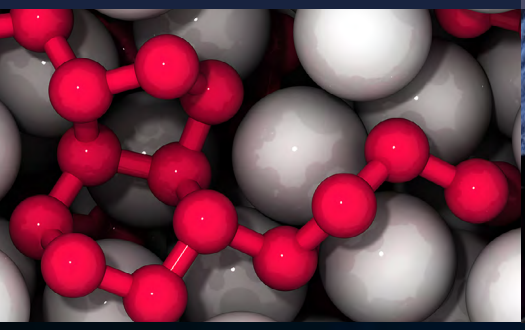
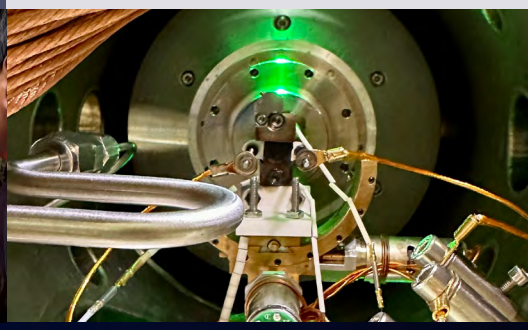
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Periodic

Magazine of the Department of Chemistry

UNIVERSITY OF OXFORD

DEPARTMENT OF CHEMISTRY

Issue 14
2026 – 27

From the Head of Department

Welcome to the new issue of *Periodic*

As always, it is a delight to introduce this issue of the magazine. We're looking forward to showing you some of the things that Oxford chemists are currently involved with.

It has been another eventful year, marked by success for many colleagues. Prof Philipp Kukura was awarded a Royal Society Faraday Fellowship – one of sixteen such awards to date, and the second in our department – while Profs Harry Anderson and Jason Davis have been awarded ERC Advanced Grants.

We've also been pleased to see how many colleagues have received national and international recognition for their work from learned societies and international agencies, and how many of our younger colleagues have made an impact on science and the world.

In the last few weeks, we've welcomed Prof Anna Peacock to Chemistry (and to a tutorial fellowship at University College). We also said goodbye (but not farewell) to some long-serving staff who have retired over the course of the year. Prof David Hodgson retired in September after more than thirty years of service to the Department, while Jennie Botham retired in May (see p. 24). Many of you will remember Jennie from the ICL teaching lab; forty years ago, Jennie was the person who issued me with safety specs when I arrived to start my undergraduate degree!

Quite a lot has changed in the last forty years, and this issue reflects how Chemistry looks today. Some things remain apparently timeless, and the cycle of undergraduate and postgraduate life looks remarkably similar. This issue showcases work by some Part II students, which is (as I hope you'd expect) at the cutting edge of research.

We also explore how the cutting edge is changing in the era of artificial intelligence. AI has been a talking point in academia and the wider world throughout the year and it is already changing how whole disciplines work in the mathematical and physical sciences. This issue touches on some of the ways we are using AI in chemistry, and harnessing its potential.

While AI streamlines some aspects of the process of research, it remains true that imagination, observation and creativity create the core ingredients for success in our subject. I hope you'll agree that Oxford chemists possess those traits in abundance.



Professor Stephen Faulkner, Head of Chemistry

Having seen many aspects of our way of working change during the course of my working life, I'm looking forward to seeing what happens next.

I hope you enjoy reading this issue. It's always a pleasure to meet or hear from Chemistry alumni, and I'll look forward to seeing many of you in the coming year. ■

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News and achievements

For more stories throughout the year, visit *www.chem.ox.ac.uk/news*













Prof Anna Peacock, Professor of Bioinorganic Chemistry, joins us this year from the University of Birmingham. She will be associated with University College, and brings an exciting research programme in bioinorganic chemistry and metallo-peptide design. (1, above)

Prof Philipp Kukura FRS received a Royal Society Faraday Discovery Fellowship. Philipp will develop new approaches for measuring the mass of individual molecules, with the aim of revealing how biomolecules interact, assemble and are targeted for destruction. (2)

Profs Harry Anderson FRS and Jason Davis each received an Advanced Grant from the European Research Council. Harry will investigate molecular quantum rings, while Jason will develop responsive nanomaterials that control interactions with water.

Prof Fernanda Duarte received a European Research Council Consolidator Grant. Fernanda's project will combine physics-based modelling, artificial intelligence and experimental data to improve predictions of chemical reactions involving metals in solution.

Prof James McCullagh is part of a £3.7 million programme to evaluate technologies for detecting falsified and substandard vaccines. The Department's Mass Spectrometry Research Facility will build on their work developing analytical methods for vaccine authentication. (4)

Profs Meera Mehta and Paul McGonigal received funding from the SCGC Fund for Innovation and Research in Sustainability and Technology. Meera's project explores sustainable phosphorus-based catalysts for energy-efficient chemical synthesis, while Paul is developing organic ionic materials intended to reduce the energy demands of future AI and machine-learning hardware.

Prof Charlotte Williams OBE FRS and Prof Iain McCulloch FRS each received Royal Society awards. Charlotte was awarded the Armourers & Brasiers' Company Prize for her work in catalysis and sustainable polymer materials. Iain received the Hughes Medal for his work on organic semiconductors and clean-energy technologies.

In this year's Royal Society of Chemistry prizes Prof Yimon Aye received the Corday-Morgan Mid-Career Prize for Chemistry for her work pioneering tools to observe and manipulate chemical signalling inside living cells and organisms. Team SMOM, several members of which are associated with Oxford, are working to develop solid-state molecular organometallic chemistry methods, and were awarded the RSC's Dalton Horizon Prize.

Waynflete Professor of Chemistry Véronique Gouverneur FRS received the 2026 Grand Prix Scientifique of the Simone and Cino Del Duca Foundation. The award recognised Véronique and her team's work towards safer and more sustainable fluorine chemistry.

Prof Jason Chin was awarded the 2026 Heinrich Wieland Prize. This international prize recognises outstanding research on biologically active molecules and systems.

Prof Christiane Timmel received the 2026 Bruker Prize from the Royal Society of Chemistry's ESR Spectroscopy Group, recognising her contributions to understanding spin dynamics in chemical and biological systems.

Dr Camilla Di Mino received an ISIS Springboard Award, recognising her as an outstanding early-career researcher using neutron techniques. (6)

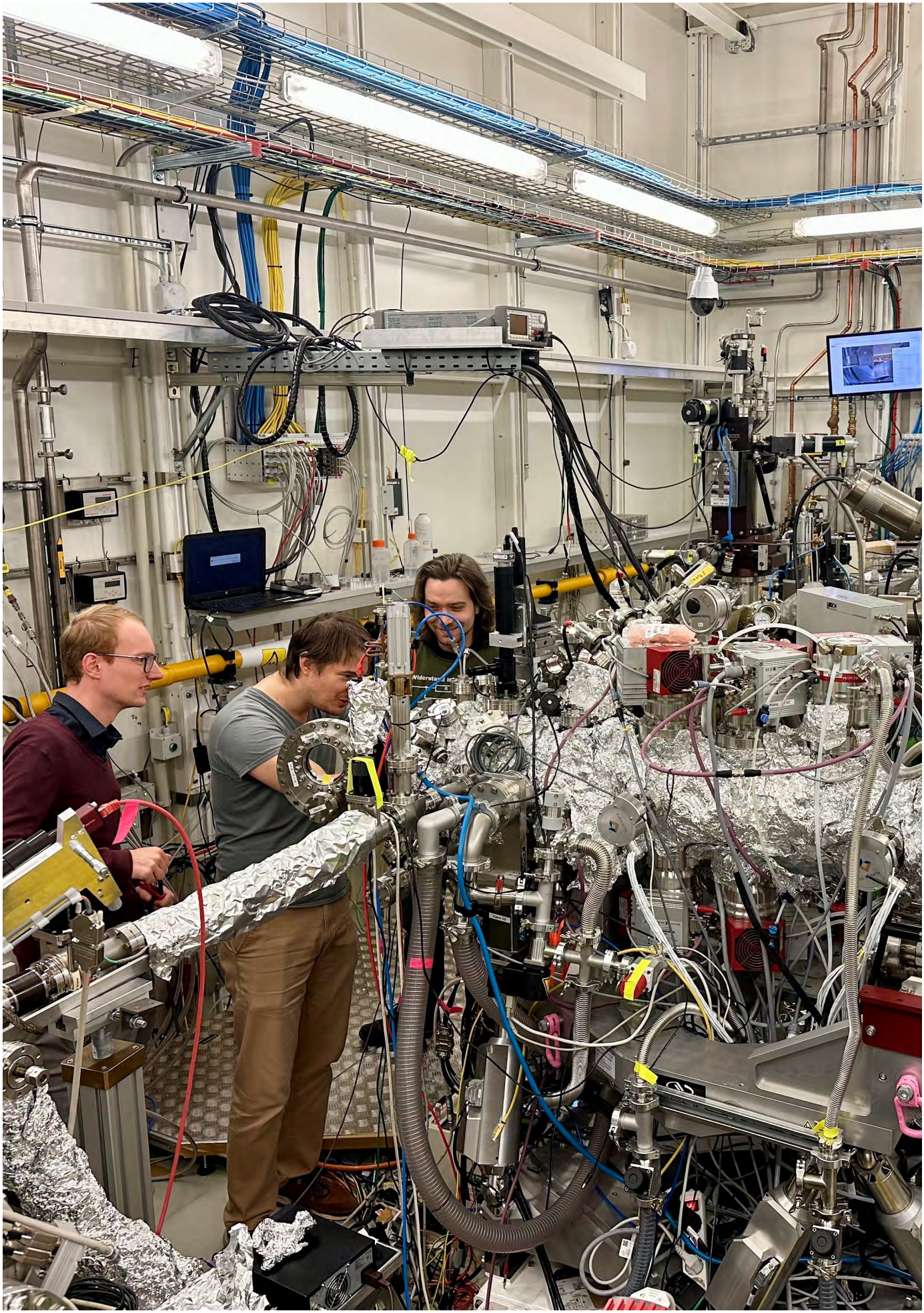
Oxford Chemistry spinout Mode Labs was awarded £100,000 in Ofwat's Water Discovery Challenge to develop and trial its CERES autonomous chemical monitoring platform. (5)

Dr Xhoela Bame was part of the 2026 Forbes 30 Under 30 Europe list in Science and Healthcare, recognised for her work on cellular degeneration and repair.

Recent DPhil graduate Dr Kieran Agg received the 2026 Katharine Burr Blodgett Award for the best PhD research in colloid and interface science.

Four projects received 2026 Jamie Ferguson Chemistry Innovation Awards. Euan Sarson is developing an MRI contrast agent for imaging hypoxic tumours; Clare McFall is investigating small molecules to treat cardiomyopathies; Matthew Williams and Emma Southall are developing materials to extract uranium from seawater; and Raman van Wee and Dan Loewenthal are advancing mass photometry for studying protein interactions directly in complex biological samples (3). Loewenthal and van Wee, alongside Alex Hannon, also took second place at the Reuben College Entrepreneurship Forum.

And finally, DPhil student Eirik Moen Liane finished in the Top 100 at the International Puzzle Championship in Munich. There are no jigsaw puzzles in this year's *Periodic* – but turn to page 31 if you fancy trying your hand at our crossword puzzle.



Seeing beyond the metal surface

Hard X-rays reveal what happens when Pd breathes in H_2

Hydrogen is a promising source of clean energy. Burning H_2 in oxygen releases energy, with only water as the by-product. Hydrogen gas, however, is famously highly flammable, and storing it safely is a major challenge for the transition to sustainable energy.

In 1869, palladium was found to be the first metal to absorb large quantities of hydrogen. Since then, PdH_x (palladium hydride – a metal with hydrogen absorbed, where x is a value below 1) has been used in hydrogen compressors, purification and sensors. Despite the long history and wide use of PdH_x, it was not well understood exactly where the hydrogen goes, and how this impacts the electronic and crystal structure of palladium beyond the surface. A better understanding of palladium hydride is important for developing better catalysts and hydrogen energy technologies.

Six research groups from across Europe, led by Prof Anna Regoutz from Oxford's Inorganic Chemistry Laboratory, have come together to see inside the bulk crystal structure of PdH_x formed from thin films. The work brings together experiment, spectroscopy and computation.

The team's recent publication in *Advanced Science* uses X-ray diffraction and neutron reflectometry to show a phase transition from α-PdH_x to β-PdH_x at 50 °C, and an expansion of the lattice when hydrogen was incorporated. The electronic fingerprint of Pd–H bonds was revealed using spectroscopy. Computational calculations confirmed the hypothesis that hydrogen atoms occupied octahedral holes, i.e. they were immediately surrounded by six Pd atoms.

Confirming the presence of Pd–H bonds in the bulk crystal answered a long-standing question: Do Pd–H bonds persist into the bulk? This question was not previously answerable by studies that stuck to the surface of PdH_x. The team's spectroscopic studies established AP-HAXPES (ambient-pressure hard X-ray photoelectron spectroscopy) as a powerful tool for seeing into the bulk electronic structure. The image to the left shows the experimental hutch of beamline P22 at PETRA III at the Deutsches Elektronen-Synchrotron (DESY), with members of the experimental team loading a sample into the spectrometer.

Conventional soft X-ray photoelectron spectroscopy only sees the outer 5–10 layers of atoms, whereas AP-HAXPES can see up to 50 layers deep, where surface effects disappear and the structure of the bulk crystal can be observed. Given that a single grain of salt contains over 1 million layers of NaCl, knowledge of the surface alone leaves most of a crystal unexamined.

Compared to soft X-rays, hard X-rays are higher in energy. Electrons knocked out of the atoms by hard X-rays can escape from deeper in the crystal as they have more kinetic energy. Measuring the ejected electrons' kinetic energy gives information about the electronic structure, and therefore the bonding in the crystal.

Obtaining spectra at variable temperatures allows correlation of electronic and structural changes as hydrogen is incorporated into the crystal. The team were able to observe exactly what the hydrogen is responsible for in the spectra as it enters the palladium.

Transnational collaboration and new instrument technologies have made this work possible. Beyond the structure and bonding in PdH_x, this research opens new possibilities for seeing into the bulk electronic structure of other metal hydrides. Furthering our understanding of metal-hydrogen interactions paves the way towards better catalysts for the splitting of water, and improved solid-state storage materials.

It is 157 years since palladium was first seen to hold hydrogen. AP-HAXPES gives us a view of exactly how it does so, bringing us one step closer to clean energy. Anna and the team are already working on the next steps. Instead of looking at PdH_x in isolation, they are now studying entire hydrogen sensors which are formed of complex multilayer structures of different materials. Following the approach developed in the palladium work, they are exploring the influence of hydrogen across several layers of the material, and at the interfaces between layers, hoping to provide a complete understanding of the structural and electronic changes underlying the sensor performance in real-world applications. ■

doi.org/10.1002/advs.202522098

Light-activated molecular switch for precision cancer treatment

Near-infrared light activates a molecule for killing cancer cells

A team from the Langton and Russell groups at Oxford Chemistry has developed a near-infrared light-activated molecule that irreversibly switches on chloride ion transport in cancer cells and triggers cell death.

Reported in *Angewandte Chemie International Edition*, the study describes a molecular system made up of two parts: a chloride ion transporter, and a boron-based photocage compound that keeps the ion transporter inactive until exposed to near-infrared light.

Cancer cells, like all living cells, depend on a carefully controlled balance of ions such as chloride, sodium and potassium to survive. Proteins transport these charged species across the cell membrane in order to regulate cell functions including homeostasis, signalling and pH. The cell's survival is therefore highly sensitive to membrane transport processes.

This study exploits that vulnerability by creating a light-activated chloride transporter: a molecule that can disrupt a cell's ion balance once switched on. The system works like a switch: while the photocage is attached, the chloride transporter remains inactive. When exposed to near-infrared light (wavelength 730 nm), the photocage is removed and chloride ion transport begins. The activated molecule then moves chloride ions across the cancer cell membrane, disturbing its carefully controlled internal balance and triggering cell death.

Crucially, near-infrared light can penetrate tissue more effectively than shorter wavelengths of light such as ultraviolet or violet, which do not pass deeply through tissue and can instead damage healthy cells. Penetrating infrared light gives researchers a way to control when and where artificial ion transport occurs, opening a potential route towards more targeted cancer therapies.

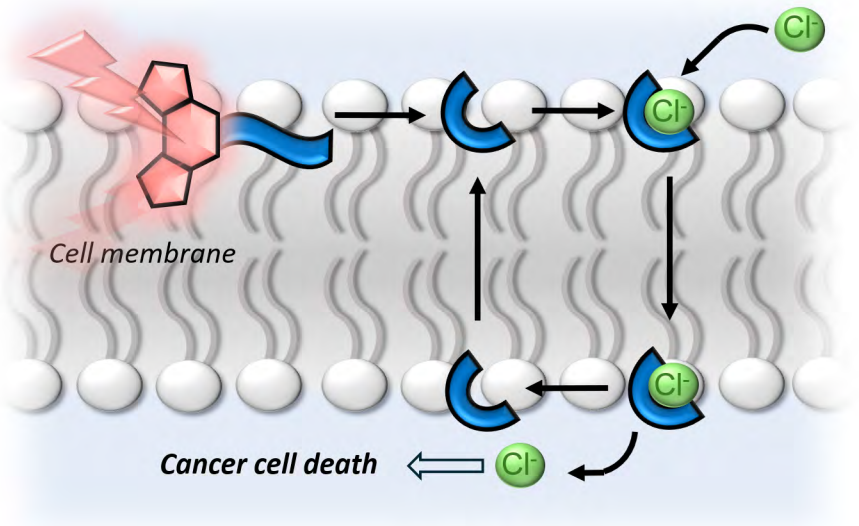
This approach offers an alternative to existing light-activated cancer therapies

This approach offers an alternative to existing light-activated cancer therapies, which usually use light to generate reactive oxygen species that damage cancer cells. Many tumours, however, have low oxygen levels, which can limit the effectiveness of current treatments. The team's new strategy avoids this limitation because it does not rely on oxygen. Instead, near-infrared light activates a molecule that disrupts chloride ion balance inside cancer cells.

The idea for this work grew from earlier work conducted by Dr Manzoor Ahmad from the Langton group, who had developed a hydrogen-bond switch that could act like a logic gate to remotely control ion transport in synthetic cells. Prof Langton said: "This earlier work inspired us to ask whether a similar concept could be used for photodynamic therapy by integrating near-infrared triggers and exploring anion transport activity in cancer cells."

The team first studied how the molecule responded to light in solution using NMR spectroscopy. They then tested it in artificial cell-like membranes called vesicles, using fluorescence techniques to show that light could switch on chloride transport. Together, these proof-of-concept experiments confirmed that the molecule worked as designed: inactive before light exposure, active after irradiation, and able to move chloride ions across membranes.

Next came the translation of this system to living cancer cells. Biological cells are far more complex than synthetic models, so it was not



The chloride ion transporter is kept inactive by the boron-based photocage (shown in red in the schematic above). When exposed to near-infrared light the photocage is removed and the rest of the molecule (blue) can reorient itself to bind chloride ions for transport across the cell membrane.

guaranteed that the molecule would still behave predictably. Working in collaboration with Dr Ríona Devereux from the Russell group, they conducted tests on breast cancer cells outside of a living organism, tracking the movement of chloride across the cell membrane and the loss of cancer cells to determine if the active transporter was able to target and kill cancer cells.

They showed that the inactive, caged transporter was much less toxic on its own, but when it was exposed to near-infrared light, chloride transport switched on and the number of live cancer cells decreased sharply. This provided clear evidence that the light-activated system works in cells. Looking ahead, the team are continuing to explore how synthetic molecules can be used to engineer new functions into lipid bilayer membranes, both in synthetic and living cells.

Although still in the discovery phase, this exciting research points towards a promising future for light-triggered, targeted cancer treatments, where cancer drugs are activated only where they are needed. This could help protect healthy cells during treatment and reduce side effects for cancer patients. ■

doi.org/10.1002/anie.202523734



A new spin on nature's compass

Engineering magnetic-field sensors for living cells

Every year, songbirds travel thousands of kilometres across continents, chasing longer and warmer days.

After 150 years of speculation, we now understand that these impressive orienteers use the Earth's magnetic field to guide their flight. Among the leading hypotheses is the theory that birds use a protein-based quantum compass located at the back of their eyes to aid navigation.

Building on our understanding of this process, a team of Oxford scientists has now used evolution to engineer proteins in living cells that respond to magnetic fields, opening up a new frontier in medical imaging.

The landmark study, published in *Nature*, introduces magneto-sensitive fluorescent proteins (MFPs) as candidates for medical imaging technologies. The team also created a prototype imaging instrument to detect fluorescence from the MFPs.

Magnetic resonance imaging (MRI) is commonly used in medicine, employing magnetic techniques to detect hydrogen and other magnetically active nuclei in the body. This work suggests that we may be able to use related principles to see MFPs in

action. Tracking these specific molecules could allow gene expression to be monitored, giving us a way to observe small changes in a tumour, for example.

> **The magnetosense stands among nature's most captivating and elusive rules of life.**
>
> Prof Christiane Timmel

The MFPs were produced using a technique called directed evolution. First author and DPhil student Gabriel Abrahams said: "What blows me away is the power of evolution: we don't yet know how to design a really good biological quantum sensor from scratch, but by carefully steering the evolutionary process in bacteria, nature found a way for us."

Professor Harrison Steel, from the Department of Engineering Science, reflects on the foundations of their work. "Our understanding of the quantum processes happening inside MFPs was only unlocked thanks to experts who have spent decades studying how birds navigate using the Earth's magnetic field."

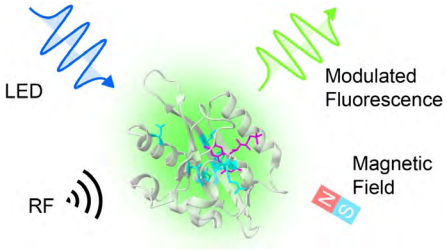
The processes that allow the function of the quantum compass used by songbirds are initiated by light. The central player in the magnetoreception hypothesis is cryptochrome, a protein found in the bird's retina. Visible light excites electrons in these cryptochromes, triggering electron transfer cascades that lead to the formation of radical species containing unpaired electrons. The Earth's magnetic field can influence the spin dynamics and subsequent reactions of these radical pairs in a way that depends on the orientation of the cryptochrome relative to the field. This could produce orientation-dependent chemical signals that the bird's nervous system uses to determine direction.

This compass behaviour comes from a remarkable property of electrons called spin, which becomes particularly important when electrons are unpaired.

Oxford has a rich history in spin chemistry. The field was pioneered at Oxford by Prof Keith McLauchlan FRS and his group in the 1980s. His student Prof Peter Hore FRS, and subsequently Hore's student Prof Christiane Timmel, extended this work to biological systems. In 2007, Prof Timmel founded the Centre for Advanced Electron Spin Resonance (CÆSR).

Now, for the first time, spin chemistry has been used to create a new biotechnology: MFPs that work in living cells.

In November 2025, an interdisciplinary project, led by the Department of Chemistry's Prof Christiane Timmel, received £6 million from the Biotechnology and Biological Sciences Research Council's Strategic Longer and Larger (sLoLa) grants scheme.



Above: Magneto-sensitive fluorescent proteins (MFP) are excited by light from a blue LED and emit a fluorescent light of a different colour (green). The intensity of this fluorescence can be modulated by applying magnetic or radio frequency (RF) fields of appropriate strengths and frequency. Previous: Prof Christiane Timmel (centre) and the interdisciplinary Oxford team investigating magnetically sensitive proteins.

"The magnetosense stands among nature's most captivating and elusive rules of life," says Prof Timmel. "By bringing together an extraordinary team of engineers, physicists, chemists, biochemists, and neuroscientists, this sLoLa initiative offers a unique opportunity to tackle this formidable task of shedding light on one of nature's best kept secrets – and to turn that discovery into powerful new biotechnologies."

Ultimately, these projects and developments prove that spin chemistry can be harnessed within living cells, opening a brand-new frontier for engineering quantum-controlled biological tools. ■

doi.org/10.1038/s41586-025-09971-3

Stop-motion crystallography reveals how a cancer-linked enzyme works

Using protein crystals to make a molecular movie

A tiny chemical change can have a big effect on how cells behave and cause diseases. For instance, an enzyme known as AspH (aspartate β-hydroxylase) adds oxygen atoms to specific sections of proteins associated with cell signalling and development. This enzyme is frequently overexpressed in a range of cancers, and has been associated with tumour progression and metastasis. Therefore, understanding how this enzyme works could help inform the development of future anticancer drugs.

In a collaborative study published in *Nature Communications*, researchers from Oxford Chemistry investigated AspH catalysis in real time using X-ray free electron lasers

(XFELs – large-scale particle-accelerator facilities found at only a few sites worldwide that produce extremely bright, ultrashort X-ray pulses).

> **...making it possible to monitor enzymes in action, and answer biological questions previously out of reach.**
>
> Dr Patrick Rabe

Led by Dr Patrick Rabe and Prof Christopher Schofield, the team combined crystallographic, spectroscopic and isotopic labelling experiments to build a detailed mechanistic understanding of how AspH functions in real-time. They worked with national and international collaborators at Lawrence Berkeley National Laboratory (US), SLAC National Accelerator Laboratory (LCLS, US), the Pohang Accelerator Laboratory (PAL-XFEL, Korea), and Diamond Light Source (Oxfordshire).

At school, enzyme activity is often explained using a lock-and-key model: a substrate fits neatly into an enzyme's active site, much like a key fitting into a lock. The reality is not so neat. Enzymes are constantly moving and changing shape as the reaction unfolds, often so quickly that experiments capture only static snapshots of the start or end of the process. Time-resolved crystallography, combined with complementary spectroscopic methods, can instead capture a sequence of snapshots as a reaction occurs, providing unprecedented insight into how enzyme structure, dynamics and catalysis are linked.

In this study, the team used XFELs at facilities in the US and Korea to take snapshots of the reaction as it unfolded within crystals of AspH, rather like filming an enzyme in action.

First, the team produced large quantities of human AspH enzyme in the lab using genetically engineered bacteria. They then crystallised the enzyme – a challenging process because proteins are much harder to crystallise than small molecules. When it works, however, the resulting crystals can be used to generate a detailed 3D picture of the protein. This is the first still image in building an understanding of how the enzyme functions.

To move beyond a single snapshot, the team grew tiny AspH crystals, each about the size of a very fine grain of sand. In solution the microcrystals formed a suspension that looked like a cloudy sludge to the naked eye. Their small size allowed oxygen to diffuse through them rapidly and initiate the enzyme reaction. In order to control exactly when the reaction began, the microcrystals were loaded under oxygen-free conditions onto a specialised tape-drive at the XFEL. By controlling the speed of the moving tape, the researchers could precisely vary the time between oxygen exposure and X-ray data collection and capture structures at different stages of the reaction, effectively assembling a molecular stop-motion movie.

The crystallographic experiments were complemented by spectroscopy, which helped pinpoint how oxygen reacts at the AspH iron centre. The researchers found that the iron has an unusual coordination environment, supported by a small network of water molecules. This arrangement leaves room for both oxygen and the substrate in the active site, and may explain why AspH can act on multiple substrates, adding an oxygen atom to both aspartate and asparagine residues. Isotopic labelling confirmed that the oxygen AspH adds to its substrates comes from molecular oxygen (O_2), and not water (H_2O).

The team's work provides the most detailed mechanistic picture of AspH obtained to date, using a variety of advanced techniques in concert to reveal its molecular forms and functions. These insights pave the way for future studies aimed at capturing additional catalytic intermediates and enzyme dynamics in real time, while also providing a foundation for efforts to selectively target AspH in disease.

Dr Patrick Rabe said: "This project brought together specialists from structural biology, chemistry, spectroscopy and large-scale X-ray facilities across Europe, Asia and the United States. It highlights how international collaboration and advances in X-ray laser technology are making it possible to monitor enzymes in action, and answer biological questions that were previously out of reach." ■

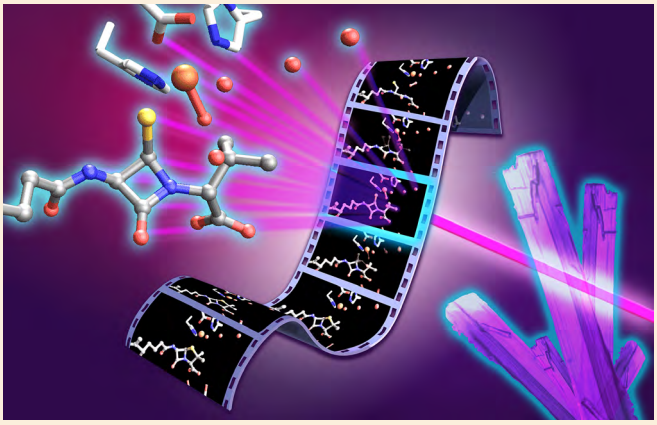
doi.org/10.1038/s41467-026-69425-w

STOP PRESS

Molecular movie reveals how penicillin is made

As this issue of *Periodic* was going to press, Dr Patrick Rabe, Prof Christopher Schofield and collaborators published a new study using similar methods in *Nature Catalysis* revealing previously unseen stages in how nature builds the β-lactam ring at the heart of penicillin. Their "molecular movie" captures fleeting steps in the reaction that have eluded scientists for decades, resolving questions about how this crucial antibiotic structure is formed. The findings could ultimately help to engineer new or improved antibiotics. ■

doi.org/10.1038/s41929-026-01618-4



Celebrating our postdocs

The gloveboxes are making a very strange noise, a new student is starting and the latest batch of experimental data looks odd. Who do you call for help? More often than not, the answer is a postdoc.

Postdocs – short for postdoctoral researchers – continue with academic research after completing a doctorate or DPhil. But that definition hardly captures the role. They are at the heart of almost every research group, developing their own research projects while mentoring students, troubleshooting experiments and equipment, sharing expertise and doing much of the essential work that keeps research moving.

"In all honesty, day-to-day postdoc life is a bit like being a magician at a children's birthday party, but instead of party tricks, it's constant chaos of sorting administrative tasks and running around with a spanner to fix equipment," says Dr Natalia Dyachenko, a postdoc in the Vincent group.

"Despite the madness, the really cool enzyme science I get to explore is what drew me to apply for a postdoc in the first place. What I enjoy most is mentoring others, while still being given the space to stay curious and pursue scientific problems."

For students, the influence of a good postdoc can extend well beyond solving an immediate research problem.



What I enjoy most is mentoring others, while still being given the space to stay curious and pursue scientific problems.

Dr Natalia Dyachenko

Periodic science writer and DPhil student in the Vincent group Shoba Laxmi says that working alongside postdocs has helped her grow as a researcher and taught her how to be a mentor.

"Postdocs in our group wear so many hats on top of conducting their own research, yet they are ready to help me whenever I approach them for help with my research," says Shoba. "I cannot express how grateful I am to learn and work alongside all of them – it has made me a better researcher and made me want to pay that gratitude forward."

Bodoo Batnaran, a final-year DPhil student in the Hayward research group, says that the postdocs he has met in Oxford have had a real influence on both his research and his outlook.

"Aside from helping with research problems, postdocs have also shaped the way I think about research and helped plan my future career," says Bodoo. "They've also had impact on my life outside of research; I've started running because of one! In short, they are a large part of the reason I view academia positively as well, despite all of its flaws."

For postdocs, Oxford offers opportunities to tackle challenging questions, work collaboratively, grow in independence and build expertise for the next stage of their careers.

"I enjoy pursuing projects that interest me while having the freedom to decide how to spend my time each day," says Dr Brad Sheath, a postdoc in the Hayward group. "I also find getting involved in the projects of Part II and DPhil students very rewarding."

"There are also some frustrating days when reactions don't work as expected in the lab or when complicated data are proving difficult to analyse, but I always try to remember that if the work was straightforward then it would have been done before."



I enjoy pursuing projects that interest me while having the freedom to decide how to spend my time each day.

Dr Brad Sheath

The postdoctoral years can also bring challenges beyond research. Unlike students and many senior academics, postdocs often have limited opportunities to become affiliated with an Oxford college. "The lack of a proper system for college affiliation for postdocs feels backward when we contribute so much to Oxford," says Natalia.

The Chemistry Department's Postdoc Committee goes some way towards bridging that gap. Run by postdocs themselves, it creates a community beyond the laboratory and gives postdocs a space to socialise, network and make their voices heard.

Short-term contracts and the expectation that early-career researchers may change institutions regularly can create another challenge, particularly for postdocs balancing research with family and other commitments.

Dr Kel Britton, a postdoctoral researcher in the Langton group working on transmembrane ion transport systems, says supporting others is one of the parts of the role she values most.

"I love the research, supporting fellow lab members and, above all, working with such an understanding and supportive supervisor in Prof Matthew Langton," says Dr Britton. "I strongly believe in supporting people, and I ensure undergrads, Master's students, DPhils and fellow [postdocs] always get the help they need, even if that means reshuffling my own work to accommodate the requirements of others."



I love the research, supporting fellow lab members and, above all, working with such an understanding and supportive supervisor.

Dr Kel Britton

But the realities of postdoctoral employment can make longer-term planning difficult: "As much as I love being a PDRA [postdoctoral research associate], being a mother to a 12-year-old son with ADHD also makes me aware of the challenge of short-term contracts and the expectation to move every two to three years, which is just not a feasible option for my family."

Around 200 postdoc researchers from across the world work in Oxford Chemistry, contributing to research across the Department. Their contribution is not confined to their own experiments and publications. They pass on knowledge, solve problems, mentor researchers, support colleagues and help shape the culture of the groups in which they work. Much of the Department's research depends on them. ■

Supporting our postdoc community

There are around 200 postdoctoral researchers in the Department of Chemistry, representing our largest staff group.

Postdoc contracts tend to be fairly short – usually between one and three years in length – because this is seen as a stepping stone role to academic and other career paths. This means that we recruit around 100 postdocs every year, many of whom are new to Oxford and the UK.

Over the past couple of years, we have worked hard to improve our induction programmes and help new postdocs settle in quickly. Most are very well supported by the research groups they join, and the Postdoc Committee have also introduced a buddy scheme to pair new starters with existing staff in order to help smooth the transition to Oxford.

Postdocs join the Department throughout the year, making it difficult to run a single welcome event. To address this, we have introduced monthly Coffee and Connect welcome sessions for postdocs who are new to the Department. These have proved a really successful way to connect small groups of new research staff, to introduce the career development support on offer, and to emphasise how much we value the research contributions of postdocs in the Department.

At the postdoc stage, career development is really important. The Postdoc Committee has introduced a series of termly panel sessions over coffee, termed Brewing Mentoring, where postdocs can discuss topics such as career transitions or how to come up with ideas for research grants.

We have also reinvigorated our Chemistry Careers Conference, aimed at DPhil students and postdocs, to introduce early career research students and staff to the variety of careers that can come from a Chemistry background. Our active Oxford Women in Chemistry Society also runs many events to support career development.

Prof Kylie Vincent
Associate Head of Department (People)

We want to hear from you

Do you have a memory of a postdoc who made a difference?

Perhaps they helped you through a difficult experiment, taught you something you still use today or simply made your time in the Department better. Share a favourite memory, a thank-you message or a few words about a postdoc who had a lasting impact on you.

Were you previously a postdoc in the Department?

We would also like to hear where your career has taken you, what you remember about your time here and whether you would like to stay in touch. The Department hosts regular events for alumni and friends and we are keen to welcome former postdocs too.

If you would like to get in touch please email *alumni@chem.ox.ac.uk*



Afua Kyei

In her element

Afua Kyei (Somerville, 2000) is Chief Financial Officer of the Bank of England. Long before she helped steer one of the country's most important institutions, she was inspired by her mother's work as a midwife and saw medicine as the obvious route. But, driven by a desire to help find a cure for cancer, she chose to study chemistry instead, completing her Part II with Professor Sir Jack Baldwin in 2004 before going on to pursue an outstandingly successful career in finance. Afua talks to DPhil student Shoba Laxmi about her roots in Oxford Chemistry, and her work today in public life.

What did you most enjoy about studying Chemistry at Oxford?

I learned to be creative. I learned resilience, and I learned to experiment. I loved learning from some of the most innovative thought leaders in chemistry, I really enjoyed the tutorials and I loved the breadth of the Oxford degree; a highlight for me was reading history and philosophy of science (and German) as extra subjects. I had a lot of fun during my Part II in Prof Jack Baldwin's group.

Tell us about your experience of Chemistry research.

I was drawn to organic chemistry, and to explore research I volunteered to work with Professor Véronique Gouverneur during my second-year summer break. I have fond memories of that time, she was a real inspiration to me. I applied for a junior research fellowship at Princeton, and after my Part I, I worked with Prof John T. Groves at Princeton and we collaborated with Harvard, so I got to spend time at both universities in the US.

In my final year, I was selected by Professor Sir Jack Baldwin to join his group to do my Part II – he only took one Part II student each year, so it was an honour. The first half was really difficult, and I was very concerned because my research seemed to be going nowhere, but my research group helped me through it.

By the end of my Part II, I had created 70 new antitumorous molecules and my research was published in *Tetrahedron Letters*.

What did research teach you in your later career?

Research taught me to experiment, to look for new solutions through innovation, and to accept trial and error as part of the process. It taught me not to be afraid of failure, because having a go and failing is how new breakthroughs happen. Research can be lonely, but chemistry taught me that progress often comes from staying open, asking questions and learning from others, which I have carried through with me.

> **It taught me not to be afraid of failure, because having a go and failing is how new breakthroughs happen.**

What motivated your move into finance?

After my A-levels and during university holidays, I worked part-time in sales at Burberry in Knightsbridge and later in Mayfair, and I was selling so much that I was able to negotiate commission. I loved the social side of it, but what really appealed was the direct link between effort and output.

That was very different from my Part II experience, which was ultimately incredibly successful, but shaped by the fact that progress can take time. I was trying to use organic synthesis to replicate molecules that occur in nature, but I discovered that synthesis is not straightforward; you can't force nature to do what nature doesn't want to do, and you can't force an experiment to work!

I realised research was a long path, and the slow pace made me want to move into a commercial, fast-paced environment – and that led me to banking.

How did you find starting in finance from a science background?

Chemistry gave me a strong foundation in problem-solving, analytical thinking, communicating complex ideas simply and mathematics; all essential in business and finance. What I did not have was the technical knowledge like some of my peers who had studied subjects like accounting or management. I had to learn that on the job working on audits at banking clients while doing my three-year qualification, which was challenging. I had to be resilient, persevere and keep learning – back then, who would have thought I would end up as CFO of the Bank of England? Certainly not me!

Why do chemists make good leaders?

I think chemists adapt so well to leadership and public life because chemistry trains you to be evidence-led, disciplined and analytical, but also creative in how you solve problems. You learn to look at the facts, test ideas carefully and then make decisions based on what the evidence shows. That is exactly what good leadership requires.

Angela Merkel stands out: a chemist who became the first female Chancellor of Germany. I was invited to a breakfast that she hosted for women leaders, and she spoke about how her science background had shaped her leadership, grounding her decisions in evidence and data. We saw the same with Margaret Thatcher (Somerville, 1943), who was also a scientist before becoming Prime Minister and who said she was prouder of being the first British Prime Minister with a science degree

than being the first female Prime Minister.

At the end of the day, as public sector leaders, we are looking at the facts and making decisions based on what outcomes will be best for society. I believe fundamentally that chemistry teaches you how to do that, by distilling complex problems into simple, clear narratives.

What was the biggest challenge at the Bank of England?

The biggest challenge I faced in my current role was leading through the pandemic. I had to manage a team, restructure it to bring together Bank of England experience and commercial-world skills, and at the same time help the Bank move towards a medium-term strategy rather than thinking about what we wanted to achieve one year at a time. This was all done during the pandemic while colleagues were suffering, experiencing both physical and mental health issues, and some of them losing loved ones. I was working from home while dealing with national critical matters, and to add to the mix I had my young children and a newborn baby around me.

I also recognised that our historic model of funding Bank of England policy costs was no longer sustainable, so I worked with HM Treasury, my colleagues and other stakeholders to change it through primary legislation. That led to the introduction of the Bank of England Levy, creating a more stable income stream and helping to reduce future losses – this is something I am very proud of.

How do you manage the pressures of your high-stakes role?

I enjoy spending time with friends and family, which helps lighten the atmosphere. In my role as CFO, and as a mother with four young kids, I meet new people all the time amidst ferrying my children to endless birthday parties! I have managed to balance work and family, but it is still a juggling act and constantly evolving. I do find time between busy stints to chill out and just enjoy my "me time" to decompress.

> **Chemistry trains you to be evidence-led, disciplined and analytical, but also creative in how you solve problems**

Earlier this year, you were a guest of honour as the Royal Society celebrated 80 years of admitting women. How can we better support women in STEM?

We know that there are many women who end up having to choose between work and having a family. I think it is really important that workplaces in STEM are supportive of women, so that they don't have to make those choices, and so that there is infrastructure in place to support them, giving women a fair shot at managing both a family and a career.

If we want more women to stay and thrive in science, the system has to support them properly in terms of promotion of STEM in schools and universities, support for maternity leave, having realistic expectations on publication timelines and flexibility in research grant funding.

What advice would you give Oxford Chemistry students today?

Chemistry gives you a set of skills that can take you in all sorts of directions. Keep an open mind: chemistry sits at the heart of so much of what is happening now – see how far it can take you. I would tell my younger self to blend a career in science with commercial innovation opportunities.

Funnily enough, I remember my Somerville inorganic tutor saying "I don't know why I'm teaching you all this. You're all going to go off and become accountants anyway." Fast forward, and out of the eight Somerville chemists in my year, we went on to do a multitude of things: one became an Olympic rower, one a fashion photographer, one a Chemistry academic. I was the only one who fulfilled her prophecy of becoming an accountant! ■



Below: Afua Kyei attends a breakfast for women in leadership hosted by former Chancellor of Germany Angela Merkel.

Chemistry gives back

A year of fundraising for Oxfordshire charity Yellow Submarine

Over the past year, staff and students across the Department have come together to raise funds for Oxfordshire charity Yellow Submarine, which supports young people and adults with learning disabilities and autism. Through its social enterprise cafés, traineeship programmes, and residential holidays, Yellow Submarine helps its members build confidence, social skills, independence and employability.

The charity particularly supports young people making the transition from school – a time when they can face social isolation, limited opportunities to develop life skills and barriers to employment. A four-person committee of Chemistry staff and students set a fundraising target of £1,000 and organised a series of events across the year.

Colleagues brought in sweet and savoury treats for a charity bake sale, which went down so well that a second one soon followed. The admin team organised a World Cup Sweepstake, bringing plenty of friendly rivalry to the Department as colleagues followed the tournament. There was some healthy competition too in the step challenge, with colleagues comparing pedometer counts and finding extra reasons to walk to work, take the stairs or get out at lunchtime.



Yellow Submarine supports people with learning disabilities and autism to live life to the full. They offer a variety of services including social clubs, activity days and residential holidays.

> **As an Oxford-based charity, it's so lovely to be supported locally!**
>
> Ellen Parker, Yellow Submarine

Alexia Leakey, Head of HR, said: "Yellow Submarine was the first charity supported through this Department initiative, and over the past year we have been proud to support an organisation making a real difference in our local community. The partnership has also brought colleagues together and given us a sense of shared purpose beyond our day-to-day work."

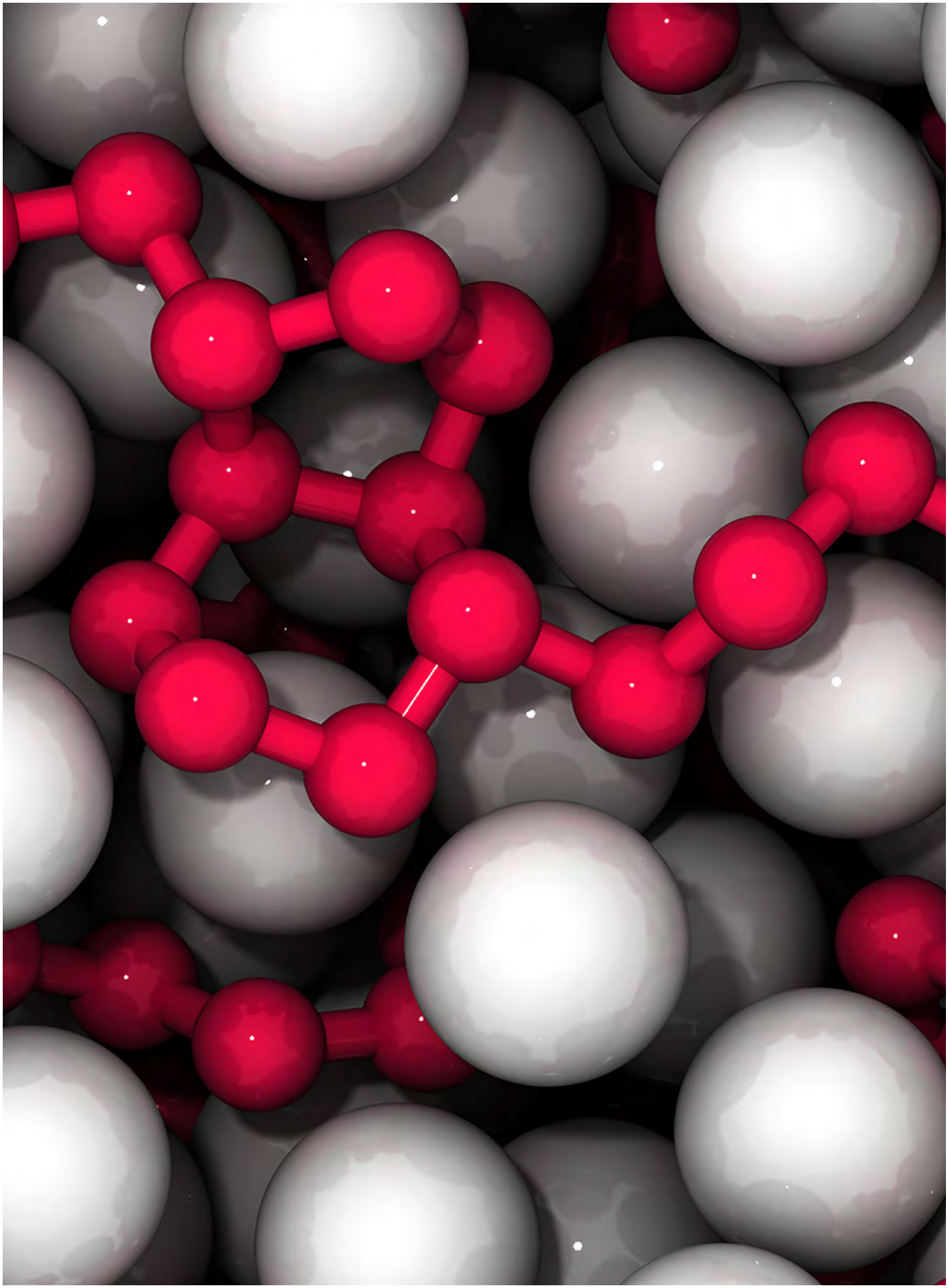
Sue Henderson, Executive Assistant to the Head of Department and Head of Administration, said: "Before we started this initiative, I knew very little about Yellow Submarine and the work they do. A colleague explained that the charity had been a great support to them and their family. I was able to see a small part of this myself when I visited their café in Oxford and ate some of the amazing bakes they make and sell. I have avidly watched the total amount raised, and am pleased that we have reached over £1,000 in support of this cause."

Ellen Parker from Yellow Submarine, said: "We are so grateful to the Oxford Chemistry Department for choosing to fundraise for Yellow Submarine. As an Oxford-based charity, it's so lovely to be supported locally! The funds they've raised will go a long way in helping people with learning disabilities and autism live life to the full. ■

You can find out more about Yellow Submarine's work by visiting *www.yellowsubmarine.org.uk*



Chemistry's fundraising organising committee outside the CRL this summer: (L–R) Ryan McGinley, Alexia Leakey, Shoba Laxmi and Sue Henderson.



Atomistic simulation snapshot of an amorphous Na–P structure, exemplifying the complex chemical environments that are relevant to using phosphorus as a sodium-ion battery anode material. The simulations were run using a custom-fitted machine-learned interatomic potential, as described in L. Wu, V. L. Deringer, *Angew. Chem. Int. Ed. 2026, 65, e08305.*

Artificial chemistry?

How AI is changing chemistry research at Oxford

Artificial intelligence is transforming how science is done. Tasks that once required weeks of coding, simulation or data analysis can now be completed in a fraction of the time, opening new possibilities for exploring chemical space. Yet such speed comes with the obvious risk of sacrificing learning and insight, especially for students at the start of their research careers.

More broadly, machine learning is not a new phenomenon in chemistry. For decades, computational chemists have used these kinds of algorithms to help identify patterns, predict properties and accelerate simulations. What has changed recently is the scale and accessibility of these tools: advances in artificial intelligence, large language models and coding agents are bringing machine learning into everyday research workflows.

How are these latest changes influencing the world of chemical research and teaching? *Periodic* spoke to three of the Chemistry Department's professors to learn more about how they are navigating the rapid progress in machine learning, large language models and coding agents.

New ways of modelling matter

Professor of Materials Chemistry Volker Deringer works at the intersection of materials chemistry and machine learning (ML). His research group develops computational approaches to investigate the atomic-scale structure of materials, with a particular interest in structures and properties of amorphous solids, which do not have a regular crystalline structure.

For decades, chemists have used quantum-mechanical electronic-structure computations to investigate materials at the atomic scale. Machine-learned interatomic potentials (MLIPs) are a fast-growing class of simulation methods that learn from such quantum-mechanical data, enabling simulations across much longer length and time scales.

"So much more is possible now," says Prof Deringer. "When I was a student, simulating a few hundred atoms at a time would have been a major effort for first-principles methods. Today, our students can look at hundreds of thousands of atoms almost routinely."

The recent advances in MLIPs build on decades of advances in theories, methods, and computational implementations. Quantum-chemical methods taught in lectures are now practically accessible in efficient, user-friendly codes.

One widely used example is CASTEP, a density-functional theory (DFT) simulation software for computing the electronic structure of materials. The code is developed by UK researchers, and is one of the core tools used in Prof Deringer's group. It can predict forces on atoms, but also properties such as NMR parameters, which are important for understanding the structure of both molecules and materials.

"DFT-based methods, and their software implementations, are now a central part of materials research," says Prof Deringer. "In the years ahead, I expect that MLIPs will similarly be fully established for mainstream chemical research – think of the opportunities that will open up!"

Prof Deringer emphasises the importance of tools and openly available software: this includes *autoplex*, which appeared in Nature Communications in 2025. The software implements automated workflows for creating accurate ML models, and is the product of a long collaborative effort with Prof Janine George, an expert on atomistic simulation workflows from the Federal Institute for Materials Research and Testing (BAM) in Berlin.



Chemists have a great lot of experience and intuition. In the age of AI, this is more valuable than ever.

Prof Volker Deringer

"The idea is to automate the parts that are tedious and error-prone," says Prof Deringer, "making it easier for the user to focus on the ideas that matter." *Autoplex* is able to interface with other materials chemistry software packages, and this open-source project is playing its part in bringing the frontier of chemical modelling to a wider audience.

To help with this, Prof Deringer and his team are active in creating resources: for example, the group published a tutorial paper

AI, decoded

Artificial intelligence (AI)
Computer systems designed to perform tasks normally requiring human intelligence, such as recognising patterns, solving problems and generating language.

Machine learning (ML)
A form of AI in which computers learn patterns from data rather than being explicitly programmed with every rule. In chemistry, ML models can learn from existing calculations or experiments to make new predictions.

Machine-learned interatomic potential (MLIP)
An ML model that has been trained on data from quantum-mechanical computations, predicting energies and forces on atoms and thereby enabling simulations.

Large language model (LLM)
An AI model trained on huge amounts of text and other data to recognise patterns in language. LLMs such as ChatGPT can generate and explain text, mathematics and computer code.

AI agent
An AI system that can go beyond answering a single prompt and carry out a series of tasks towards a goal. Coding agents, for example, can write, run, test and revise computer programs.

Training a model
The process of exposing an ML model to data so that it can learn patterns and relationships that can later be used to make predictions.

Benchmarking
Testing a computational method against agreed reference data to find out how accurate and reliable its predictions are.

on validating MLIPs in 2023, and group members contribute to "practical" exercises on some of the Department's courses. They ran a first Oxford MLIP workshop in May 2026, as part of the Oxford Advanced Materials Network's initiatives, with more activities planned in the future.

Prof Deringer emphasises that, with ML entering the mainstream, the collaborative aspect of chemistry becomes increasingly important. "We have seen a qualitative shift: from simplified models of the world towards the real thing. Atomistic simulation results can now often be compared directly with experimental settings, which in many cases was not possible before. If you look across the department, and across Oxford more widely, there are a lot of exciting possible use cases for MLIPs, and there are world-leading experts on subjects across the chemical sciences. My hope is that we can help these colleagues and their teams to incorporate ML-driven simulations into their research programmes."

With easily accessible ML models, it is more important than ever to consider the results of computational experiments carefully. Prof Deringer leads work creating benchmarking datasets, which provide a way to test new ML models: for example, on Li–P–S electrolyte materials, published in the *Journal of Chemical Theory and Computation*. "Chemists have a great lot of experience and intuition. In the age of AI, this is more valuable than ever: it means that chemists know what looks right, and what tests an ML model would need to pass in order to be trustworthy."

Exploring chemical reactions under more realistic conditions

Professor of Computational and Theoretical Chemistry Fernanda Duarte Gonzalez uses ML in two complementary ways: to extend her research group's ability to model reaction mechanisms, and then to navigate chemical spaces where traditional computational approaches to mechanistic modelling cannot reach.

"On the mechanistic side, we are particularly interested in accounting for dynamics, solvent and concentration effects in chemical reactions," says Prof Duarte. "This provides us with a more realistic picture of how reactions occur in the lab."

One way her group is doing this is through automation. They have developed *autodE*, a software package for automated reaction mechanism exploration, and coupled it with MLIPs via their code *mlp-train*. Together, these tools enable the efficient exploration of complex chemical systems and pathways in solution by reducing the need for computationally expensive electronic-structure calculations at every configuration along the different reaction pathways.



> **Ignoring this current transformation would mean missing an extraordinary opportunity, not just to participate in the shift, but to help shape it.**
>
> Prof Fernanda Duarte Gonzalez

In a recent study published in *Nature Communications*, Prof Duarte's group demonstrated this approach by using MLIPs to model a chemical reaction in water and methanol, capturing how interactions with individual solvent molecules affect

the reaction mechanism and producing reaction rates that agree with experiment.

"On the data-driven side, we use ML to identify structure–activity relationships and to explore chemical space. We have also used larger ML models for retrosynthesis predictions, where mechanistic exploration is not feasible given the scale of systems to be explored." In a recent publication in the *Journal of Chemical Information and Modeling*, her group explored how machine learning models can improve retrosynthesis predictions for challenging chemical transformations, including the prediction of synthetic routes for heterocycle-forming reactions where available reaction data is limited.

Looking ahead, she thinks that the rapid development of AI tools represents a major shift in how chemists work. "I recently read an article in *Chemistry World* which made the point that every previous new tool in the toolbox – tools like NMR spectroscopy, and DNA sequencing – has resulted in a shift of focus for chemists. I like that way of looking at it. Ignoring this current transformation would mean missing an extraordinary opportunity, not just to participate in the shift, but to help shape it. Many things can go wrong, and we really need the experts at every step."

For Prof Duarte, this also shapes how students are taught. "How do you teach students who use AI? By teaching the scientific method: how to ask good questions, challenge assumptions, and think critically. Perhaps this is one reason why philosophy, with its focus on fundamental questions, is regaining popularity in the age of AI."

One of the central challenges for AI in chemistry is knowing when models can be trusted. Knowing the domain up to which a given ML model is reliable, whether it can work reliably beyond the examples it has been trained on, and recognising when it is uncertain about its predictions are key. "So far, there is no simple solution," she says. "Keeping the chemistry in the loop seems the safest option."

New tools for new ways of working

The Oxford Colloid Group, led by Professor of Chemistry Dirk Aarts, combines experiment and theory to understand soft and biological matter. This year, the group found a new level of productivity by adopting LLMs, agentic workflows and ML into their practices.

Prof Aarts described his first encounters with AI: "I was very intrigued by LLMs at the level of writing limericks, until the beginning of 2026 where I found it really could do mathematics."

The way Prof Aarts and his team used these AI tools has developed over the months. Initially they were simply a convenient way to translate code from one programming language to another. But now, by using generative AI systems known as agents, they are finding new ways to share ideas and delegate programming tasks.

"The coding agents blew my mind. Now you can work in ideas and do maths really well, for example extending a theory from 2D to 3D." AI systems can be used to discuss ideas, while autonomous coding agents can write, test and refine delegated programming tasks. The group found that when they used these agents to generate code from scratch, the style was more embellished than necessary. However, when given a basic program written in their own style, the AI models could match it.

Prof Aarts agrees that while AI assistance provides an extraordinary speed-up: "The importance of going through ideas and mathematics with pen and paper remains. With better data analysis tools, experimental data now also become more important."

"The field of machine learning is new for the group. With the help of AI, what was previously a somewhat daunting and certainly time-consuming task became much easier." They found that AI had a particularly large impact on recent work using ML methods to classify antibodies from their amino-acid sequences. They are now extending this approach using experimental immune-repertoire data from their collaboration with the Frater group (Nuffield Department of Medicine), with the longer-term aim of identifying and ultimately predicting antibody sequences associated with responses to specific pathogens.



> **The importance of going through ideas and mathematics with pen and paper remains.**
>
> Prof Dirk Aarts

Artificial intelligence and machine learning are already changing how chemists model materials, analyse data, write code and explore chemical space. As these tools become faster and more capable, we are finding that chemical judgement matters more, not less. The opportunity presented by artificial intelligence is not simply to automate what chemists already do, but to use the new tools to ask new questions, exploring chemistry that was, until now, out of reach. ■



In what has become a recent tradition, Part II students come together in the Chemistry Research Laboratory at the end of Trinity Term to celebrate handing in their theses.

Part II perspectives

In the fourth and final year of the Oxford Chemistry degree, students join research groups to complete their Part II projects under the guidance of academic supervisors. *Periodic* science writer and graduating MChem student Charlie Muston spoke to his cohort about their experiences of research, what they learnt from Part II and why so many consider it their favourite part of the degree.

Phase phenomena and mixing mechanisms

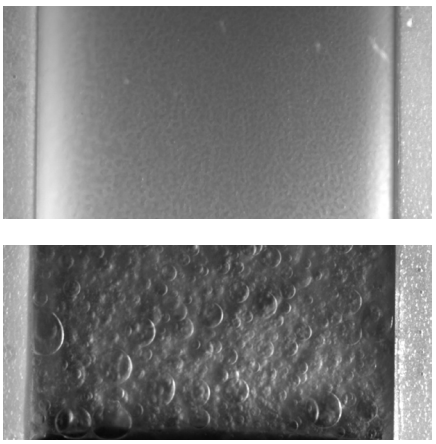
Dinah Lewis

Dinah enjoyed the liquids and solutions, statistical mechanics and theoretical chemistry courses during her first three years studying at Lady Margaret Hall. Prof Susan Perkin's group in the Physical and Theoretical Chemistry Laboratory offered a friendly and welcoming environment to combine her interests. A visit to the lab during her third year confirmed the Perkin group as her top choice, where she worked on understanding how certain liquids mix.

Understanding how, when and why liquid phases separate has applications across medical, food and environmental sciences: from delivering drugs across cell membranes to creating a stable salad dressing, or cleaning up an oil spill.

C_6E_2 (diethylene glycol *n*-hexyl ether) and water are partially miscible. Certain ratios of the two liquids in a sample will dissolve in each other, or mix, while other compositions will form two separate liquid phases – like olive oil and water.

The mixing behaviour of C_6E_2 and water is also temperature-dependent: the two liquids mix at low temperatures, and separate at high temperatures. Mixing occurs at low



Photograph of a bicontinuous morphology (top) and bubbles (bottom) taken through a microscope.

temperatures because of intermolecular forces between C_6E_2 and water. As the temperature is raised, these forces are overcome and phase separation takes place. Dinah studied the process of phase separation by heating the mixture above the threshold temperature.

Heating the mixed phase quickly to bring about phase separation is called quenching. There are two mechanisms at play during phase separation. Quenching gives us a window into these mechanisms but comes with the challenge of measuring changes that happen very quickly.

Dinah began her project by building an apparatus to quench mixtures of C_6E_2 and water while simultaneously photographing the phase separation process through a microscope. Over the course of the year she collected a dataset of 180,000 images, documenting phase separation caused by quenching over various temperature ranges.

Dinah then used computer vision techniques on this large bank of images to analyse the effect of temperature on phase separation. She was able to see the transition between the two mechanisms of phase separation, and how this varied with the size of the temperature range during the quench.



Dinah Lewis (right) and the Susan Perkin research group.

Liquid-liquid phase phenomena show up in many areas of science. Dinah's work brought together theory, design and experiment to reveal what happens during a quench.

Dinah told us that she enjoyed her project "because of the creativity involved. Building the apparatus from scratch was particularly fun because of the problem solving involved to get the experiment working. I also enjoyed learning about the field of computer vision, which was new to me, and applying these tools to analyse the images and distinguish different types of texture and bubbles."

With her coding and design skills, Dinah is continuing her work in the group. "I am staying in Oxford over the summer to complete more experiments, then taking a gap year to apply for PhDs."

Using light to open new pathways in organic synthesis

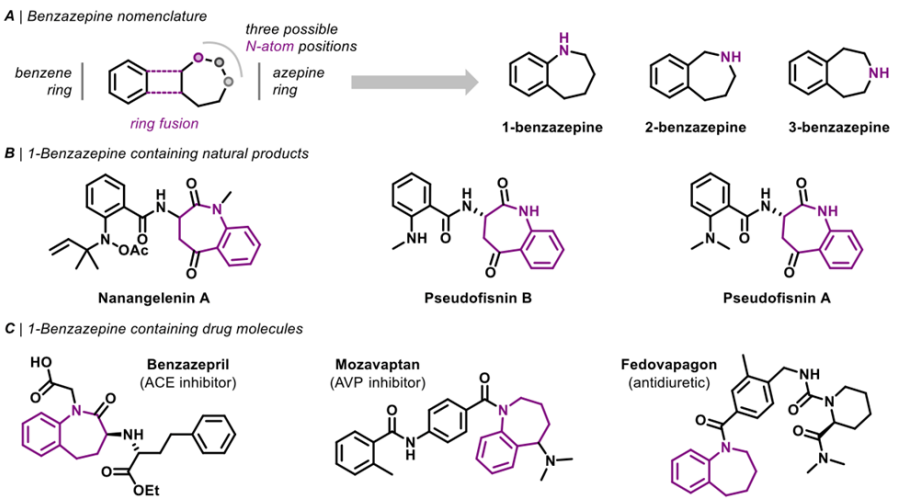
Grace Hagan

Light can give molecules access to excited states and open reaction pathways that are unavailable under normal thermal conditions. Grace joined Prof Martin Smith and DPhil student Valentin Veselinov to use photochemistry in the synthesis of benzazepines.

Grace got in touch with Martin to hear about his work. She was welcomed with a tour of the lab followed by a meeting to discuss his research. "He explained the projects he was aiming to do for my year and I thought all three ideas sounded cool and innovative."

Benzazepines are of interest owing to their many medicinal properties, including anti-inflammatory, anaesthetic and antimicrobial activity. Benazepril, for example, is a benzazepine-derived medicine used to treat high blood pressure (see figure).

The key step in the synthesis uses light to access a reaction pathway that is unavailable under normal thermal conditions. Photons of violet light bring one of the reactants into an excited state, allowing the reaction to proceed through a triplet-state pathway to form the desired product.



Benzazepine nomenclature (A), natural products (B) and drug molecules (C) containing 1-benzazepine.

Grace reflects on this key reaction: "The photochemical step was novel and required repeated trials, with many unsuccessful attempts before the initial hit." After months at the bench, Grace finally made it work. Her favourite moment was "getting the initial reaction hit. After isolating the compound and assigning the NMR spectrum, I could see that I had made the correct product. That moment was so special."

Beyond benzazepines, Grace enjoyed the lab environment. "It was nice having structure every day and going into the lab with a goal in mind. The lab is very social and often had group lunches, so I got to see different colleges that I would otherwise never have seen."

Grace was initially inspired to pursue organic chemistry by Dr Christie, her sixth-form chemistry teacher, and now, after a year of research experience, she hopes to continue to work in science. "I have a few holidays booked, but then I am job hunting. I would love to work in pharmaceuticals, so I'm looking for work experience in industrial labs."



Grace Hagan (second right) and the Martin Smith research group.

Solid-state synthesis and a magnetic mystery

Sarah Browne

Sarah, from North Somerset, joined Prof Simon Clarke and Dr Robert Smyth for her research project. She said: "I enjoyed the solid-state chemistry courses and became interested in crystallography, taking the supplementary course. I chose the Clarke group specifically because of its friendly atmosphere."

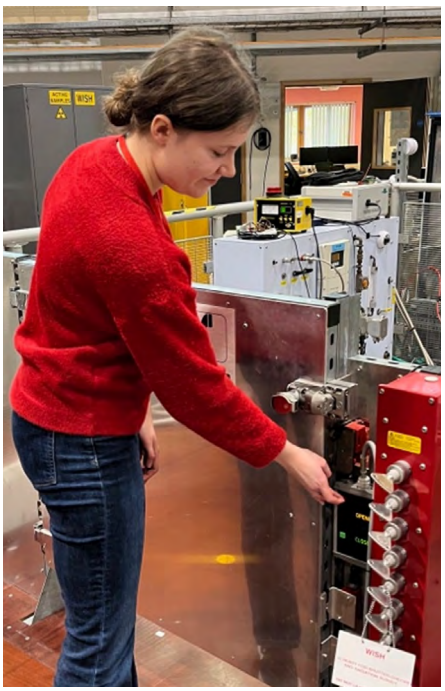
Sarah worked in the Inorganic Chemistry Laboratory to synthesise and study the magnetic properties of transition metal gallium sulfides $M_2Ga_2S_5$, where M is a transition metal such as manganese, iron, cobalt or nickel.

MGa_2S_4 are known as spin-glasses: they lack long-range magnetic order. This magnetic disorder arises from a non-repeating alignment of the electrons in the crystal structure. Sarah focused not on MGa_2S_4 but $M_2Ga_2S_5$ – a similar crystal with an extra layer of M ions in the repeating structure. Her project set out to solve a mystery in the magnetism: would the two compounds have the same magnetic disorder?

Previous attempts to make $M_2Ga_2S_5$ suffered from large levels of Ga_2O_3 contamination. Commercially produced Ga_2S_3 starting material contained significant levels of impurities that obscured the true magnetic behaviour of $M_2Ga_2S_5$. Sarah's first step, therefore, was to obtain a pure sample of Ga_2S_3. "Making the pure gallium sulfide took months of trial and error," she said. "It was so rewarding when the X-ray finally showed no impurities."

Now with pure Ga_2S_3 starting material, Sarah was able to synthesise a clean sample of $M_2Ga_2S_5$ and investigate its structure and magnetism. She recalls her favourite moment during the project: "Going to Harwell's ISIS Neutron and Muon Source and seeing the neutron diffraction data for my sample in real time." The spin-glass behaviour was observed for the pure product, which is attributed to imperfections in the crystal.

With the successful synthesis and the magnetic mystery solved, Sarah had a great year. "It was such a fun group to be a part of. The friendly atmosphere and breaks to play games made for a great end to my degree." After spending the summer with her family, Sarah is going to King's College London to train as a chemistry teacher. ■





Top: Sarah Browne using the neutron diffractometer at Harwell's ISIS Neutron and Muon Source. Bottom: Samples of Ga_2S_3 sealed in glass ampoules.

Do you have memories of your Part II project that you would like to share?

We would love to hear about your experiences. Please write to us at *alumni@chem.ox.ac.uk*.



Compounds of Interest

Chemistry at Oxford has changed the modern world

Glucose sensors, rechargeable lithium-ion batteries, sustainable polymers and new antibiotics – all of these discoveries, and many more, owe something to fundamental chemistry research that took place here in Oxford.

At a time when research is increasingly expected to deliver immediate economic and societal benefit, and younger generations show greater ambivalence towards science, making the case for fundamental research has become more important than ever. But the path from curiosity-driven, blue-sky research to something that changes healthcare, industry or society is rarely straightforward – or predictable.

A new Oxford Chemistry project, *Compounds of Interest*, aims to open up that process by taking audiences inside areas of research that are still developing. Borrowing its name from the Inorganic Part 1B examination paper question that will be (in)famous to many *Periodic* readers, the series brings together Oxford researchers with teachers, writers and film-makers to explore areas of active research through complementary formats designed for different audiences.

The inaugural series involves Prof Ed Anderson, three postdoctoral researchers and two DPhil students, working with an A-level chemistry teacher, professional film-makers, a science writer, and the Department's Outreach and Public Engagement with Research team.

Each edition begins with an area of active Oxford research and approaches it in several ways. A *Compounds of Interest* film connects the research with chemistry that is familiar to A-level chemistry students, while *In a Nutshell* offers a short introduction through social media. *Research Companions* take readers into the journal articles themselves, exploring the challenges, breakthroughs and wider significance behind the published work.

For post-16 students who want to go further, *The Lit Lab* uses those same research papers as its starting point. Carefully adapted text, explanatory notes, curriculum links and guided questions help students to engage directly with the research, before an interactive webinar gives them the opportunity to meet the researchers behind it.

Across academia, teaching, industry, policy, entrepreneurship and public engagement, Oxford Chemistry alumni have first-hand experience of where curiosity-driven science can lead. We all have a stake in making the case for fundamental research. *Compounds of Interest* is one contribution to that wider effort. ■

The Department is grateful to Wadham College for supporting the development of the inaugural *Compounds of Interest* series through its Access programme.

Image: Dr Joe Ford (Gouverneur Group) during filming for the *Compounds of Interest* series.

Jennie Botham retires

In April, members of the Department of Chemistry gathered to celebrate the retirement of Jennie Botham, a familiar face to many readers of *Periodic*. Over 46 years, Jennie supported and encouraged generations of students through their degrees in chemistry.

Jennie joined the Department in 1980 as a trainee laboratory technician in Inorganic Chemistry, shortly after completing her A levels. On her very first day, she met Chris Botham, who would later become her husband – the beginning of a lifelong partnership rooted in the Department.

For 38 years, Jennie worked in the Inorganic Chemistry Laboratory, where she played a central role in undergraduate practical teaching. Whether preparing experiments, ensuring laboratories ran smoothly or offering reassurance to nervous first-years, Jennie became an integral part of the student experience. She also looked after the lecture theatre, producing vast quantities of lecture handouts and dealing with lecturers who needed to use the slide projectors, and subsequently IT systems, with which they may not have been familiar. Lecture demonstrations also formed part of the job – many alumni will remember Dermot O'Hare's oxygen lectures, with the liquid oxygen produced by Jennie.

When the new teaching laboratories opened in 2018, Jennie continued her work with characteristic dedication, helping to design and set up practical experiments across the breadth of chemistry teaching for a further six years. In 2024, she moved into an administrative role supporting graduate students and contributing to the running of the Faculty Office and the various Centres for Doctoral Training, bringing the same warmth, professionalism and commitment to a new generation of researchers.

Over the course of Jennie's long career, countless students progressed from undergraduate practical classes to successful scientific careers. Remarkably, the current Head of Department, Prof Steve Faulkner, along with all three Heads of Section and many current faculty members, completed their undergraduate practicals here during Jennie's time working in the lab.

Speaking at Jennie's retirement celebration, Prof Faulkner recalled Jennie being the person who handed him his lab coat and safety glasses on his first day in the teaching lab. He praised her dedication to the Department and the care she showed to generations of Oxford chemists.

The event was also attended by University's Proctors, Profs Andrew Farmery and Caroline Warman, who congratulated Jennie on her remarkable contribution and reflected on the strong sense of community here.

In her own remarks, Jennie reflected on the many students and colleagues she had met over the years: "Over 8,200 undergraduates did their practical work in the labs I worked in over the years and one of the most satisfying things for me has been helping them to develop skills and confidence. I am very happy to think I played a part in encouraging them to do their best.

"Along the way I also met lots of DPhil students who demonstrated in the labs. Many have become friends



who I think fondly of and follow their career progress on LinkedIn.

"When I had to give up lab work for health reasons, the Department were very caring and helpful and found me an office-based role where I enjoyed 18 months working with old and new friends alike. I'm sure I will miss all the people here, but I am looking forward to spending more time with my husband Chris, who I met in the lab on my very first day at work!"

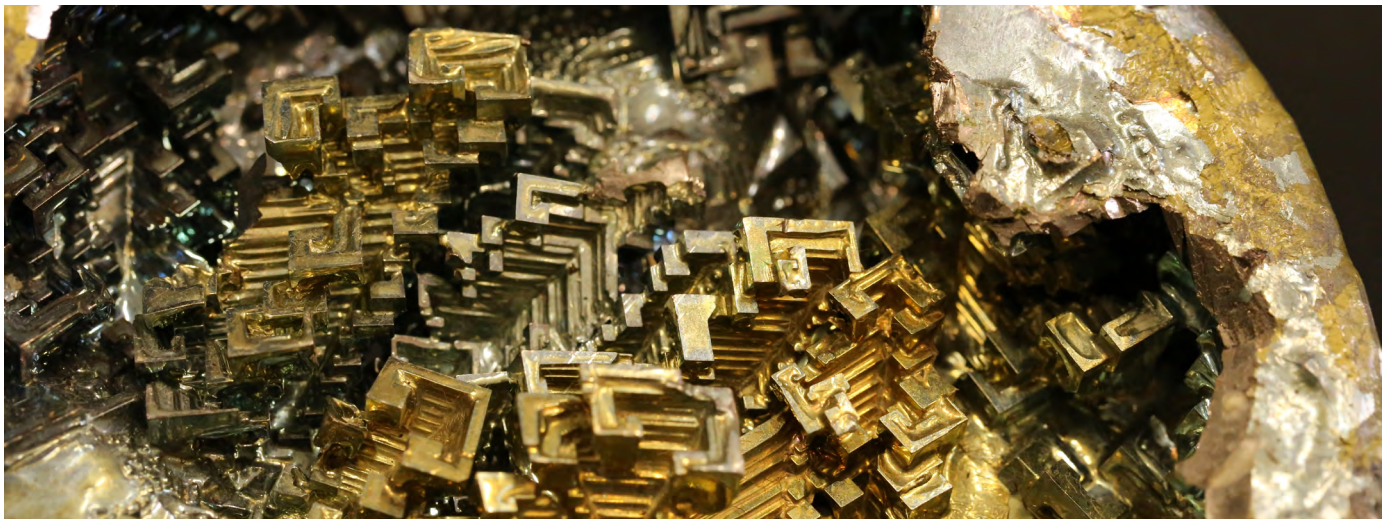
Jennie's contribution to Oxford Chemistry has been immense, not only through her technical expertise and long service, but through the kindness, encouragement and continuity she brought to generations of students and staff. Everyone in the Department wishes her a long, happy and well-deserved retirement. ■



L–R: Junior Proctor Prof Caroline Warman, Jennie Botham, Senior Proctor Prof Andrew Farmery and Head of Chemistry Prof Steve Faulkner, taken during Jennie's leaving party in the CRL this year.

Unearthing the minerals shaping our future

The hidden materials behind everyday life are front and centre in a special exhibition at the Museum of Natural History, University of Oxford



From the smartphones in our pockets to the imaging equipment in our hospitals, modern life depends on materials drawn from the Earth's crust.

Lithium, iron, aluminium, graphite, cobalt, titanium… these are important materials, and highly familiar to chemists.

Now, a timely exhibition is bringing the stories of 34 critical minerals deemed essential to the UK's future to a wider audience.

At the heart of *34: The Critical Raw Materials Shaping Our Future* are raw materials such as iron and aluminium, alongside the rare earth elements and other less well-known but equally vital substances.

As governments seek to decarbonise energy systems, electrify transport and expand digital infrastructure, demand for these materials is rising at speed. The International Energy Agency predicts that global demand could require around five times as much lithium by 2040, and twice as much graphite and nickel. Critical materials are those essential to a country's economy or national security, but which may not have a secure supply chain.

By bringing together geological specimens, industrial products, historic objects, contemporary technologies and cutting-edge scientific research, *34* asks how we can meet rising demand for critical raw materials without further endangering ecosystems and communities.

The exhibition takes a long view of humanity's relationship with the Earth, from a 40,000-year-old iron-rich ochre from Ngwenya Mine in southern Africa to lithium extraction today in Chile's Atacama Desert. Aerospace components, wind-turbine magnet replicas, battery modules and medical devices sit alongside the rocks that made them possible.

Extracting these materials can be dangerous and cause damage to the environment. *34* highlights research from Oxford and beyond into how rising demand might be met more sustainably, including lower-impact extraction, recycling, repair and substitution.

One of the exhibits is a camcorder that was originally powered by the first lithium-ion battery. This technology was developed in Nobel Prize-winning work, some of which was conducted in Oxford's Inorganic Chemistry Lab by John B. Goodenough, and Oxford alumnus M. Stanley Whittingham, who both shared the Nobel prize with Akira Yoshino.

Lithium-ion batteries have transformed everything from smartphones and laptops to electric cars. They depend on lithium extraction, which can be highly water- and land-intensive and place serious pressure on fragile ecosystems and local communities.

Now, Oxford EARTH is exploring whether geothermal brine resources in New Zealand and Montserrat could offer a more environmentally sustainable supply route. ■

***34: The Critical Raw Materials Shaping Our Future* is free to visit until 13 April 2027 during the Museum's normal opening hours.**

A series of events will accompany the exhibition. For more information, visit *www.oumnh.ox.ac.uk*, follow *@morethanadodo* on social media, or read the Museum's blog at *www.morethanadodo.com*.

Beyond Oxford Blue

Two remarkable pigments help a new generation connect with chemistry past and present

No colour is more closely associated with the University than Oxford Blue. But for Oxford chemists, two other remarkable blue pigments – Egyptian Blue and Prussian Blue – now connect the Department's work in heritage science, modern materials research and public engagement.

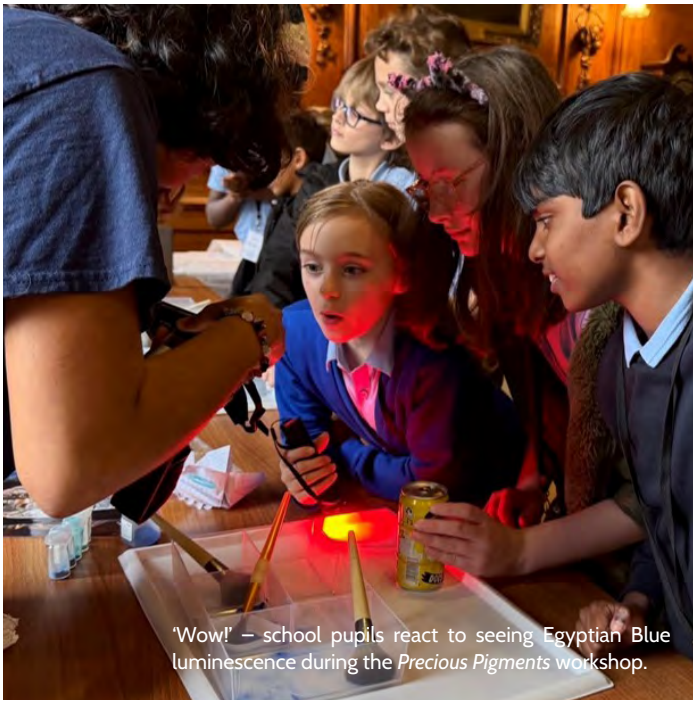
Widely regarded as the world's first synthetic pigment, Egyptian Blue is a calcium copper silicate, first produced around 5,000 years ago. In 1996, researchers discovered that it emits strongly in the near infrared when illuminated with visible light – an unexpected property that allows traces of the pigment invisible to the naked eye to be detected thousands of years after they were applied.

Dr Luciana da Costa Carvalho (McCullagh Group and School of Archaeology) introduced the Department's Outreach and Public Engagement with Research team to Egyptian Blue through her heritage science work with the British Museum in Sudan.

Inspired by her work, Oxford Chemistry's Building Bridges Partnership Project acquired an adapted camera capable of detecting the pigment's luminescence, allowing primary school pupils to investigate Egyptian Blue for themselves during a visit to the Ashmolean Museum.

One of the most striking examples of Egyptian Blue's enduring properties can be found on the west wall of Taharqa's Shrine, which is displayed in the Ashmolean Museum. Millennia of weathering have removed almost all visible traces of its original decoration, but infrared imaging can reveal a depiction of the ancient Egyptian god Amun-Re in vivid detail.

Nearby, pupils can examine a small Egyptian funeral figure known as a shawabti whose surviving blue decoration glows with striking intensity under infrared imaging. This figure is featured in a *Heist at the Museum* board game, which pupils play before visiting and which was developed to build familiarity with Oxford, its museums and the careers that connect chemistry with cultural heritage.



'Wow!' – school pupils react to seeing Egyptian Blue luminescence during the *Precious Pigments* workshop.

The same optical properties have taken Egyptian Blue far beyond archaeology. The pigment has also been investigated in modern forensic science as a means of enhancing latent fingerprints.

The second blue pigment at the heart of *Precious Pigments* has a very different history. Prussian Blue was first synthesised in the early eighteenth century, and later became central to one of the earliest forms of photography: the cyanotype.

Oxford Chemistry undergraduates developed the cyanotype activities used in *Precious Pigments*, in which pupils use the chemistry of Prussian Blue to create their own cyanotype keyrings. In doing so, they encounter the work of Anna Atkins, whose 1843 Photographs of British Algae – widely regarded as the first photographically illustrated scientific book – used the same process. A copy is now held by Oxford's History of Science Museum.

Atkins produced her pioneering work decades before Oxford awarded degrees to women. Today, students from Lady Margaret Hall and Somerville College – both founded to widen access to university education to women – use the same chemistry to introduce a new generation to Oxford science.

Like Egyptian Blue, Prussian Blue is much more than a pigment only of historical interest. Here in Oxford, Prof Andrew Goodwin's research group has shown that its analogues possess previously hidden structural organisation, opening possibilities for applications ranging from batteries to gas storage.

Through *Precious Pigments*, primary school pupils discover that the story of chemistry is carried by people as much as pigments: from the makers of Egyptian Blue and Anna Atkins to today's Oxford researchers and undergraduates.

By exploring the people and discoveries behind these colourful chemicals, pupils build familiarity with Oxford Chemistry, and begin to see themselves as part of its story. ■



The first CSHP CDT cohort during a visit to Syngenta, one of the programme's industrial partners.

What should modern synthesis look like?

Oxford and York are training a new generation of synthetic chemists to make sustainability a part of how they think from the outset

For much of the last century, generations of synthetic chemists had a clear challenge: can you make the molecule, in good yield and with the selectivity you need? Today, another question is becoming just as important: can you make your molecule sustainably?

That means considering not only the final molecule, but – from the very beginning of the project – the energy, materials and waste involved in getting there. Could a renewable feedstock be used? Is there an alternative to a scarce metal catalyst? Could a different route avoid problematic solvents or reduce waste? This approach encourages researchers to think about the whole life cycle of a synthetic route, rather than its outcome alone.

These questions are at the heart of the EPSRC Centre for Doctoral Training in Chemical Synthesis for a Healthy Planet (CSHP CDT), established by the Universities of Oxford and York in 2025 with support from the EPSRC (Engineering and Physical Sciences Research Council) and major pharmaceutical, materials and agricultural companies. Led by Professor Michael Willis, with Co-Directors Professors Edward Anderson, Véronique Gouverneur and Helen Sneddon, the programme aims to make sustainability part of the instinctive behaviour of the next generation of synthetic chemists.

"Making molecules has always been exciting," says Prof Willis, Director of CSHP CDT. "Now, in addition to the challenges of making the key bond with the selectivity required, we need to address the sustainability demands of modern synthesis. This can be hard, but the challenge of employing a renewable feedstock, or finding a catalyst derived from an abundant metal, adds to the reward, and the excitement."

The programme welcomed its first 14 students in October 2025. Rather than treating sustainability as a specialist topic, the CDT embeds it throughout its training programme. Students are encouraged to consider not only whether a reaction is possible, but how it can be achieved using more sustainable reagents, catalysts, solvents and synthetic strategies.

> **Green chemistry shouldn't be seen as a constraint on great synthesis; it's what great synthesis now looks like.**
>
> Prof Helen Sneddon

After an initial period of training in both Oxford and York, including two intensive weeks at York's Green Chemistry Centre of Excellence, the students have now begun their research projects. The taught element combined synthetic methodology, catalysis and green chemistry with industry engagement and the development of public engagement skills as Sustainability Ambassadors. Their research ranges across reaction innovation, sustainable feedstocks and molecular design, with potential applications including medicines, agrochemicals and advanced materials.

Industry is also closely involved in the programme from the outset. Industrial partners collaborate on research and help to design and deliver the students' training, bringing a wide range of perspectives from large companies and SMEs. Entrepreneurs in Residence share first-hand

experience of building science-based businesses through workshops, mentoring and training. Together, these different forms of involvement give students insight into the opportunities and challenges of turning new chemistry into practical applications.

For Professor Helen Sneddon, Co-Director of the programme and Director of York's Green Chemistry Centre of Excellence, the aim is ultimately to make the distinction between synthetic chemistry and sustainable synthetic chemistry disappear. "The students joining this CDT have grown up in a world where sustainability is already an expectation, not an aspiration," she says. "Green chemistry shouldn't be seen as a constraint on great synthesis; it's what great synthesis now looks like. We want our graduates to have the skills, confidence and instinct to deliver on this expectation."

As the first students begin their research, and new cohorts join them, the programme is building a network that extends beyond Oxford and York and into the wider academic and industrial community. Embedding sustainability alongside scientific excellence from the outset will help shape how the next generation of synthetic chemists approach their discipline – and what they consider when deciding whether a synthesis is successful.

Oxford Chemistry alumni and friends can be part of that community too. The CSHP team are keen to hear from people who could contribute their experience and expertise, whether through mentoring, industry perspectives, entrepreneurship, careers, public engagement or other forms of involvement. ■

Interested in getting involved? Write to *cshp-cdt@chem.ox.ac.uk*, find us on LinkedIn, or visit *cshp-cdt.chem.ox.ac.uk*.

Applications for 2027–28 entry are now open

New doctoral training programme in generative biology

Applications for 2027–28 entry are now open

The Generative Biology EIT Doctoral Training Programme is a fully funded four-year DPhil that brings together outstanding researchers from chemistry as well as biology, engineering, computer science, mathematics and the physical sciences to tackle some of the most exciting challenges in modern biology. Supported by the Ellison Institute of Technology (EIT) and hosted by the Department of Chemistry in collaboration with departments across the Mathematical, Physical and Life Sciences Division and the Medical Sciences Division, the programme offers an interdisciplinary training environment at the forefront of biological research.



Rendering of the Ellison Institute of Technology campus, currently being built in Littlemore.

Generative biology seeks to transform our ability to engineer living systems for the benefit of humanity. Achieving this vision requires overcoming two fundamental challenges. First, we must be able to write in the natural language of biology, enabling the rapid and precise synthesis of entire genomes. Second, we must understand what to write by predicting which DNA sequences will produce biological systems with desired functions.

Together, we aim to unlock transformative advances in healthcare, agriculture, sustainable manufacturing, clean energy and beyond. ■

For more information on the programme, visit *generativebiology-eitdtp.chem.ox.ac.uk*

Building industrial perspectives into a DPhil

Before starting their main research projects, IMAT CDT students spend two months working with an industrial host

The placements give students an early opportunity to apply their academic training to a focused industrial challenge, and to experience how scientific decisions are shaped by commercial and practical considerations.

Students on the EPSRC Centre for Doctoral Training in Inorganic Materials for Advanced Manufacturing (IMAT CDT) begin with four months of intensive cohort-based teaching, delivered by academics and industrial partners, followed by two months in industry.

During the taught element of the programme, students are encouraged to consider the complete journey of an inorganic material, from raw materials and synthesis through to processing, product design and circularity. The subsequent industry placement gives them an opportunity to apply that thinking in a setting where scientific questions sit alongside considerations such as sustainability, commercial priorities and customer need.

For Tabitha Seymour, a DPhil student in IMAT's second cohort, that meant joining HydRegen, an Oxford Chemistry spin-out developing biocatalytic technologies for sustainable chemical manufacture.

"My internship allowed me to experience first-hand the challenges a start-up company faces, but also the exciting opportunities available to scientists working in new small businesses," she says. Tabitha was able to develop her project management skills and adaptability, including learning to redesign experiments and reassess project goals quickly. Working in a small company also meant she could interact with colleagues at every level, from research scientists to the company's senior leadership team.

The benefits of these industrial placements are not only for the students. Johnson Matthey has hosted four IMAT CDT students across the programme's first two cohorts, and External Programmes Manager Dr Paul Collier compared the quality of the students and their work to that of fourth-year doctoral researchers.

The focused two-month projects can help accelerate innovation by enabling scientists to explore ideas that might otherwise be difficult to pursue alongside existing priorities. In some cases, Paul described students as delivering around six months' worth of work. Hosting students can also provide development opportunities for employees, including experience in supervision and project management.

The internships are one part of IMAT's wider collaboration with industry. A network of 19 industrial partners and national facilities contributes throughout the programme, from site visits, workshops and teaching to mentoring, networking and collaborative research. Students are connected with scientists working across industry, giving them insight into real-world challenges and allowing them to share ideas and expertise.



An IMAT CDT student sharing their research at the annual Science Day for Industrial Partners

For Prof Simon Clarke, Director of the IMAT CDT, building close relationships with industry has been an important part of the programme from the outset.

"The first-year internship programme is one key to that," he says. "We are proud of our students for being such great ambassadors for the IMAT CDT and the University, and excited by the enthusiasm which the host companies have for providing these internship opportunities."

By the time IMAT students begin their research projects, they have already experienced how chemistry and materials science operate outside of the University. That perspective continues to shape their research, helping them consider not only how new materials can be developed, but how they might ultimately be manufactured, applied and used.

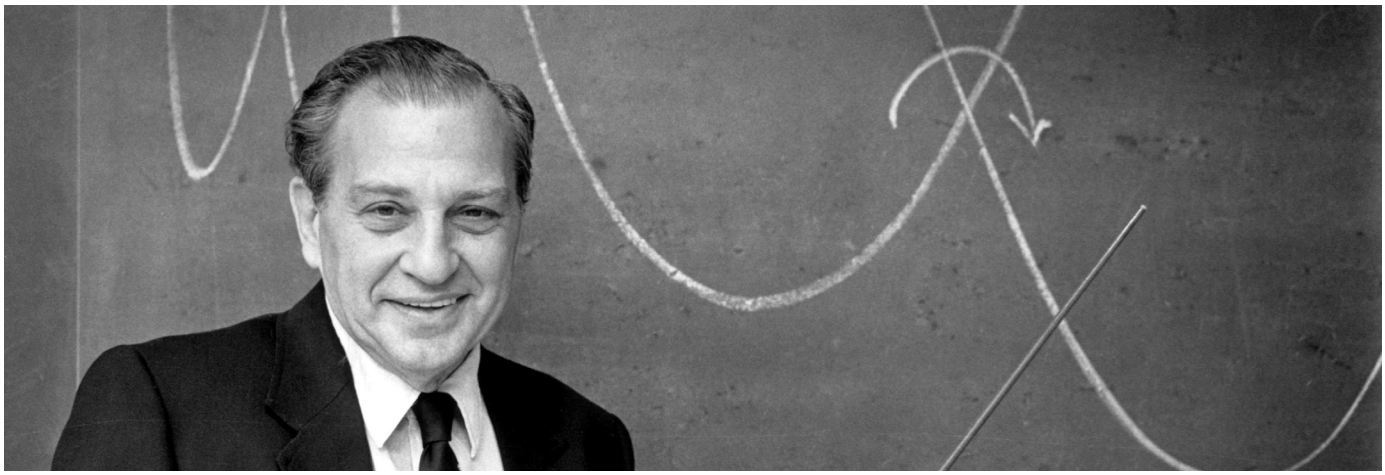
The IMAT team welcomes conversations with Oxford Chemistry alumni and others who could bring relevant experience or expertise to the programme, whether through internships, mentoring, teaching, site visits or other forms of engagement. ■

Interested in getting involved? Find us on LinkedIn, email us at *imat-industry@chem.ox.ac.uk* or visit *imatcdt.chem.ox.ac.uk*.

Applications for 2027–28 entry are now open

Professor Rudolph 'Rudy' Marcus

One of the most influential theoretical chemists of the twentieth century, and a longstanding friend of Oxford, Prof Rudy Marcus died on 16 July 2026, five days short of his 103rd birthday



Prof Rudy Marcus was best known for developing the theory of electron transfer reactions that bears his name. Beginning in the 1950s, his work provided a theoretical framework for understanding how electrons move between molecules, explaining why apparently simple electron-transfer reactions can proceed at very different rates.

Marcus theory went on to become fundamental to understanding processes across chemistry and biology, including photosynthesis, electrochemistry and many photochemical reactions. In 1992, Professor Marcus was awarded the Nobel Prize in Chemistry "for his contributions to the theory of electron transfer reactions in chemical systems".

Born in Montreal in 1923, Marcus studied chemistry at McGill University, completing his PhD in 1946. After research positions in Canada and at the University of North Carolina, he joined the Polytechnic Institute of Brooklyn in 1951, where he began the work on electron transfer reactions for which he would become famous. He moved to the University of Illinois in 1964.

Following Charles Coulson's death in 1974, funds became available to bring distinguished visiting professors to Oxford's Department of Theoretical Chemistry, which Coulson had established in 1972. In 1975, Marcus was invited to Oxford by Prof Mark Child as Visiting Professor of Theoretical Chemistry, with University College offering him a Visiting Fellowship. Prof Child said: "Rudy was by far the most distinguished theoretical chemist in my own immediate field, so I was delighted to be able to use the IBM fund to attract him to Oxford."

The Coulson Chair of Theoretical Chemistry was established the following year in 1976 and attached to University College. Marcus was approached about becoming its first holder, but declined. In 1978 he moved to the California Institute of Technology (Caltech), where he spent the rest of his career.

Marcus's connection with Oxford, however, continued for the rest of his life. He was elected an Honorary Fellow of University College in 1995 and received an honorary DSc from the University of Oxford in the same year.

His scientific career was remarkable not only for its impact but for its longevity. Marcus continued lecturing at Caltech until the age of 95, and maintained an active research group for the rest of his life. Even during his final illness he continued working on scientific papers and discussing research with colleagues.

Prof David Logan, Emeritus Professor at University College and former Coulson Professor of Theoretical Chemistry, said: "Rudy Marcus was a scientific legend – a towering giant in the field of chemical theory, whose phenomenal intellectual legacy will continue to influence chemists for generations to come."

Prof Justin Benesch, Fellow of University College, said: "He provided a rigorous conceptual framework for electron-transfer reactions, arguably the very centre of chemistry and the cornerstone of some of the most important mechanisms in life. This transformed the interpretation of kinetic measurements and established a lasting dialogue between molecular theory and experiment."

Marcus remained proud of his Oxford connection. Although he visited relatively rarely in later years, he returned for Professor John Albery's 70th birthday celebrations in 2006, and in 2014 chose to wear his Oxford DSc robes at the inauguration of a new President of Caltech.

Marcus helped establish ways of thinking about chemical reactions that have shaped generations of physical and theoretical chemists, and his legacy extends far beyond the theory that carries his name. ■

Oxford Chemistry: Then and now



Thank you to alumnus John Needham (Hertford, 1975), who recently shared with us a copy of an Oxford Chemistry brochure from the seventies, offering a glimpse of undergraduate life in the Department fifty years ago.

Some things remain the same today – *"Lectures are held at 9 and 10 a.m. on most weekdays; attendance, although recommended, is not compulsory"* – but plenty has changed.

To see what studying Chemistry at Oxford looks like today, scan the QR code or visit the link to watch our new undergraduate course video. ■

youtube.com/watch?v=t0iVk3b7agM



Do you have memories of your time at Oxford Chemistry to share?

You can write to us at *alumni@chem.ox.ac.uk*, or by post to the address on the back cover.

Chemistry crossword

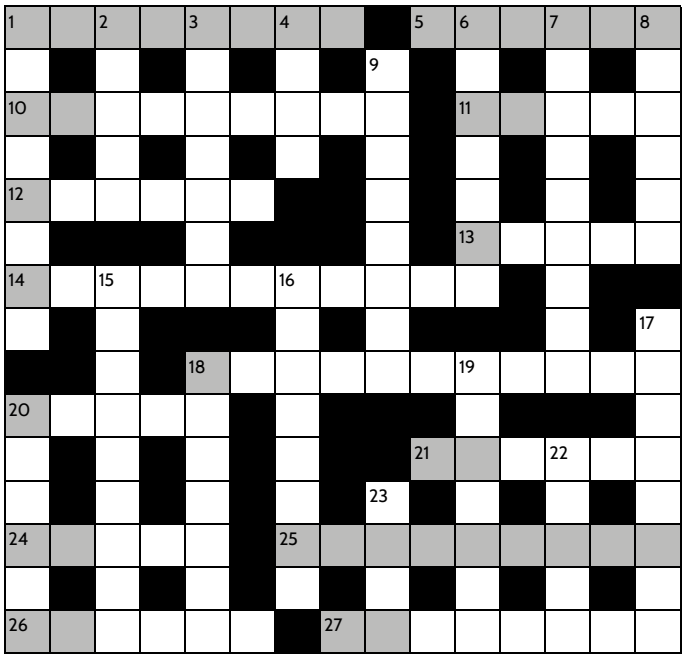
Look to the shaded squares for a *Periodic* helping hand.

Across

1 Hindenburg filling (8)
5 Squeaky-voice gas (6)
10 Relating to sexual desire (9)
11 Brute (5)
12 Wicker container (6)
13 *Killing Eve* and *Prima Facie* actor Jodie ____ (5)
14 Keats's "immortal bird" (11)
18 Protective atmospheric layer rich in O_3 (11)
20 Jedi or Sith power (5)
21 Lower (6)
24 US civil rights organisation (5)
25 Metal at the heart of chlorophyll (9)
26 Gene variant (6)
27 Mutton chop, perhaps (8)

Down

1 Fiercely determined (8)
2 Financial liabilities (5)
3 Leftover piece (of fabric) (7)
4 Volcano (4)
6 Hug (7)
7 Lifeless (9)
8 Stuff (6)
9 Land of gold (2,6)
15 Safety barrier (9)
16 Midday (8)
17 Charon, for instance (8)
18 Like a son too fond of Mum? (7)
19 Come before (7)
20 _____ Fáil, Irish political party (6)
22 Five, seven, five (5)
23 Farming prefix (4)



Email *alumni@chem.ox.ac.uk* for the crossword's solution.

Overcrowded aromatics

McGonigal group

This molecule's crowded propeller-like phenyl rings allow the π systems to interact and shift its fluorescence to longer wavelengths. If the molecule is under pressure its crystals change colour, going from colourless to yellow.

JACS 2023, 145, 19780–19789

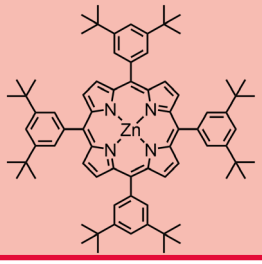


Porphyrins

Harry Anderson group

Porphyrins are natural pigments related to those in blood and used for photosynthesis. By modifying their structure you can tune their colour and build extended π-systems for light harvesting, molecular wires and nanorings.

Science 2025, 390, 290–293

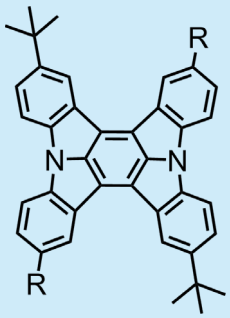


Indolocarbazoles

Congrave group

Organic molecules offer unusually precise control over colour: small changes to their atomic structure can tune both absorption and emission. Fused indolocarbazoles have rigid structures that produce unusually pure blue-light emission. Bulky substituents have been used to control energy transfer between molecules to develop efficient blue OLEDs for high-definition screens.

Nat. Mater. 2024, 23, 519–526





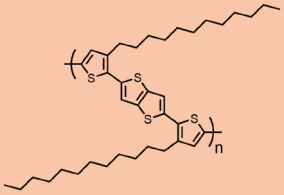
Several Oxford Chemistry groups make and work with chromophores. Some chromophores can release the energy stored in their excited states as light (luminescence). The colour of the luminescence is linked to the chromophore molecular structure. Samples from organic molecular materials groups across the Department were combined to create this striking image. Read on to discover the chemistry behind the colours.

Conjugated polymers

McCulloch group

This conjugated polymer has an electron-rich backbone, promoting an ordered, crystalline morphology in the solid state that allows charges to move efficiently, hence its family of analogues can be used in transistor applications. Its lamellar structure can also accommodate small dopant molecules without disrupting this order, enabling high conductivities, making it well suited to organic thermoelectric devices that convert heat into electrical power.

Nat Mater 2006, 5 (4), 328–333

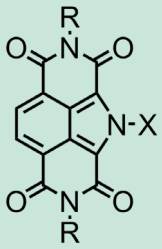


Isoindole diimides

Avestro group

Isoindole diimides (IDIs) are a new family of electron-deficient molecules that produce strong, tunable green fluorescence. Their optical and electronic properties can be adjusted by changing the groups attached to the central core or through interactions with nearby atoms, making them promising materials for light-emitting and optoelectronic applications.

ChemPlusChem 2019, 84, 1638–1642

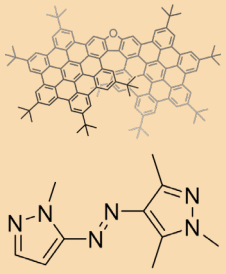


Chiral and switching molecules

Fuchter group

Both these molecules use carefully controlled three-dimensional shapes to create unusual properties. Their twisted (top) or switchable (bottom) structures influence how they interact with light, electrons and neighbouring molecules, enabling functions ranging from unique optical and electronic behaviour to light-controlled thermal energy storage.

Nat. Photon. 2025, 19, 1361–1366



Contact us

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DEPARTMENT OF CHEMISTRY

UNIVERSITY OF OXFORD