small protein scaffold that can be engineered. This protein scaffold is designed to confer the properties needed to allow the active site to function as well as the one in the natural enzyme, with the advantage that we can engineer it to tune its properties. We can use site-directed mutagenesis to modify the first and second coordination spheres in the protein scaffold to improve the activity or stability, or tune the reactivity, of our artificial enzymes.

Why do you need a protein scaffold – isn't the active site enough?

No, the active site alone isn't enough. The rest of the protein 'tunes' the activity and properties of the active site. In our proteins the metals in the active site are the location of the reaction, but the substrate needs to get there and the product need to get out; there are gas channels, proton pathways and electron relays. That's why we need to understand the rest of the enzyme and not only the active site.

What techniques do you use to understand these enzyme systems?

The main techniques that we use are infrared spectroscopy and electrochemistry. We also use molecular biology techniques to produce different recombinant enzymes, both the natural proteins and our small protein scaffolds, and then typical biochemical techniques to quantify the activity of these enzymes. There's also crystallography, electron paramagnetic resonance (EPR) spectroscopy, and X-ray spectroscopy, which we use in combination to elucidate the binding and catalytic mechanisms of proteins.

Wow, that's a lot of techniques – your research must be quite interdisciplinary?

Yes, it is a lot of different techniques! The goal is gaining an intrinsic understanding of the enzymes. Sometimes you see things with one technique that you don't see with others.

I like to call my research inter-multidisciplinary. I'm expert in certain techniques but sometimes you need to collaborate with people who can bring different expertise. That's the beauty of science – one person can't do everything themselves; we need to have a pipeline of knowledge transfer between the different disciplines. Talking to people outside your immediate field can really open your mind to possibilities in your research that you would never have thought of yourself.

How do you see your research being applied?

The main focus of my research is hydrogen conversion, which is needed for renewable energies: producing hydrogen from water electrolysis that can be then used in a fuel cell. My second biggest focus is CO_2 reduction, capturing CO_2 from the atmosphere to produce carbon monoxide or formate that can be used in industrial processes.

We're developing new catalytic materials that could be used for these reactions. The best thing about the catalysts we're producing is that they are based on earth-abundant metals such as nickel and iron and don't need high pressure or high temperature to work.

Your studies and career have taken you to quite a few different countries and cities so far – how are you finding Oxford?

Oxford is great because there are so many different topics being researched within the department, from chemical biology to supramolecular chemistry. I've really enjoyed the seminars that the department has; it's nice to be aware of what is going on outside of your research niche.

The college system is also great for meeting different academics, in completely different disciplines. It's so interesting to interact with academics teaching and researching music, law, literature and so on, and it can really make an impact on you.

One of my other favourite things about Oxford is the mix of teaching and research that you don't get when working at a research institute (such as the Max Planck). The teaching experience helps you to be a better researcher, and vice versa.

Final question: what excites you most about the future of your research?

The possibility of understanding an enzyme system so well that we can generate much simpler catalytic materials that could work as well as the natural enzyme. We've moved from natural enzymes to semi-synthetic and artificial ones; one day we hope to be able to replace the protein scaffold with a completely metal-lo-organic framework, using our deep knowledge of how an enzyme works. ■

Patricia studied Chemistry at the University of Alicante before a PhD at the Max Planck Institute for Chemical Energy Conversion, Muelheim, under Wolfgang Lubitz' supervision. Her doctoral work focused on using electrochemistry and infrared spectroscopy to study hydrogenases and bio-inspired synthetic catalysts. A postdoctoral position in Serena DeBeer's group followed, where she applied X-ray spectroscopy to various metalloenzymes. Patricia joined the University of Oxford in 2020 as a PDRA in Kylie Vincent's group. In 2021 she was appointed Glasstone Research Fellow to start her independent career.

Figure top of p.24: homodimeric structure of a dehydrogenase enzyme from C. hydrogenoformans, a thermophilic bacterium that reversibly reduces CO_2 to CO, producing hydrogen as a waste product. The Ni-Fe active site can be seen at the right and left edge, and the iron-sulfur cluster redox cofactors in the middle (PDB ID 3B51).

John Goodenough's 100th birthday

Nobel Laureate Prof John Goodenough celebrated his centenary on July 25th 2022.

Professor Goodenough was Head of the Inorganic Chemistry Laboratory (ICL) at Oxford from 1976–1986, and it was during this time that he and his group conducted ground-breaking research that led to the widespread use of lithium-ion batteries and a revolution in modern life.

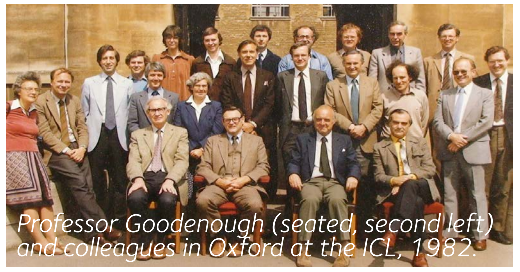
Working in the ICL with Koichi Mizushima, Phil Wiseman, and Phil Jones, Prof. Goodenough expanded on previous work by M. Stanley Whittingham and found that by using Li_xCoO_2 as a lightweight, high energy density cathode material, he could double the capacity of lithium-ion batteries. The seminal work conducted at the ICL was commemorated in 2010 by a blue plaque from the Royal Society of Chemistry, designating the laboratory as a National Chemical Landmark.

After his departure from Oxford, Prof. Goodenough joined the University of Texas at Austin, where he has continued to advance battery research ever since. In 2019, at the age of 97, he became the oldest ever Nobel Laureate, winning the Nobel Prize in Chemistry together with Akira Yoshino and Oxford alumnus M. Stanley Whittingham.

To celebrate Prof. Goodenough's 100th birthday in 2022, the University of Texas at Austin held a symposium attended by representatives of the US Department of Energy, leaders in battery research from around the world, and several former colleagues from Oxford, including Sir Tony Cheetham, Bill David, Peter Battle and Mike Thackeray.

Professor Simon Clarke, Head of the ICL, said: "Congratulations to John Goodenough on reaching a fantastic milestone. Members of the Oxford Chemistry community at all levels continue to be inspired by his and his group's achievements in developing lithium cobaltate as a viable Li-ion battery material. This has given so many around the world access to technology and services on portable devices – something of which he is justly proud.

"He also has a towering legacy in many other areas of fundamental and functional inorganic chemistry, formulating an understanding of the interactions between magnetic ions in solids and making significant contributions to the development of RAM. His longevity in research remains an inspiration." ■


Professor Goodenough (seated, second left) and colleagues in Oxford at the ICL, 1982.

Rex Richards

2022 marks the centenary of the birth of Rex Richards, who died in 2019. Rex was Dr Lee's Professor of Chemistry in the Department from 1964–69 before becoming Warden of Merton College and, later, Vice-Chancellor of the University of Oxford. Here Graham Richards, former Chairman of the Department of Chemistry, remembers Sir Rex's life.

Sir Rex Richards

© Bryan Organ and The Warden and Fellows of Merton College, Oxford.

Rex's massive scientific contributions were celebrated in several published obituaries, perhaps most notably the one by David Gadian. Here I want to concentrate on his impact on the PCL, the Physical Chemistry Laboratory as it then was, and on science in Oxford.

Scientifically he was a major figure in the application of nuclear magnetic resonance (NMR). He was one of the first to realize its potential in chemistry, and not just in physics. Later, again showing massive intuition, he foresaw and exploited its application to biochemical problems.

Being a pioneer, there were of course no commercial machines, and he had to build his own in the laboratory. In this he had some notable students, including Robert Gasser, part of whose apparatus is now in the Science Museum, and Ray Freeman, later of Varian, before returning as an academic in Rex's department.

Notably, the building of NMR machines was heavily dependent on the Departmental electronics workshop technical staff, in particular Doug Cook as its head. Years later Rex ensured that Doug received an Honorary MA. One notable feature of those early days was that the PCL housed the world's biggest permanent magnet: quite a problem when it had to be decommissioned.

In 1964 Rex succeeded Sir Cyril Hinshelwood as Dr Lee's Professor of Physical Chemistry and Head of the Department. Hinshelwood was a giant figure: Nobel laureate; Order of Merit; President of The Royal Society in its Tercentenary year and fluent in as many as twenty languages including Chinese and Japanese. That might seem a very hard act to follow – in fact, in many ways, it was like night turning to day.

The mid 1960s saw a huge national University expansion. More than a dozen new universities were created all at the same time, and existing ones grew in size. Jobs were easy to get and facilities were greatly improved.

In Hinshelwood's time staff were referred to by their surnames. The only outside telephone line went into the office of Hinsh's secretary, the redoubtable Miss Binnie who constituted the entire administrative staff. If a call came for a member of staff she went into the corridor and bellowed his name. Students did gather for coffee and for tea, but in general the academic staff did not join them. In slightly earlier days the rare women students were allowed to make the tea, but not join in. This included Rex's wife to be, Eva.

Rex changed everything. Outside telephone lines went to every office and pagers were picked up from a panel in reception. We started to use first names. Two extra floors were added to the building, incorporating most notably the communal PCL Common Room, then a total novelty across the Science area. The physicists had the habit of meeting for coffee in a corridor, but an attractive common room was novel. Academics mixed with students and the impact was huge. Rex actually wanted to include the technical staff, but they chose to have their own separate common room.

Another major innovation was Rex's Monday afternoon tea party in his office for the academic staff. We had cake and discussed laboratory business. It was very informal and totally democratic, although to my memory we always came to decisions matching what Rex wanted.

We lost Rex as Head of the Department when he was elected as Warden of Merton, almost immediately becoming Vice-Chancellor. He was the first scientist to take on this role. This too was something of a revolutionary change, marking a huge switch in the power balance in the University. Previously much of the power was in the hands of the Humanities faculties and the Science and Medical faculties struggled to get their way.

Rex changed not just the PCL, but science in Oxford. Indeed, he was notably influential in my academic career; he examined my Part II, he was my DPhil examiner, and he hired me. ■

Glass model of NMR equipment for Rex and Eva Richards. Photo courtesy of Oxford Chemistry alumna Mrs Sheila Mawby (Somerville, 1962).

Life-like chemical oscillations

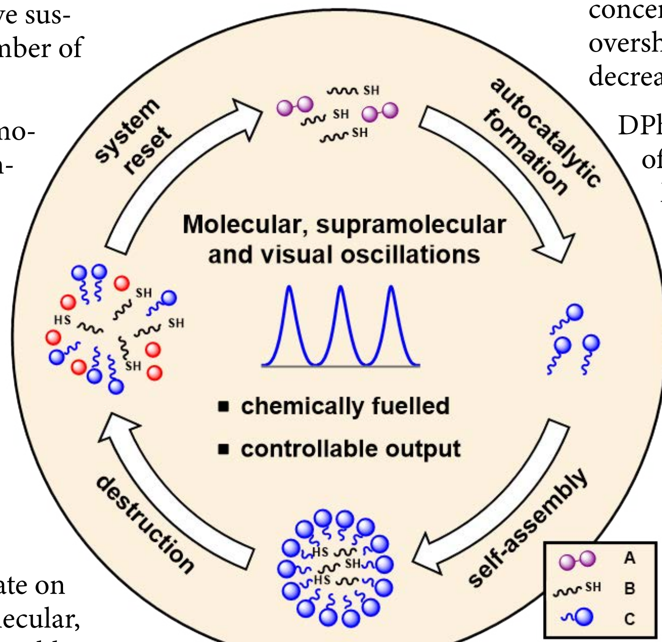
A team from Stephen Fletcher's research group has shown how a chemical system of self-assembling, self-replicating molecules can exhibit oscillations in time. In a paper published in Nature Chemistry they showed how simple cell-like structures can emerge, decay, and then repeatedly arise again in a network of relatively simple chemicals.

In the study the team analysed the reaction between a hydrophilic disulfide (A, purple molecule in figure) and hydrophobic thiol (B, black) to form a molecule (C, blue) that can self-assemble into micelles. By carefully controlling the reaction parameters, for example stirring rate, they were able to observe sustained oscillations in the number of micelles formed over time.

Micelles are spherical supramolecular structures held together by weak intermolecular forces. As well as being important in many biological processes they are also used in drug delivery and in chemical syntheses, because the interior of the spherical shell can hold molecules like a mini reaction vessel and lead to enhanced yields.

All known forms of life operate on length scales beyond the molecular, with supramolecular structures like micelles, vesicles and protein host-guest complexes critical to countless important biological functions. Designing supramolecular replicators capable of sustained oscillations would be a big step towards creating systems with this lifelike complexity, and would give insight into how complex systems could emerge and evolve.

Because the diameter of the micelles in their oscillating system is on the order of nanometres, the team could image their growth and decay in the solution by performing super-resolution scattering microscopy (iSCAT), taking snapshots at regular intervals and counting the number of particles. On a timescale of hours, the number of micelles rose and fell reliably and repeatedly, a result that was also demonstrated using liquid chromatography on samples from the reaction mixture.



The proposed sequential processes that lead to oscillations in the amount of micelles is shown in the figure above. Both the formation and destruction of micelles requires the black thiol B, which is taken up into the centre of the spherical structure. Importantly, only the micelle formation requires A. When both A and B are present the production of C is favourable, whereas when A is depleted the micelles release B to cause the breakdown of C and therefore the micelles themselves. This process represents one oscillation, or one loop around the circle in the figure, after which the system resets.

The balance between the catalysed formation and destruction of component C is critical for the observation of oscillations – the reaction swings back and forth like a pendulum, oscillating between enhanced production of micelles and enhanced destruction. All oscillating chemical reactions require some kind of autocatalytic process that can lead to chemical feedback, whereby large increases in the concentration of one component overshoot and then lead to large decreases.

DPhil student Michael Howlett, of the Synthesis for Biology and Medicine CDT and joint lead author alongside Anthonius Engwerda, describes the long experiments the team ran in order to track the progress of the oscillations over a day: "When first discovered, the oscillations were very chaotic and we spent a lot of time taming them, but with the two of us working together to monitor the reactions in high resolution, we could even track the oscillations over multiple days and are really proud of how far it has come!"

The dynamic behaviour of this oscillating system across different length scales may have relevance in drug delivery, signal transduction, and in the design of functional nanoscale machines. Going forwards the aim is to further control these oscillations not only in time but in space – because the micelles can take up and release chemicals, it is hoped that in the future it may even be possible to design systems that could directionally transport chemicals. ■

Keep up to date with all of the latest research and news from the Department of Chemistry at www.chem.ox.ac.uk/news.

Green chemistry revolution

There has been a rapid surge in the setting of net-zero targets in recent years, with over 135 countries now having one in place. Individual, national and international actions are moving us in the right direction. However, as the chemical industries underpin virtually all manufacturing, it will be impossible to meet these targets without radical changes being made there first.

Although the chemical industries already enable green growth, vast infrastructure and process changes still need to be made. For example, an additional 3.2 petawatt hours of renewable energy could be needed each year to power the EU chemical industries with renewables – that's about five times the total amount currently produced by the EU. Although the need is clear and the drive is strong, the challenge is enormous.

Central to the solution is green chemistry. In broad terms, this is the design of processes and products that reduce or eradicate the use and production of harmful substances in manufacturing, address existing waste, and help us understand, analyse, and limit pollution. Its guiding principles are helping pave the road to a future in which the needs of our growing global population can be met sustainably.

Innovation in academia is one of the great drivers of change in industry. Our 'Energy & Sustainable Chemistry' research theme (led by Professors Bill David FRS and Kylie Vincent) synergises expertise from across the Department of Chemistry to shape approaches to sustainability challenges. Here are some examples of our cutting-edge work:

Green hydrogen and ammonia

To realise the enormous environmental potential and economic benefits of a hydrogen economy, research in Oxford Chemistry focuses on areas including sustainable production, storage and transport and improved fuel cells. One area of strength is green ammonia, which, beyond its use as a ubiquitous feedstock for fertilisers, offers huge promise for global zero-carbon fuel storage and internationally traded green energy. Future green power provision, built upon optimised ammonia-hydrogen blends all the way from the direct use of ammonia to the complete conversion of ammonia to hydrogen, offers the possibility of a complete transition from fossil fuels. However, production currently accounts for c. 2% of the world's fossil fuel consumption and c. 1.3% of global CO_2 emissions.

Professors Bill David FRS and Edman Tsang are leaders in green ammonia research, working to make it environmentally, logistically, and economically attractive. Research in the area includes: using renewables to synthesise and decompose ammonia; designing catalysts and electrocatalysts for hydrogen production; catalytic cracking of polyolefins; and nitrogen activation chemistry. This research could provide clean energy solutions and help us meet growing global food demands sustainably, and has led to two spin-out companies – Sunborne Systems (Professor David) and OXGRIN (Professor Tsang).

Sustainable manufacturing

Professor Kylie Vincent has developed an enabling-platform technology for cleaner, safer, faster and cheaper chemical production, which forms the basis of spin-out company HydRegen. The technology uses hydrogen-powered biocatalysis, replaces toxic metal catalysts, lowers energy demand in manufacturing, increases product purity and enables continuous flow processes. It could offer big changes for the production of, for example, pharmaceuticals, flavours and fragrances, so supports direct and indirect reductions in environmental impact.

Harnessing the power of light

Oxford chemists are designing better materials for solar conversion and enhancing photocatalysis. For example, Professor Iain McCulloch FRS is working to increase the efficiency of organic semiconductor photocatalysis and developing porous frameworks for CO_2 reduction. The group also designs new photovoltaic materials that generate larger voltages, absorb more light, avoid recombination losses and have optimal transport properties.

Professor Ludmilla Steier focuses on the design of photo- and electrocatalysts to convert water, CO_2 and industrial waste products into energy-rich fuels and chemicals. Her group specialises in the use of atomic layer deposition coupled to operando spectroscopy to study the role of defects, surface composition and interfaces in determining efficiency, selectivity and operational stability of these catalysts.

Making a circular economy possible

A number of research groups are working to accelerate our move towards a more circular economy. Professor Charlotte Williams OBE FRS, for example, looks at ways to use and recycle renewable resources, such as plants or carbon dioxide, to produce useful products like polymers. You can read more about her work on page six.

Another example is Professor Véronique Gouverneur FRS, who is shifting paradigms in fluorine chemistry and providing solutions for a circular economy. Fluorine is used in many products, from refrigerants and non-stick coatings to agrochemicals and pharmaceuticals, so increasing its circularity has great potential to lower the environmental impact of many sectors. Fluoro-organic compounds are rare naturally, and can only be accessed through chemical synthesis. Today, production requires hydrogen fluoride (HF), a very dangerous chemical that renders its manufacturing from fluorspar highly laborious. The Gouverneur group is developing new technologies that bypass HF, and instead, use directly the mineral fluorspar (CaF_2) as a fluorinating reagent. Her laboratory also develops methods to repurpose waste fluorine-containing organic products.

Designing better batteries

Oxford chemists have made hugely important contributions to battery technology over the years. This focus remains strong today, with a breadth of research into sustainable batteries (much in collaboration with the Faraday Institute in Oxford and other institutions). Research includes: the development of safer solid-state batteries with longer lifespans; improving the durability, sustainability, and power of battery cathodes; the development of carbon dioxide polymer electrolytes; replacing cobalt with iron and manganese; and theoretical modelling and prediction.

The next generation of green chemists

To equip our graduates to be drivers of change wherever their careers take them, we are placing more focus on sustainable chemistry in our teaching and training. For example, the Oxford Inorganic Chemistry for Future Manufacturing Centre for Doctoral Training includes green chemistry focuses like a Siemens' green ammonia demonstrator (the first of its kind, behind which Professor Edman Tsang was a driving force). Even our outreach programme features green chemistry, with, for example, the 'Plastics from Another Perspective' workshop.

The future of green chemistry in Oxford

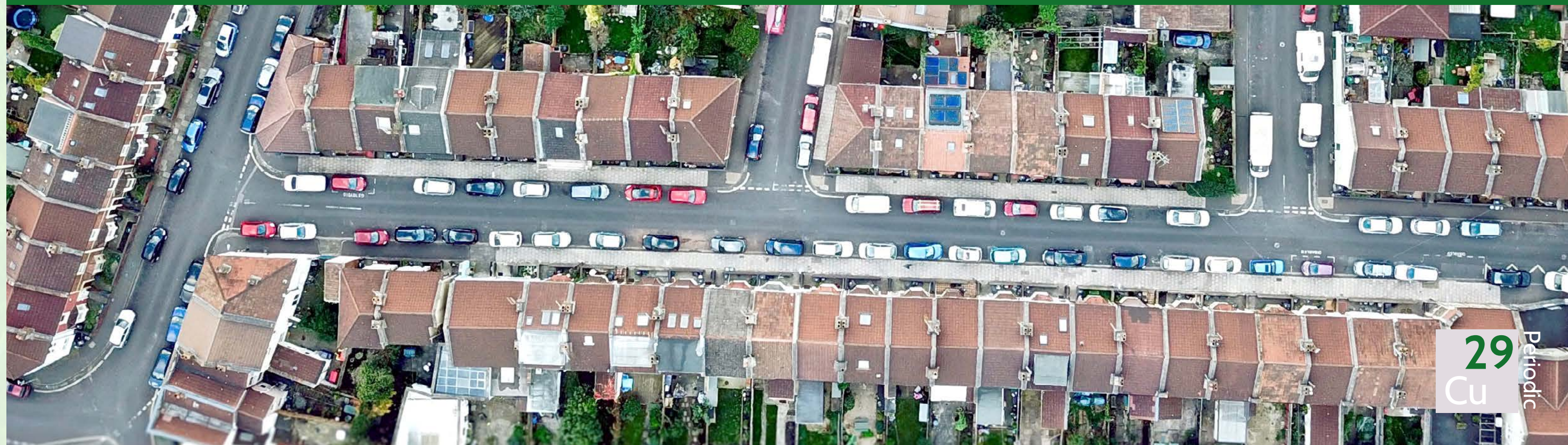
The University has made green chemistry one of the inaugural philanthropic priorities in its new development strategy. This recognises Oxford Chemistry's strengths in sustainable chemistry and acknowledges the vital role that chemistry will play in achieving net-zero targets.

Our mission is to be the global leader in sustainable chemistry and to accelerate the translation of lab-based discoveries into real-world solutions for industry and society more broadly. To achieve these goals, we hope to support chemists at every stage, develop partnerships and invest in our laboratory infrastructure. We will shine a spotlight on green chemistry in Oxford and beyond to help catalyse the green growth that the world needs in order to build a future in which we can thrive sustainably. ■

Do you want to keep up to date with green chemistry at Oxford? Can you help us pave the road to a sustainable future?

Please get in touch to receive research updates or to discuss partnerships or supporting our research.

Jane Rice, Senior Development Manager
jane.rice@chem.ox.ac.uk
Physical and Theoretical Chemistry Laboratory, South Parks Road, Oxford OX1 3QZ
To make a gift, please contact Jane or visit:
https://www.development.ox.ac.uk/chemistry



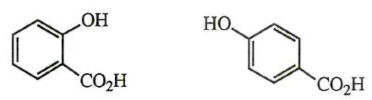
Periodic puzzles

Organic Chemistry

Explain, with reasoning, which member of the following pairs is the stronger acid (a-c) or the stronger base (d-e): [5x5]

a) CH_3CO_2H — Cl_3CCO_2H

b)



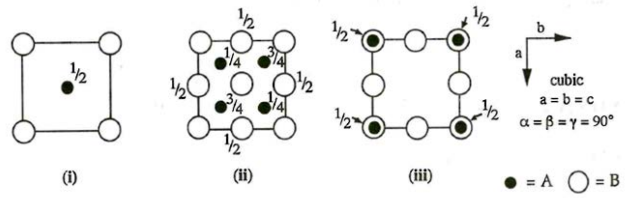
c) $HC{\equiv}CH$ — $H_2C{=}CH_2$

d)

e) CH_3CN — $CH_3CH_2NH_2$

Inorganic Chemistry

Plans of unit cells of several common A_nB_m crystal structures are shown below (viewed down the *c-axis* in each case).



Heights of the atoms above the z = 0 plane are expressed as fractions of c.

(a) Identify the formula units A_nB_m in (i) — (iii). [12]

(b) State the coordination about A and B in each case. [8]

(c) Assign the following compounds to their correct structure type and give reasons for your choice.
AlF_3 ; CsBr ; ZnS [5]

Are you smarter than... yourself as a student?

University exams: a hazy memory, or a walk in the park?

Have a go at these questions from 30 years ago and see how you think you'd do today. All are adapted from 1992's Preliminary Examinations in Chemistry.

No periodic table allowed...

Physical Chemistry

(a) Sketch (i) the radial wavefunctions and (ii) the radial distribution functions for an electron in the 1s, 2s and 2p orbitals of the hydrogen atom. [6]

(b) The normalised wave-function for an electron in the 1s orbital of the H atom is

$$\Psi = \left(\frac{1}{\pi a_0^3}\right)^{\frac{1}{2}} exp\left(\frac{-r}{a_0}\right)$$

where r is the electron-nucleus separation and a_0 is a constant.

i. Write down an expression for the radial distribution function describing the probability of finding an electron between r and $r + dr$. [4]

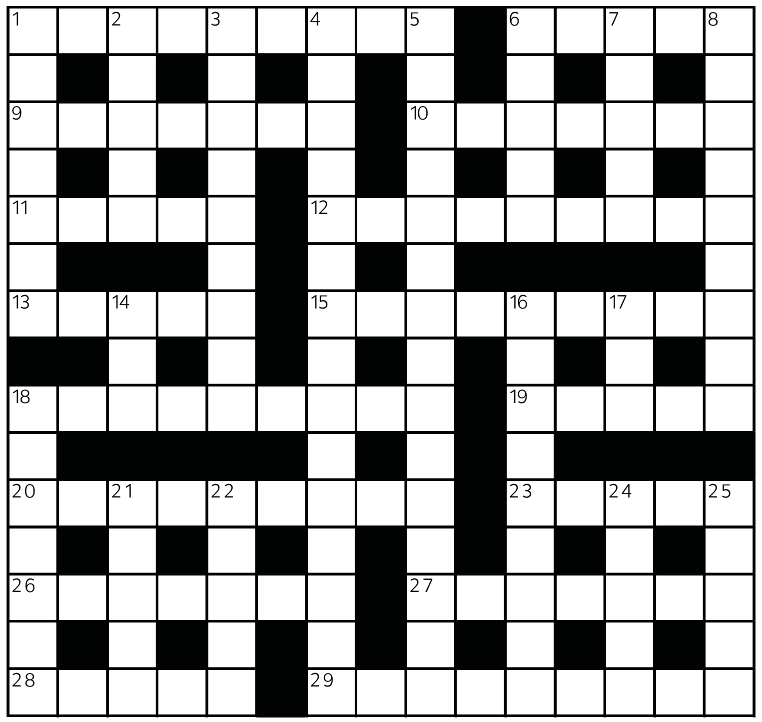
ii. Using your answer to part i, calculate the most probable electron-nucleus separation in terms of a_0. [7]

iii. By calculating the expectation value $< r >$, determine the mean distance of the electron from the nucleus in terms of a_0. [8]

$$\left[\int_0^\infty r^n e^{-an} dr = \frac{n!}{a^{n+1}}\right.$$

for $a > 0$ and n positive integer.]

Crossword, with added chemistry



Across

1 Of a thermodynamic process with no heat transfer (9)
6 Fatty acid in animal and vegetable fats and oils (5)
9 Bye bye! (7)
10 One of four elements named for the Swedish town of Ytterby (7)
11 Reach inside and search for something (5)
12 $CH_2CHCHCH_2$ (9)
13 Prefix meaning English (5)
15 3D oval shape (9)
18 Green edible seed from the cashew family (9)
19 Raised parts of a tyre (5)
20 TV detective drama prequel set in Oxford (9)
23 Hydrocarbon group, e.g. $-CH_3$, $-C_2H_5$ (5)
26 Series of large waves (7)
27 People obsessed with minor details (7)
28 Doctoral degree at the University of Oxford (5)
29 Sugars that serve as glucose storage in the body (9)

Down

1 Department of Greece; utopic vision of natural splendour and harmony; Tom Stoppard play; P&O cruise ship (7)
2,14 Many randomly moving non-interacting particles (5,3)
3 Spanish city (9)
4 Finding problems and fixing them (15)
5 Dorothy Hodgkin's field of research (15)
6 Exposed (5)
7 Expel, bar (5)
8 Praised (9)
16 Stopped abruptly (3,4,2)
17 Rock containing valuable minerals (3)
18 Folded back and forth upon itself (7)
21 Thick malleable substance made from grains and liquid (5)
22 Help, benefit (5)
24 _____ West, rapper and former husband of Kim Kardashian (5)
25 Destroys, for instance a cell (5)

Explore the periodic table of... Oxford Chemistry

Find your way around with this handy guide to the people, research, and facilities that make up Oxford Chemistry.

- **13** winners of the Nobel Prize in Chemistry
- **4** doctoral training centres
- **450** postgraduate research students
- **20 000+** followers on Twitter
- **200** postdoctoral researchers
- **720** undergraduate MChem students
- **38+** RSC awards and prizes since 2013
- **120** professional support staff
- **51** nationalities of students on research degrees
- **1** UK Prime Minister
- **26+** spin-out companies

- **19** NUS Green Impact awards
- **4** chemical landmark plaques

- **1** Athena SWAN silver award
- **52** journal articles published per month
- **8** cross-disciplinary research themes
- **11 490** square metres of lab space
- **5** department buildings
- **85** academic staff
- **70+** research groups
- **35** technicians
- **£140m+** active research portfolio
- **1** Outreach team
- **15** department lecturers
- **11 000** living alumni
- **1500** undergraduate admissions interviews per year
- **10** Fellows of the Royal Society

Keep in touch...

www.chem.ox.ac.uk

/ OxfordChemistry

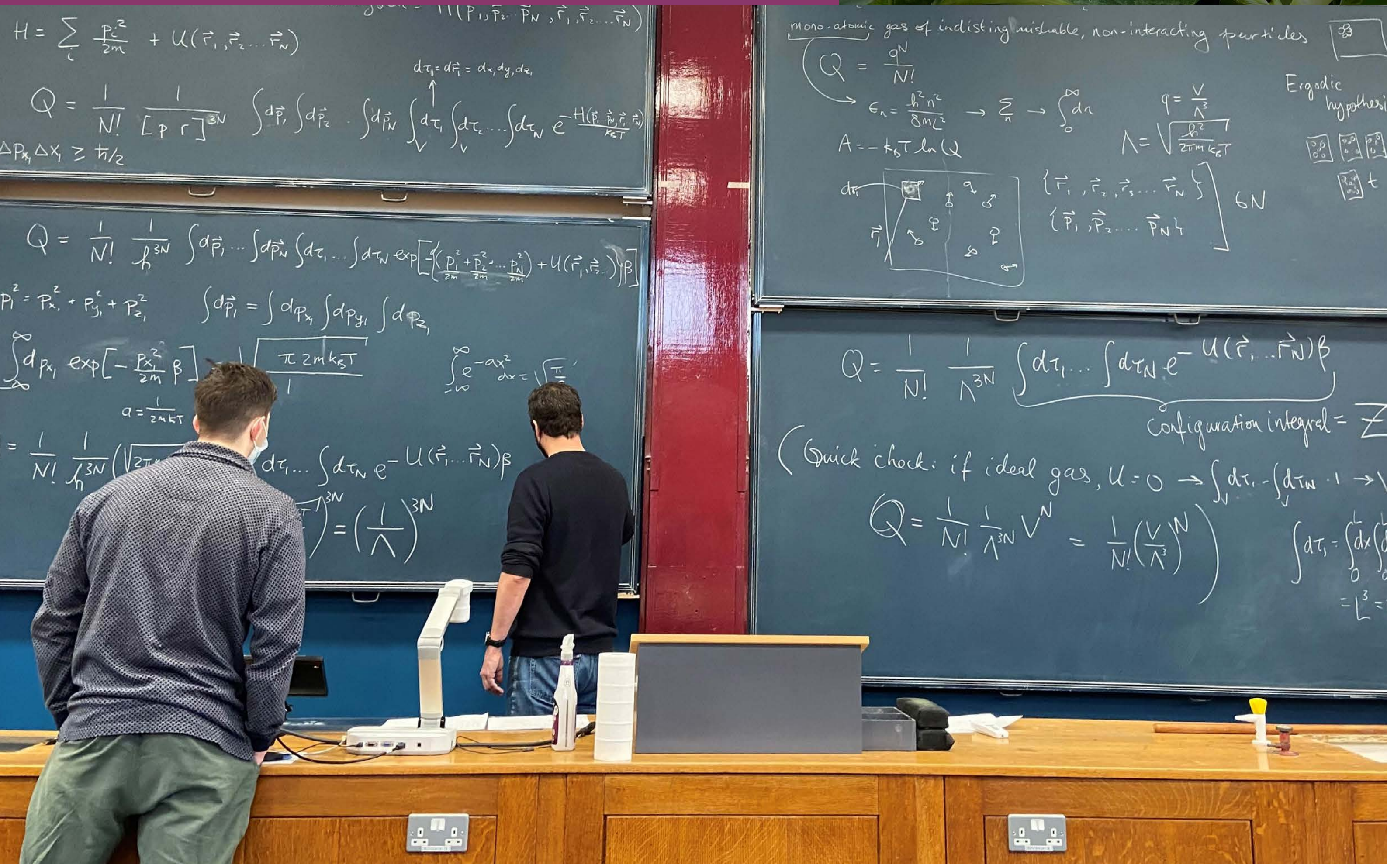
/ OxfordChemistry

The front and back cover images for this year's copy of Periodic were the winners in the Department's photography competition.

Front cover *The doughnut-shape structure is made of fluorescent-ly-labeled ovarian cancer cells. Each bright spot represents one cell that has a diameter of several micrometers. All cells were embedded in UV-cross-linked silk hydrogel – a natural biocompatible macromolecular protein network – that finally formed this ecliptic structure using hydrogel droplet printing techniques. Photographers: Yujia Zhang, Xingyun Yang.*

Back cover, right *This photo combines experimental chemistry, computational chemistry, and nature. The code in the background is from a Python software package being developed to calculate free energies. Computational chemistry can be aesthetically uninteresting, so the photographer combined plants from their office, tiny glassware, and flowers to add some colour to the standard computational chemist's view. Photographer: Tristan Johnston-Wood*

Back cover, below *Chemist's view of the blackboard from a Hilary Term lecture in the Physical and Theoretical Chemistry Laboratory. Photographer: Beth Watkins*



Contact us

Periodic magazine is published annually and distributed free to Chemistry alumni, researchers, staff, students and friends of the Department. We are always delighted to hear from readers, and if you have any pictures or stories you would be willing to share please do get in touch.

Susan Davis, Alumni Relations & Communications Manager

alumni@chem.ox.ac.uk

Alumni Relations and Communications Office,
Physical and Theoretical Chemistry Laboratory,
South Parks Road, Oxford OX1 3QZ

Editors Susan Davis and Thomas Player

Science Writer Karen Heathcote

Design Thomas Player

Distribution and Printing windrushgroup.co.uk

Images: IBM gallery, bottom of p.4; Northwestern University, portrait p.13; Nobel Foundation archive, portrait p.20; Alexandre Caron and Louis Reed via Unsplash, p.29.

UNIVERSITY OF OXFORD