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2020-2021

Periodic

The Magazine of the Department of Chemistry

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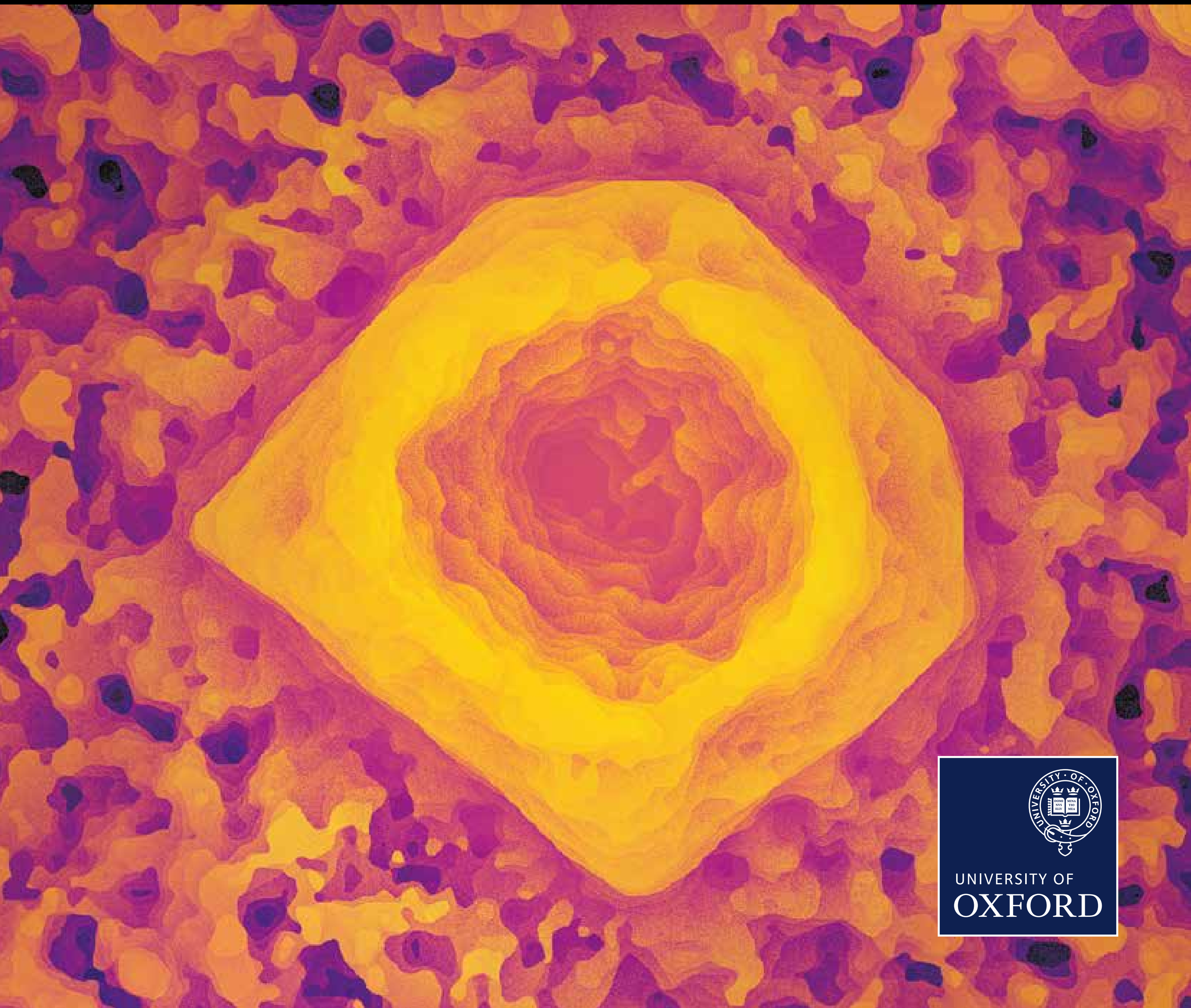


UNIVERSITY OF OXFORD

From the Head of Department

After an academic year like no other, it gives me pleasure to introduce the 2020-21 edition of Periodic magazine. Despite the most challenging of circumstances, since June my colleagues have been able to continue their wide range of ground-breaking research, including research into combatting Coronavirus; you can read about some of their work on the following pages. I applaud their ingenuity and dedication and I am very grateful for the efforts of our talented team of administrative and support staff, whose tireless efforts have helped to make safe working possible and practical.

Of course, we are currently still some way away from our normal routine, but over the coming academic year we hope to offer our students and researchers the very best environment possible. I have been supported in these endeavours by Associate Heads Nick Green (Teaching) and Tom Brown (Research). As Tom prepares to step down from his Associate Head role, I offer him my thanks and very best wishes, and extend a warm welcome to Charlotte Williams, who became Associate Head for Research in October 2020. The Chemistry Management Board also welcomes Grant Ritchie, who becomes Head of Physical and Theoretical Chemistry as Stuart Mackenzie's term of office ends, and Janice French, who joins us as our new Head of Administration, following the retirement of Rosie Mortimer, Head of Administration from 2014-20, and Malcolm Bradbury, who has served as interim Head of Administration since spring 2020. I owe a debt of gratitude to these colleagues who have made outstanding contributions to the life and work of the Department. Three members of our academic staff, Rob Adlington, Peter Battle and Steve Davies, retired in 2020. Their long-standing commitment to the Department and their great achievements and are too numerous to list, but I believe that I speak for everyone here in thanking them for their enormous contributions to Oxford Chemistry and in wishing them long and happy retirements. I am delighted to welcome some outstanding new faculty members: David Tew (Physical and Theoretical Chemistry) joined us earlier this year and we welcome Iain McCulloch to the Organic section staff, and Matthew Langton to Inorganic. Thanks to the efforts of my colleagues old and new, the Department continues to go from strength to strength.

Our wider community of alumni and friends continues to strengthen too, and we were delighted by the very positive response to our centenary campaign to support student research. After a century, the role played by Oxford Chemistry DPhil students is still crucial; they are using chemistry to help address many of the world's most pressing challenges, from COVID 19 to climate change. I hope that you will enjoy reading about some of their amazing work in the following pages.

We were saddened to learn of the deaths of three great former members of the Department this year: Jack Baldwin, Peter Day and Malcolm Green. Their pioneering work and achievements brought so much to chemistry and the world beyond, and continue to inspire the young chemists of today.

On the cover: A collaborative study from the Timmel, Aarts and Mackenzie groups uses confocal microscopy to image the spatiotemporal evolution of magnetic field effects (MFEs) in flavin-doped lysozyme crystals. Due to a number of competing effects, including diffusion and photobleaching of the flavin molecules, the MFE is not uniform within the crystal. The figure is an artistic representation by Dr Marcin Konowalczyk of data collected by Victoire Déjean and Jamie Gravell. This work was published in RSC Chemical Science (Volume 11, Number 3014 August 2020. Pages 7733–8042. https://doi.org/10.1039/D0SC01986K). Image copyright Dr Marcin Konowalczyk (licence CC-BY-SA).

News & Achievements

A selection of recent highlights. More news can be found at **www.chem.ox.ac.uk**

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

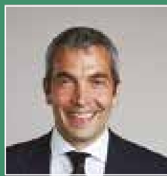
Professor Ed Anderson was named the winner of the **Bader Award** for his creative contributions to organic synthesis and synthetic methodology. Ed's work involves creating molecules with function, and creating new ways to make them more efficiently and selectively for synthesis as antiparasitic agents, antibiotics and anticancer molecules.

Professor Andrew Baldwin won the **Norman Heatley Award** for his development and application of chemical methods for understanding the biology of membraneless organelles. Andrew's work focuses on large protein assemblies, or 'aggregates', whereby one of the aggregates is linked to disease and the other dictates normal cellular function.

Professor Vernon Gibson of the University of Manchester, Imperial College London, and MPLS Visiting Professor of Chemistry at Oxford, received the **Lord Lewis Prize** for his seminal contributions to fundamental and applied inorganic chemistry, and for critical work in policy setting at the interface of academia with industry and government.

Professor Madhavi Krishnan won the **Corday-Morgan Prize** for her invention of a 'field free' trap for confining and manipulating a single colloidal particle or molecule, enabling accurate and precise measurements of molecular charge in aqueous solution.

Professor Christiane Timmel received the **Tilden Prize** for her seminal contributions to the fields of Spin Chemistry and Electron Paramagnetic Resonance of spin polarised systems. Christiane's work is focused on molecular structures that interact with magnetic fields to explain their physical, chemical and biological properties.



Professor Ben Davis has been awarded the Davy Medal from the Royal Society. Professor Davis, of the Rosalind Franklin Institute and the Department of Chemistry, was awarded the medal for inventing powerful chemical methods that directly manipulate complex biological molecules, enabling elucidation and control of biological function and mechanism in vitro and in vivo, beyond the limits of genetics.

Sebastian Kopp and Dr Vanessa Restrepo-Schild were selected to represent the University at the 2020 Lindau Nobel meeting. Vanessa is a postdoctoral researcher in the Bayley group, and Sebastian is a DPhil student in the Anderson group and OxICFM CDT. The in-person meeting had to be postponed, but a virtual conference was held to allow for scientific exchange and networking.

Dr Emily Flashman was awarded a prestigious Consolidator Grant from the European Research Council (ERC). The award will fund her research on plant oxygen-sensing enzymes and how to manipulate them in order to make plants better able to tolerate flooding. Emily has also been appointed a Fellow of Reuben College, Oxford's new graduate college, which will focus on 21st century interdisciplinary research.

Dr Brianna Heazlewood is to receive an ERC Starting Grant from the European Research Council for her pioneering research project 'Taming the reaction dynamics of paramagnetic species.' The ERC grants aim to help outstanding scholars and scientists to pursue their most innovative ideas.

Jack Baldwin

(1938 – 2020)

Organic chemist whose rules aided the synthesis of natural products.

Georgina Ferry

Professor Sir Jack Baldwin FRS.

"Chemistry," Jack Baldwin once said in his direct way, "is about making forms of matter that have never existed." Baldwin was best known for formulating a set of rules that predict how likely it is that atoms (mostly carbon) in a synthesis will link into rings, a structural feature of many biological molecules and drugs. Published in just three pages (with a one-sentence abstract) in 1976 (J. E. Baldwin J. Chem. Soc. Chem. Commun. 734–736; 1976), Baldwin's rules have been fundamental to organic synthesis in the pharmaceutical and agrochemical industries, and to understanding biology from a chemical perspective. He died on 4 January, aged 81.

His passions also encompassed finding out how nature makes chemicals that researchers cannot. This led him to 'biomimetic' synthesis: using the principles of nature to improve the generation of biomolecules in the laboratory. He particularly relished the challenge of 'molecules from Mars', his term for natural products whose biosynthesis was baffling.

Baldwin's interest in rings led him to study antibiotics that contain a β-lactam ring, the best known of which is penicillin. He worked initially with Edward Abraham, who had been part of the team that developed penicillin and who went on to reveal the activity of broad-spectrum antibiotics known as cephalosporins. Baldwin uncovered the mechanistic basis of the enzyme action that catalyses the formation of the two rings at the heart of the penicillin molecule. Others have since found that related enzymes are involved in many biological processes, including how the human body responds to low levels of oxygen.

Baldwin was born in London, and studied chemistry at Imperial College London, where he also did a PhD. He was supervised by Derek Barton, a pioneer of conformational analysis — the idea that the reactivity of a molecule could predict its preferred 3D shape — who later won a Nobel prize. Barton had a major impact on Baldwin's career.

After four years on the staff at Imperial College, Baldwin spent more than a decade in the United States, working first at Pennsylvania State University in State College and then at the Massachusetts Institute of Technology (MIT) in Cambridge. With an able young team and the latest instruments, his MIT period was particularly productive. To develop a detailed picture of how atoms arrange themselves during organic reactions, he combined theoretical and geometric considerations with structural information. His team obtained this using techniques such as nuclear magnetic resonance and X-ray crystallography. At MIT, he created a class of biomimetic molecule that reversibly binds oxygen when complexed with iron, just as haemoglobin does in the blood, and formulated his rules for ring formation. It was also where he met his future wife, Christine Franchi, who built a career in academic publishing.

In 1978, Baldwin was recruited to head the Dyson Perrins Laboratory at the University of Oxford, UK. As only the fourth person to hold the chair in organic chemistry since the laboratory opened in 1916, he transformed his discipline at Oxford, in terms of both scientific ambition and equipment. Baldwin brought with him researchers from his internationally diverse lab at MIT, and continued to recruit people with a wide range of backgrounds.

Many of his students, who knew him as 'J.E.B.', went on to lead research all over the world. The output of his lab was prodigious: he is an author on at least 700 papers. In 1988, he became the founding director of the Oxford Centre for Molecular Sciences, which he headed for 10 years. The centre helped to link physical and biological sciences in Oxford.

AI designs organic syntheses

The pioneering role of Oxford scientists in the extraction, testing and structural analysis of penicillin during the 1940s inspired Baldwin's extensive work on trying to make the drug from scratch. His respect for the optimally efficient process by which microbes produce the molecule — even now, most penicillin antibiotics continue to be produced through fermentation — led him further into the field of biomimetic synthesis. His favoured approach for building complex multi-ring structures was to try to mimic nature's strategy of making a relatively simple linear framework that is predisposed to react to give multiple rings in a single step. The 'molecules from Mars' he made using this approach included unusual alkaloids derived from marine sponges and rare rainforest plants.

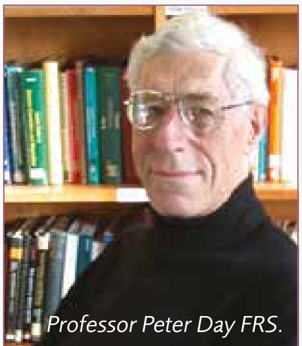
Baldwin had little time for the academic conventions of Oxford: he spoke his mind, and could seem pugnacious in scientific debate. But his forceful leadership style belied a generosity in his treatment of junior colleagues. Wholly committed to research, he never sought seats on prestigious committees, although his distinction brought many honours, including a knighthood in 1997. He developed links with the chemical industry and championed its role in society, encouraging his students to pursue industrial careers. Aside from science, he enjoyed good food, fine wine, powerful motorbikes, fast cars and his dogs. After he retired in 2005, he continued to co-author publications until just months before his death.

Reprinted by permission from Springer Nature Customer Service Centre GmbH: Springer Nature. Nature (Nature 578, 212 (2020) doi: 10.1038/d41586-020-00357-1. Jack Baldwin (1938–2020), Georgina Ferry, Feb 7, 2020.

Professor Peter Day FRS

(1938 – 2020)

The Department was sad to announce the death of Professor Peter Day FRS. Professor Day's major contributions included systematising and rationalising the properties of inorganic mixed-valence compounds (The Robin-Day classification), and in the synthesis of numerous and diverse complex solids in the search for unusual magnetic and electronic materials properties.



Professor Peter Day FRS.

Elected fellow of the Royal Society in 1986, Professor Day's RS biography describes him as 'a pioneer of materials chemistry, seeking unusual physical properties in inorganic and metal–organic compounds and models to explain them. He played a major role in the development of mixed-valence chemistry, and carried out important and elegant experimental and theoretical work on the spectra, magnetic properties and conductivity of solid, inorganic complexes'.

Day was born on 20 August 1938 in East Malling, Kent, and educated at Maidstone Grammar School. He was an undergraduate and then a DPhil student in Chemistry at Wadham College and completed a doctoral thesis entitled "Light induced charge transfer in solids" under the supervision of Bob Williams in 1965. During his time at Oxford he was a Junior Research Fellow (1963-65) at St John's College, and then Official Fellow and Tutor in Inorganic Chemistry (1965-88) at St John's and a University Lecturer. During this time he and his colleague Tony Cheetham co-edited what became a standard undergraduate text book on solid-state chemistry.

Having become a leading advocate for the use of neutron scattering in chemistry he took up the Directorship of the Institut Laue-Langevin in Grenoble in 1988, returning to the UK in 1991 as the Director of the Royal Institution of Great Britain where he was the Fullerian Professor of Chemistry. He retired from the Royal Institution in 1998 and in the years since 2008 was Emeritus Professor of Chemistry at the University of London.

Day received numerous awards from learned societies around the world; in 2008 The Royal Society of Chemistry honoured him by inaugurating the Peter Day award in Materials Chemistry, reflecting his championing of this discipline.

In retirement, Day and his wife Frances divided their time between Oxford and their home in Roussillon in south-west France. In 2012 he published a memoir *On the Cucumber Tree*, full of fascinating anecdotes about his life and career. He died at his home in Marsh Baldon in Oxfordshire on 19 May 2020 at the age of 81 and is survived by his two children, Alison and Christopher, and five grandchildren. He will be sadly missed by many around the world.

Professor Malcolm Green FRS

(1936 – 2020)

Professor Malcom Green FRS.

The Department was sad to announce the death of Professor Malcolm Green FRS in July 2020. Malcolm was a global figure in the field of organometallic chemistry and was known for his creativity in devising new compounds and in pioneering new ways of making them. He was awarded the prestigious Davy Medal of the Royal Society in 1995 "In recognition of his contribution to organometallic chemistry with particular application to catalytic reactions". He was an inspiration to the huge number of undergraduates, Part II & D.Phil. students and postdocs whom he taught or guided, and all will have their own fond memories of him.

Malcolm graduated from Acton Technical College in 1956 and obtained his PhD from Imperial College in 1959 in the group of Geoffrey Wilkinson. He was briefly an Assistant Lecturer in Cambridge before moving to Oxford for the rest of his career, becoming Fellow of Inorganic Chemistry at Balliol College in 1963 and a University Lecturer in Inorganic Chemistry in 1965. He was a Royal Society Senior Research Fellow from 1979-86, and in 1989 he was elected to the Statutory Professorship of Inorganic Chemistry and Headship of the Inorganic Chemistry Laboratory, becoming a Fellow of St Catherine's College, until his retirement in 2004. He was elected Fellow of the Royal Society in 1985 and was the recipient of many other major awards and prizes from learned societies around the world. He will be sadly missed by all those who knew him.

Harry B Gray, Arnold O. Beckman Professor of Chemistry at Caltech, pays tribute to Malcolm's life and work:

Malcolm Green was a towering figure in inorganic and organometallic chemistry. His work on metal-alkyl compounds led to the discovery of noncovalent interactions between C-H bonds and empty orbitals in coordinatively unsaturated early transition metal complexes. Likely after a fun dinner with colleagues at Balliol, he coined the name "agostic" for these relatively weak electronic interactions. Agostic "bonds" play roles in many C-H activation processes of great importance in the chemical industry.

We are greatly indebted to Malcolm for his brilliant development of scalable metal vapor synthesis methods to obtain useful quantities of organometallic compounds of titanium and other early transition metals. He and I spent many enjoyable hours discussing applications of his game changing work during my year in Oxford. I also was greatly impressed by his development of scalable methods for the syntheses of carbon nanotubes. His work, which led to single walled nanotubes that can include metals and other materials, made a huge impact on the course of nanoscience.

Malcolm had many close friends at Caltech. There was never a dull day during the year he and Jenny spent with us. Both in the lab or mixing it up with students and faculty at the Green house on Hill Avenue in the late afternoon and evening, he was in his element. No one here will ever forget the hugely positive impact he had on our science.

I have lost a great friend, one who put his stamp on my field as no other.

New Research

Thomas Player reports on some exciting new research highlights

Anderson Group

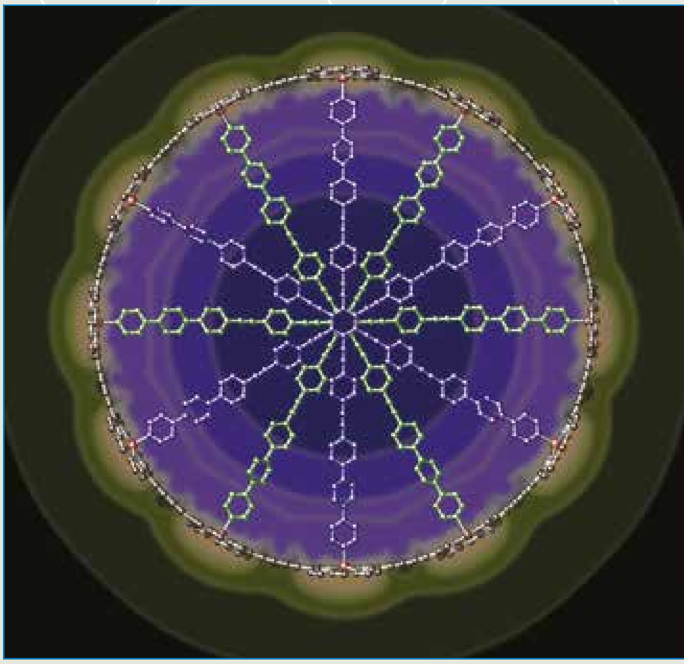
Large aromatic rings

Harry Anderson's group has been exploring the upper size-limits of aromaticity, whereby certain ring-shaped molecules have special electronic and magnetic characteristics compared to non-aromatic compounds, and exhibit distinctive electric currents when in a magnetic field. It can be important to know whether or not a particular molecule will be aromatic: but how can we tell?

All organic chemistry textbooks will tell you to use *Hückel's rule* for counting pi-electrons. This simple rule is very reliable for small molecules. What was not clear was whether it can be extended to far larger rings that contain many more electrons.

The Anderson group's research into these larger rings was recently featured on the cover of *Nature Chemistry*, where they measured ring currents in nanoscale porphyrin ring structures containing up to 162 pi-electrons, corresponding to n = 40 in Hückel's rule. They observed the presence of aromatic (and anti-aromatic) ring currents for various oxidation states of these nanorings, and were able to control whether or not the molecules were aromatic by varying their structure, oxidation state, and conformation.

This work involved many NMR oxidation titrations, some of which threw up results that were at first confusing. It eventually came good though, and with "all the observations falling into place, we knew we had just proved the validity of Hückel's rule". This is how former group member Michel Rickhaus, now leading his own research group at the University of Zurich, described the team effort he, Michael Jirasek, and other group members made to reach their conclusions.



The molecular structure of one of the large ring complexes over which the aromatic electrons are delocalised.

Most textbooks say aromaticity is limited to rings with less than about 22 pi-electrons, which makes it interesting to study this effect in much larger rings. It is also intriguing because, at low temperatures, small non-molecular rings of metal display persistent ring currents and behave like aromatic molecules. This research is exploring to what extent molecular wire rings behave like small rings of wire.

Professor Anderson has recently been awarded an Advanced Grant from the European Research Council (ERC), which will be used to continue exploring the boundaries of aromaticity in nanoscale structures.

References: Rickhaus, M. et al., *Nature Chemistry* **12** (2020) 236–241 (doi.org/10.1038/s41557-019-0398-3); Behind the Paper (2020) https://go.nature.com/30CS7pa.

Hückel's rule: if a delocalised loop of p orbitals in a flat molecule contains 4n + 2 electrons (where n is an integer), then the molecule is expected to be aromatic. Benzene is the classic example with six pi electrons, meaning n = 1.

Benesch Group

Unravelling protein origins

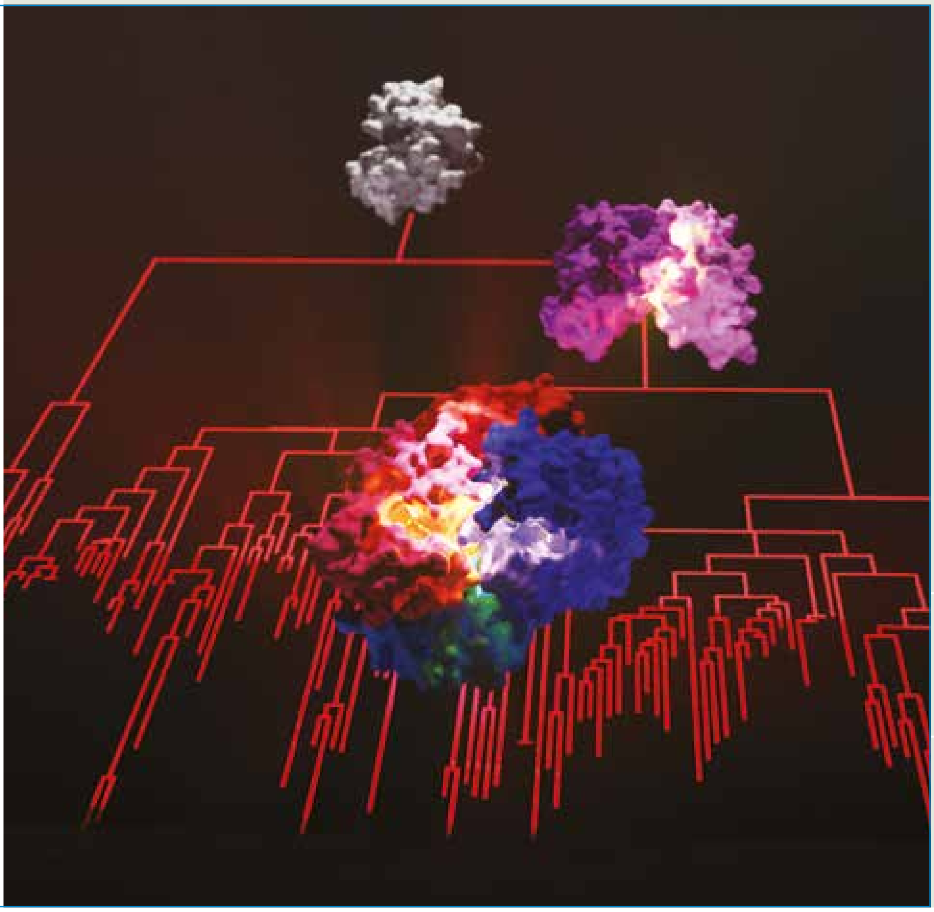
The Benesch group, working alongside researchers from the Universities of Chicago, Nebraska, and Texas A&M, have demonstrated that the structures responsible for specialised functions of complex proteins can come about via surprisingly simple mechanisms.

The evolution of proteins that perform all the specialised functions in our bodies is one of the biggest puzzles in biology. Haemoglobin – responsible for oxygen transport in blood – is made of four protein sub-units that form the vital oxygen-carrying complex.

In the collaborative study, published in *Nature*, the researchers identified the "missing link" that explains how haemoglobin's remarkable oxygen-transport abilities evolved. By reconstructing ancient proteins, they found that just two changes to the structure of an ancestral protein led to both the formation of the four-part complex and the optimisation of its oxygen-binding ability.

A traditional view of evolution says that complexity in nature comes about through many successive small mutations with gradual improvements in function – this study showed that, on a molecular level, a couple of simple mutations sometimes lead very quickly to complex behaviour.

Reference: Pillai, A. S. et al., *Nature* **581** (2020) 480–485 (doi.org/10.1038/s41586-020-2292-y).



The collaborative study traced the evolutionary roots of haemoglobin's structure and function.

New Research *continued*

Timmel Group

Imaging magnetic field effects

A collaborative study between the Timmel, Aarts, and Mackenzie groups has demonstrated for the first time the use of confocal microscopy to investigate the magnetic field sensitivity of chemical reactions.

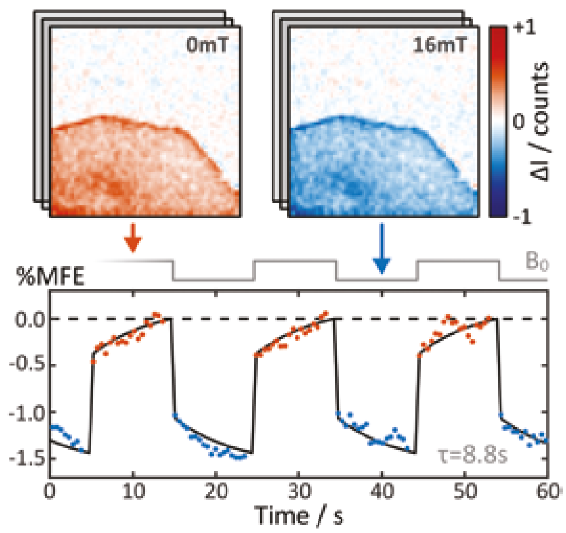
Confocal microscopy is an optical imaging technique that blocks out-of-focus light, allowing a thin plane containing the fluorophore of interest to be distinguished from that of the surroundings.

The technique was used to observe magnetic field effects (MFEs) both in solution and in single crystals. The systems were irradiated to form excited states that can quickly undergo electron transfer to produce radicals: chemical species containing unpaired electrons. The excited state can also fluoresce to reform the initial state, and it is this fluorescence that is observed using confocal microscopy.

How does a magnetic field affect this process? The radicals formed carry an unpaired electron (have non-zero spin) which is associated with a non-zero magnetic moment. This magnetic moment in turn interacts with an applied magnetic field. The direction and intensity of this field can affect the products formed from these radical states, and thereby affect the fluorescence intensity for the photochemical cycle.

In the team's experiments a weak magnetic field was repeatedly switched on or off, and step changes in the intensity of fluorescence were observed at coincident times, providing clear evidence for the magnetic field sensitivity of the reaction in the imaged solution or crystal. The main aim of the work was to explore the potential of confocal microscopy to investigate spatially resolved MFEs, with possible applications including investigating the effects of magnetic fields on light-induced processes in living tissues or in synthetic materials and devices.

As well as viewing the effect of the magnetic field on diffusing flavin molecules in a single crystal of a small protein, they were able to observe directional differences in response when the field was applied parallel or perpendicular to a single crystal of tetracene, a molecular organic semiconductor.



Variation in percentage magnetic field effect (MFE) in a flavin-doped lysozyme crystal in synchrony with magnetic field steps between 0 mT (red) and 16 mT (blue).

An exciting application of this work will be to test the directional magnetic sensitivity of immobilised samples of cryptochrome, a blue-light sensitive protein that is thought to be crucial in the mechanism by which birds detect the direction of the Earth's magnetic field when they migrate.

Victoire Déjean, DPhil student in the Timmel group, said that "this paper is the first big achievement of a fantastic collaboration between three research groups. I am very excited about the new avenues of research it opens up, especially regarding our goal to show that cryptochromes, the blue light photosensitive proteins found in birds' retinae, can act as chemical compasses."

Reference: Déjean, V. et al., *Chemical Science* **11** (2020) 7772–7781 (doi.org/10.1039/D0SC01986K).

Profile

Periodic magazine sat down with Volker Deringer, recently appointed Associate Professor of Theoretical and Computational Inorganic Chemistry, to discuss atomic-scale computer simulations, allotropes of carbon, and plenty more…

Professor Volker Deringer.

How would you describe your research?

We use accurate computer simulations to understand the atomic structure of inorganic materials. Our aim is to link that structure to practical applications, and ultimately we hope to suggest new synthetic materials. I'm most interested in materials that are hard to characterise, like amorphous matter, where we don't yet know the whole atomic structure.

Using quantum mechanics, we're able to model materials very accurately, but only for a couple of hundred atoms at a time. A central part of my research is using machine learning to reach much larger system sizes, while keeping the same accuracy. This allows us to attain an entirely new degree of realism in structural modelling, and we're starting to reach quantitative agreement with what experimental colleagues are measuring in the lab.

We hear a lot about machine learning nowadays – how are you applying it to chemistry?

Many established ideas in materials modelling are based on physical concepts – for instance, thinking of bonding in terms of spring constants between atoms. This has been extremely successful for decades. In our machine learning models, we don't pre-define what these interactions look like: all the information is somehow encoded in the data, and we have to use the right algorithms to tease it out.

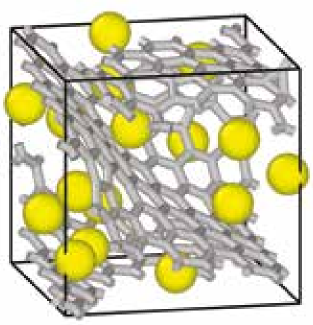
We spend a lot of time building databases – sets of relatively small-scale, highly accurate, quantum mechanics simulations – for fitting machine learning models, covering structural space as efficiently as we can. If we are looking at elemental carbon, we'd want to "teach" our model with data for diamond, graphite, nanotubes, but also liquid and amorphous structures. We want to expose it to lots of possible arrangements of atoms, including unfamiliar ones. Then we can answer really broadly relevant questions in chemistry and materials science.

In modelling inorganic materials, there's often a choice: use quantum mechanics for highly accurate results, or empirically fitted force fields for very large systems. The hope is now to achieve both at the same time – of course this is a highly simplified, and optimistic, view. We won't be making established methods obsolete, but I expect that machine learning methods will complement them much more widely in the future. And we aim to be at the forefront of that!

What applications of these methods are you currently working on, and what's the next big challenge?

I always say that we must first understand existing materials properly, and only based on that can we hope to design new ones.

For example, we've been looking at how sodium ions can intercalate into disordered carbon, just like how lithium in graphite is used for batteries. You might think that the two alkali metals behave in a similar way, but they really don't. And carbon is still "only" an elemental system! In the coming years we hope to branch out into more complex chemical compositions, with lots of implications for practical applications.



A disordered carbon structure (grey) with sodium ions interspersed (yellow): one of many atomic-scale challenges for computer simulations.

Image credit: J. Mater. Chem. A (2019) 7 19070.

Making machine learning modelling broadly accessible, coming up with the right datasets to capture complicated structures, and using all that knowledge to predict all-new materials: those are some of the major challenges for the coming years.

deringer.chem.ox.ac.uk @vl_deringer

Volker Deringer completed his doctorate at RWTH Aachen University in Germany before moving to the University of Cambridge in 2015 as an Alexander von Humboldt Foundation fellow. He was subsequently awarded a Leverhulme Early Career Fellowship at the same institution before joining Oxford Chemistry in September 2019. In addition to his post in the Inorganic Chemistry Laboratory, he is a Tutorial Fellow at St Anne's College.

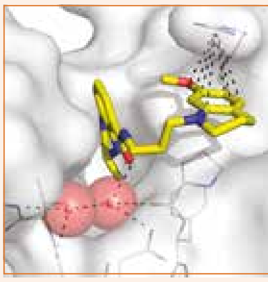
Chemistry in Cells

Understanding the interplay between chemistry, biology, and physics in the natural world is more important than ever, and so we are pleased to announce the establishment of a new cross-divisional doctoral training programme that aims to develop innovative physical science-based approaches to answer key biological questions relevant to diagnosis and treatment of disease.

The Chemistry in Cells DPhil programme is newly established with £5.8 million of funding from the Wellcome Trust and industrial partners, offering multidisciplinary training to a generation of outstanding graduate physical scientists. Its aim is to break new ground by accurately and directly quantifying the interactions of molecules, and their consequences, in biological settings such as cells, tissues and organisms. This research will have applications in the understanding and development of treatments of diseases including cancer, Alzheimer's disease, and conditions such as diabetes.

Break-through technologies emerging from the physical sciences that the new students will harness are not yet widely used or applied in complex biological systems of relevance. By focusing on specific biological questions and fostering collaborations between physical and biomedical researchers, the Chemistry in Cells programme will help to test and apply these cutting-edge lab-based methods, translating their use into medicine.

Alongside the development of these emerging techniques the programme will provide training and support to promote and nurture a diverse and supportive research environment. Led by Profs Stuart Conway, Angela Russell, Akane Kawamura, and Frances Platt (Department of Pharmacology), the programme brings together around 50 physical and biomedical lead scientists from across the university, other institutions, and industry.



X-ray crystal structure of a molecule developed in Oxford binding to the CREBBP bromodomain, a protein involved in cancer.

The first cohort of students will begin in Michaelmas 2020 with taught courses, followed by a 16-week Springboard phase that allows the students to orientate themselves within the laboratories of their prospective supervisors, before their substantive DPhil project starts in the spring of their first academic year. The students will have the opportunity for 1–3 month placements in industry relevant to their projects, and will also experience clinical placements so that they can contextualise the medical setting and importance of their research. Transition funding at the end of their projects will enable the students to explore diverse routes into postdoctoral careers, be they in academia, in industry, or in other areas.

http://chemistry-in-cells.chem.ox.ac.uk
@chem_in_cells

"We believe that embracing and supporting diversity in all forms will lead to a collaborative research culture in which science and scientists can flourish"
Directors, CiC programme

"The Department is very excited to be hosting the Wellcome Trust doctoral training programme Chemistry in Cells. The initiative is perfectly aligned with our vision of supporting collaborative multi-disciplinary research, from which ground-breaking discoveries are so often made."
Mark Brouard, Head of Chemistry

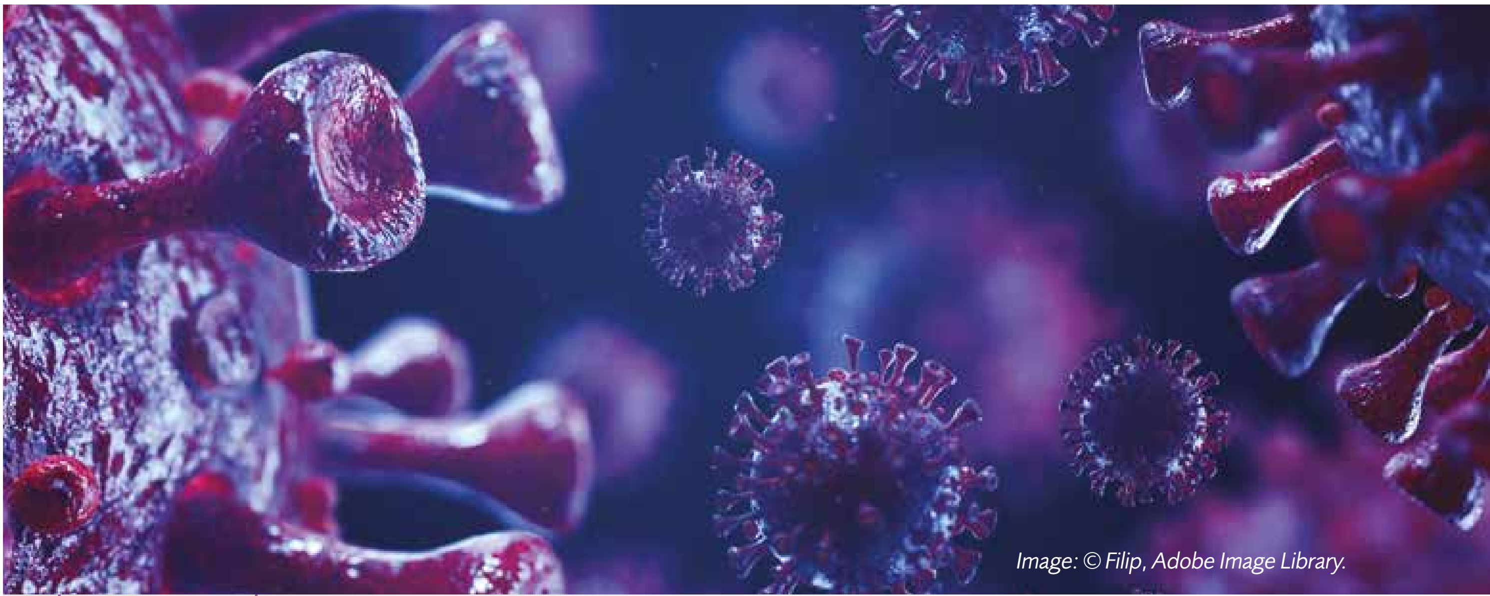


Image: © Filip, Adobe Image Library.

Coronavirus Research

The Department of Chemistry has been playing its part in the fight against COVID-19. Thomas Player explains some of the most recent research.

Funding new research

Chris Schofield was part of the committee responsible for distributing the University's COVID-19 Research Response Fund, which has received very substantial philanthropic donations during the crisis. It has funded projects related to COVID-19 across the University, including four in the Department of Chemistry.

Inhibiting the virus

One project in the Schofield group saw DPhil student Tika Malla and postdoctoral researcher Tony Tumber developing a mass spectrometry based assay to screen many different compounds and assess how they may inhibit viral enzyme targets, as prepared by Martin Walsh and his team at the Diamond Light Source. The aim of this project is to identify existing drugs that may be effective against the virus, as well as developing new treatments.

The assay was designed to monitor the inhibition of the main protease (M^{pro}). Unlike human proteins, the viral proteins are synthesised in long polypeptide chains. The function of M^{pro} is to cleave these polypeptide chains and release the proteins to carry out their downstream roles either individually or by forming a complex with other proteins. As the polypeptides are up to 20 kilodaltons long and synthetically less feasible, short peptide substrates were synthesized to monitor the activity of M^{pro}.

Tika Malla, member of the Schofield group, next to a RapidFire mass spectrometry sampler and injecting a sample from a 96-well plate. This equipment was crucial for the screening assay developed by the Schofield group.

Tobias John, a DPhil student in Schofield group, spent many days synthesizing and purifying natural peptide substrates of viral enzymes. This key work was carried out during the peak of the lockdown period this spring, with many late nights but always with stringent consideration of health and safety and increased hygiene practices. The work was fantastically well supported by the CRL staff including stores members, Adam Hardy, and the wonderful cleaners.

Unsure how the disease would progress, members of the Schofield group were able to optimise a method for comparing how effective many different compounds are at impairing the coronavirus protein – a vital tool for assessing the efficacy of new drugs. Based on these results, novel protease inhibitors were designed and synthesized by Lennart Brewitz; some of these show encouraging protease inhibition activities.

Along with in-house screening of drugs, this assay has also been used in collaboration with PostEra Inc. and a multidisciplinary cohort of scientists from academia and industry to screen compounds from the COVID Moonshot Project: a crowdsourced and collaborative initiative that aims to speed up discovery of the COVID-19 antiviral compound.

Drugs and treatments

The Schofield group has also been part of a highly collaborative investigation into repurposing the existing respiratory drug almitrine to treat COVID-19 patients. Many coronavirus patients die on ventilators because their lungs cannot take in enough oxygen. Almitrine, previously used to treat chronic obstructive pulmonary disease (COPD), is a respiratory stimulant that helps increase uptake of oxygen into blood in the lungs.

A collaboration across departments of the university, led by Peter Robbins from the Department of Physiology, Anatomy and Genetics, aims to determine if almitirine will have a similar effect in COVID-19 patients and prevent them being put on ventilators. The Schofield group, and in particular Tharindi Panduwawala and Alistair Farley, have developed routes to synthesise and analyse almitrine, and the drug will now be tested in clinical trials funded by LifeArc at three UK hospitals. Since almitrine is a relatively cheap drug it could be particularly useful where ventilators are not readily available, improving patients' lung function before the disease progresses too far.

"We hope that this massive and very productive set of national and international collaborations on COVID-19 will be maintained over the longer term," said Professor Schofield, "to address not only potential future pandemics but also viral diseases in general, particularly in middle and lower income countries where diseases like dengue and Zika fever are major killers. There is just a chance that these efforts will change the way the world works for the better in terms of infectious diseases."

Stephen Fletcher's research group has received a grant from UK Research and Innovation in order to develop COVID-19 specific viral RNA polymerase inhibitors. This is a type of drug that prevents replication of the virus' genetic material. Their work is inspired by Remdesivir, an antiviral drug that is

Florian Modicom, Sourabh Mishra and Conor Dean – members of the Fletcher group working on COVID-19 research – relax outside the lab.

administered intravenously and was previously tested as a treatment for hepatitis C and the Ebola virus. This new research will use rhodium-catalyzed reactions, developed in the Fletcher lab, to make a variety of candidate molecules that look similar to Remdesivir. These will then be assessed based on their biological activity, with the ultimate aim being effective inhibition of COVID-19 viral replication.

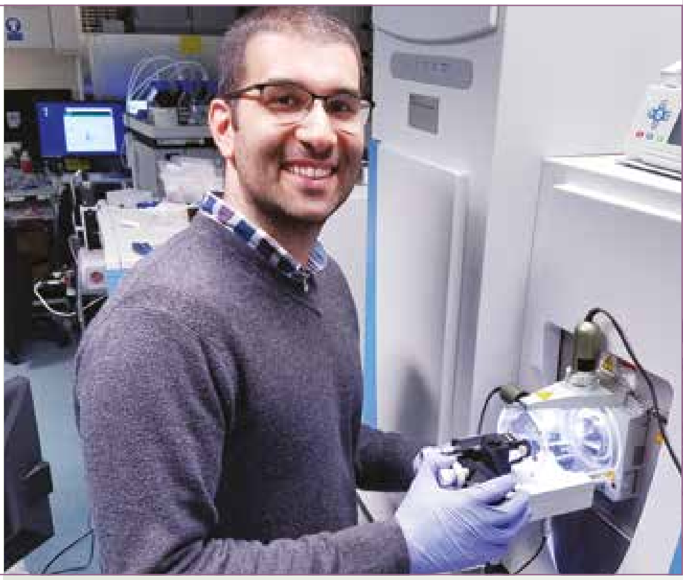
References: Goetzke, F. W. et al., *Angew. Chem. Int.* Ed. 58 (2019) 12128–12132 (doi.org/10.1002/anie.201906478), Schäfer, P. et al., *Nat. Commun*. 8 (2017) 15762 (doi.org/10.1038/ncomms15762).

Analysis and screening

Potential methods for inhibiting the virus responsible for COVID-19 are being investigated using mass spectrometry in native conditions in a collaboration between **Carol Robinson**, Chris Schofield, and colleagues in the Department of Biochemistry. They have been considering the effect of small molecules that can bind to the virus far from its active site. Drugs that bind non-covalently in this way can limit its activity, and may also be more stable and have less toxic effects than other drugs that bind irreversibly. Using mass spectrometry they characterised a section of the SARS-CoV-2 protein M^{Pro} – the main protein responsible for processing mature SARS-CoV-2 – and found that several small molecules can bind non-covalently to this protein and slow its activity. This is a promising and straightforward route to test and optimise potential antiviral drugs.

Biophysics of COVID "spike" protein

The university's COVID-19 response fund has also awarded funding to **Philipp Kukura's** research group in order to investigate the molecular biophysics of the protein responsible for COVID-19. In particular, they will be using their state-of-the-art mass photometry



Tarick El-Baba and Corinne Lutomski, members of the Robinson group, performing key COVID-19 research on their favourite machines. A husband and wife team – no masks necessary!

techniques to consider the role that the SARS-CoV-2 "spike glycoprotein" may play in coronavirus infections. Similar protein features are known to play a role in HIV, Ebola, and SARS-CoV-1 (responsible for the 2002–2004 SARS outbreak), but it is currently unknown how they work in the SARS-CoV-2 protein that causes COVID-19.

References: Young, G., and Hundt, N. et al., *Science* **360** (2018) 6387 423–427 (doi.org/10.1126/science.aar5839), Soltermann, F. et al., *Angew. Chem. Int.* Ed. **59** (2020) 27 10774–10779 (doi.org/10.1002/anie.202001578)".

Working to change the landscape of COVID-19 testing

Tom Brown, postdoctoral researcher Lapatrada Taemaitree, and spin-out company ATDBio are working with several research groups, companies and NHS Trusts to make chemically modified synthetic DNA for use in improved COVID-19 point-of-care diagnostic testing and high-throughput screening. Widespread testing will be increasingly important in determining the true scale of the spread of the COVID-19 pandemic by identifying both infected individuals and asymptomatic carriers.

These tests are used in several different contexts including the screening of healthcare workers in hospitals and care homes, surveillance of travellers at airports, and to determine the main mechanisms of COVID-19 infection. The tests are also designed to allow mutations in the virus to be characterised. This is an important element in the study of the epidemiology of this new virus.

Reference: Wu, Q. et al. (2020, doi.org/10.1101/2020.06.01.127019).

Oxford Nanopore – a spinout company from the Department of Chemistry (see page 15), that also works with Professor Brown's research group – has developed the LamPORE test for COVID-19. This diagnostic tool can detect the presence of the SARS-CoV-2 virus in a patient's sample within 90 minutes. The UK Department of Health and Social Care has ordered hundreds of thousands of these tests for rapid testing in settings like screening healthcare workers.

As well as detecting the COVID-19 virus, a further test using the same technology is being developed that will be able to detect not only coronavirus but more common winter respiratory illnesses such as influenza. Being able to distinguish between these diseases will be vital as we approach the winter flu season with the coronavirus pandemic still ongoing.

Thank you

The Department has been beginning to re-open over the past weeks and months, and special thanks should go to all the buildings and facilities staff who ensured that the labs remained safely operational for crucial work during the lockdown period, and who have worked tirelessly over the past months to help make a safe working environment as people return to work.

Sequencing SARS-CoV-2 RNA

Divya Popat (Jesus, 2017), DPhil student in the Vallance group, reports on how Oxford Nanopore Technologies Ltd, a spin-out company from the Department of Chemistry, has enabled the surveillance of the RNA sequence of SARS-CoV-2 to understand its transmission and evolution.

Oxford Nanopore Technologies was founded in 2005 by Hagan Bayley, Professor of Chemical Biology in the Department of Chemistry. The company specialises in the nanopore sequencing of DNA/RNA and focuses on increasing the ease of use of the nanopore sequencing technique and automation. The company's first product was the 'MinION', the only portable, real-time device for direct nanopore sequencing of DNA and RNA. In this device, ionic currents are passed through up to 512 protein nanopores; characteristic modulations of the currents are measured as the nucleic acids pass through the nanopores, enabling their sequences to be read. The MinION has the capacity to read 7-12 million RNA sequences within hours and stream the data directly to a computer in real-time, enabling the rapid identification of viral pathogens.

The company sent hundreds of their handheld 'MinION' devices to China's Centre of Disease Control and Prevention, which allowed the first RNA sequences of SARS-CoV-2 to be recorded.

Their technology was key to identifying the strain of the coronavirus when it first appeared and understanding its transmission and evolution.[1] The MinION device was also used in work published in late January 2020 which indicated person-to-person transmission of the virus through air travel.[2] The scientific community had previously used the MinION device in several outbreak situations in the past including Lassa Fever, Swine Flu, Yellow Fever, Zika[3] and Ebola[4]. This experience supported the rapid deployment of MinION devices for the current outbreak. Oxford Nanopore Technologies is supplying the devices to countries all around the world to enable rapid, large scale sequencing analysis of samples from patients testing positive for COVID-19.

The surveillance of the rapidly mutating sequence of SARS-CoV-2 RNA can help to provide information about the degree to which it is related to other viruses, the mode and speed of evolution, geographical spread and adaptation to human hosts. This information can be used to assist in epidemiological investigations. Fast generation and sharing of data can lead to a better public health response as well as supporting vaccine development and diagnostic capabilities. For these reasons, the rapid nanopore sequencing MinION devices have been of paramount importance in the monitoring of COVID-19.

Nanopore technology is also applicable to the detection and identification of small molecules (e.g. pharmaceuticals) and reactive molecules (e.g. chemical warfare agents), as well as additional biological macromolecules including proteins and their post-translationally modified forms, all of which are important in medicine.

References:
[1] N. Zhu et al., N Eng J Med, 2020, 382;8, 727-733
[2] J. F. Chan, The Lancet, 2020, 395, 514-523
[3] N. Faria et al., Nature, 2017, 546, 406-410
[4] J. Quick et al., Nature, 2016, 530, 228- 232.

MinION device from Oxford Nanopore.

Chemistry Nobel Laureate Professor M. Stanley Whittingham

Thomas Player (Keble 2013), DPhil student in the Hore group, interviews 2019 Nobel Laureate Professor M. Stanley Whittingham

Has Stanley Whittingham had enough of being congratulated for his Nobel Prize in Chemistry, awarded last December? His simple reply: it comes and goes.

Whittingham shares the prize with John Goodenough and Akira Yoshino for research that began in the late 1960s and led to the development of lithium-ion batteries. Commonly used for portable electronics, as well as electric vehicles and other applications, they are a type of high energy-density rechargeable battery that relies on lithium ions moving between the electrodes. It is perhaps surprising that such a ubiquitous invention – you likely have one in your pocket – had until now remained unacknowledged by the Nobel committee.

Whittingham's early work at US energy company Exxon in the 1970s, developing intercalated materials where molecules or ions are incorporated into a layered solid, preceded that of both of his Nobel co-recipients. Goodenough was at Oxford in the late 1970s and early 1980s when he expanded on Whittingham's work, using lithium cobalt oxide as a material for battery cathodes, and this was later developed and commercialised at Sony by Yoshino. Nowadays lithium batteries are vital in a multitude of settings, from smartphones and laptops to electric cars and national grids. "It's very gratifying. I think everybody in the field is happy because it [lithium battery technology] is being used."

In the early days investigating the fundamental properties of lithium electrode materials, did Whittingham have an inkling of how widespread this technology would become? "We were working on all kinds of energy problems at Exxon, and I think they recognised that oil was going to run out." This led to lots of work on batteries, with Whittingham pitching his lithium project to the board of directors in "what they call an elevator speech these days".

Professor M. Stanley Whittingham.

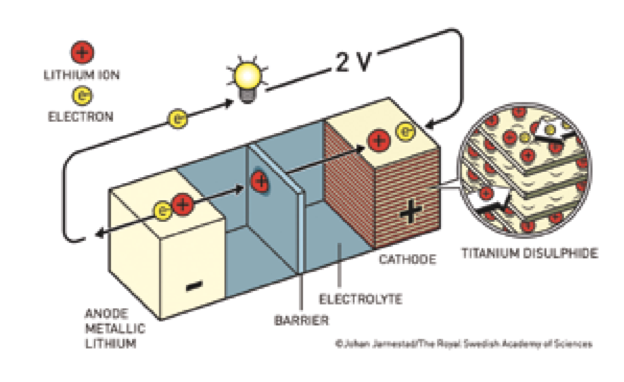
Even at that time, the development and manufacturing teams at Exxon had goals that remain familiar today. Developing electric vehicles, still a major concern for the automotive industry, was one. "Back at some of the old talks I gave we even talked about smoothing the [national] grid using large batteries – I think people were thinking along the same lines [as we do today]".

"There's a huge push here, particularly in New York State and California … to install solar and wind power and combine them with batteries". One advantage of this is that you can quickly turn the batteries on to meet peaks in electricity demand – faster than pumped hydro-electric generators, and greener than fossil fuel stations. "It's very clear now: I don't think anyone's going to build new coal power plants, they're just too expensive compared with wind and solar. [Renewables] may be a bit more expensive in the beginning, but the fuel is free and it needs almost zero maintenance." Battery technology is similarly low-maintenance – Whittingham cites a battery facility that he visited where they proudly informed him that their biggest maintenance task is mowing the grass.

Whittingham is unsure that receiving the award has had a large impact on his research, although the associated publicity has certainly raised the profile of lithium-ion batteries and their importance. But if the Nobel Prize has not had much impact on his work over the last few months, something that certainly has is the COVID-19 pandemic.

"Obviously we've stopped all experimental research for several months. It's kept me basically at home, and I would have been on the road 60–70% of my time during March to June." He is curious whether Oxford will be opening up to students in October, and it seems the academic struggles related to the virus are similarly felt all over the world. Whittingham states the problem simply: "chemistry has to have labs".

Whittingham has been based at Binghampton University in New York state for the last 31 years. Before emigrating to the US he studied for both his BA (1964) and DPhil (1968) in the Chemistry department at Oxford. He remembers that tutorials with Peter Dickens took place in his house on Sunday mornings, complete with tea and biscuits. Dickens – New College tutor in Chemistry at the time, and later Whittingham's Part II and DPhil supervisor – died in October 2019, just two weeks before it was announced that his former student had been awarded the Nobel prize.



The Whittingham Battery. © Johan Jarnestad/The Royal Swedish Academy of Sciences.

During his Part II year, Whittingham's research was funded by the office of the US Air Force in London. It was the peak of the space race and they were particularly interested in topics such as the reactions of oxygen atoms with rocket nose cones, leading to Whittingham's early work on tungsten bronzes. His DPhil, funded by the British Gas Council, was supposed to focus on catalysts for converting coal gas into natural gas. "They gave me the fellowship, and then I think it was early August when they struck natural gas in the North Sea and said 'we're not interested in that anymore – you can do whatever you like, send us a report at the end, and don't bother us with anything in the interim'." They honoured the funding, and this gave Whittingham the freedom to follow his interests during his doctoral studies.

"I think my lab was a little bit infamous in the Inorganic Chemistry Laboratory. I still remember dismantling part of a hood in there: to generate the draught under the hood you had to light gas that caused the flow up the exit pipe. So, if we had organics then they burnt up the exit pipe too."

Other students were looking at reactions of chlorine atoms. "There was always a slight sniff of chlorine in the air. In the three years I was there I think no-one caught a cold."

"I was doing microbalance studies on reactions of hydrogen with these tungsten bronzes, so I had to build all the electrical systems to control it. We built an automatic liquid nitrogen refilling system, you learnt how to be an electrician, glassblower – you did everything yourself. The glass blowers … would help train you, but they only did specialised stuff, so you had to become almost a jack of all trades." Data was measured using chart recorders rather than computers, so if an experiment was running for a long time you might be in the lab for 24 hours or longer, dozing off when possible to get a bit of sleep.

Whittingham sees a distinction between the custom setups he used in his doctoral studies, which involved a lot of forethought and design, and current approaches. "You've got the opportunity of thinking now. In those days you couldn't do what most students tend to do now, which is to try everything."

Outside of the lab there was still time for leisure, with fond memories of living in Oxford in the 1960s. "In the summer, if you got bored you'd go and watch the cricket; in those days Oxford played international tourists and most of the county teams. If you were in Chemistry you'd just walk, almost out the back door, and into the field."

"[When I was] an undergraduate it snowed between Christmas and New Year once, and the traffic just packed it down … the snow was still there until the beginning of March. If anybody says climate warming isn't happening then they haven't lived long enough to see it."

For Whittingham, science is certainly an international business. "In solid-state chemistry people move from country to country, with collaborators in all different countries. Some of my colleagues use the light beam just outside Oxford rather than ones in the US."

“I said in the banquet speech for the Nobel prize: John [Goodenough] made his inventions in Oxford and I made mine in the US, so in a sense we switched nationalities to do that.”

Following his DPhil, Whittingham moved to Stanford for a postdoctoral position. “I moved in 1968, it was cold and miserable in England. I caught a 707 direct to San Francisco ... 70 degrees, sunshine. And that was one of the reasons I went! I think all DPhils, if they wanted a good academic or industrial job, had to go to the US in those days for a postdoc.” Subsequently he took a research position at Exxon’s new corporate labs, studying “anything energy related that wasn’t petroleum or chemicals”. He remembers it as a great time to be in industry, and contrasts it with the situation today. “Exxon, Bell Labs, DuPont, General Electric, IBM: they all had these very fundamental research labs – more basic research than academics could ever do – but they’re all gone.” In his opinion this has been driven by a focus on short term returns, where inventions may still be made in Britain or the US but then “the engineering is shipped off to Asia. They’re willing to invest ten years, or whatever it takes, to turn an idea into a product”.

He and Goodenough now form part of the Battery500 Consortium, a collaboration that aims to increase the energy density in lithium battery cells to 500 watt hours per kilogram. “That’s about double what it is today.” Another of his projects is more fundamental, aiming to “understand all the chemical reactions that can occur in battery electrodes”. The area for which he has recently been honoured remains ripe for exploration, almost 50 years after he began working in the field.

So, what would his move be today, if he were a DPhil student just finishing up his studies? “Certainly in Britain it will be very stressed in research with Brexit and things like that. I don’t know what the British government is going to do, whether they will invest in research to get out of the doldrums or whether they’ll worry more about the virus and stop investing in everything. I’m at the end of my career, it’s not going to affect me, but I think it’s much more worrisome for new folks getting into the field.”

Alongside his scientific projects, Whittingham also sits on a task force for the governor of New York State that aims to elucidate the factors limiting the uptake of electric vehicles. He cites range as one of the major limiting factors, but sees no reason why fleets of delivery vans and buses in large cities could not be

John Goodenough – co-recipient of the Nobel Prize alongside Whittingham – and colleagues outside the Inorganic Chemistry Laboratory in 1982. Goodenough is second from the left in the front row.

totally electric. “Most of us believe that large cities like London, New York, and San Francisco will ban internal combustion engines within the next 10 or 15 years.”

There are stark differences in attitudes to climate change across the US. In Whittingham’s view the Democrat-led states, in particular California, are leading the way in the automotive industry. “You’ve got these big areas pushing for a greener environment, and car manufacturers won’t make two different sets of cars so they have to follow the California standards. That’s what Trump is trying to change, but I don’t think auto manufacturers will change because they want to make cars they can sell around the world.”

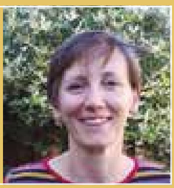
He remains optimistic about a global response to climate change, explaining that Nobel laureates as a group are certainly in favour of action. “Even Trump will have to listen when his mansion in Florida gets flooded, it’s only about two feet above water level now.”

One current debate is whether the impacts of COVID-19 related lockdowns on the way we work – more working from home, less commuting – will have a long-lasting impact on our attitudes to travel and pollution. Possibly in the long-term, says Whittingham, but “in the short term it’s going to make things worse. People are going to be loath to carpool, they’re not really going to want to go on full buses or full trains, but instead they’ll opt to drive themselves”. He does concede that in Oxford, perhaps, more people might just ride bikes.

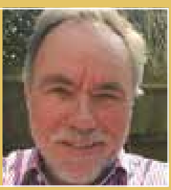
In light of his Nobel Prize, Whittingham was recently made an Honorary Fellow of New College. “What are the perks?” he enquired, on hearing the news. “Well, you can park your car inside the quad” came the reply. Perhaps, if Whittingham’s predictions on the future of internal combustion are to be believed, when he next pulls up into the quad his car will need to be powered by one of his own lithium-ion batteries.

Contributing to the fight against climate change

Divya Popat reports on some of the ways in which chemistry research can contribute to mitigating the effects of climate change as we strive towards a cleaner and greener future.



Dr Emily Flashman's main focus is on how cells sense and respond to environmental stresses, particularly in plants. Since the onset of climate change, plants are increasingly subject to flooding resulting in a lack of oxygen; plants are able to detect how much oxygen is available using oxygen-sensing enzymes called plant cysteine oxidases. Flashman works on understanding how these enzymes trigger a stabilisation mechanism and adaptation response in plants, so that they can engineer these enzymes and genetically alter the enzymatic behaviour in plants to help them survive longer when they become submerged in water, making them capable of withstanding the inevitable extreme weather conditions. Crop yield loss due to flooding is a threat to food security so this type of engineering could help make crops more tolerant of climate extremes and enhance submergence tolerance in agriculture.



Professor Fraser Armstrong's research includes the exploitation of nature's catalysts, enzymes, for energy production with the aim of contributing to the development of future renewable energy technologies. His group has pioneered a technique called 'protein film electrochemistry' and they are using it to study how enzymes function so efficiently. Evolution has ensured that electrical/solar and chemical energy are interconverted with maximum rate and minimal wastage, so enzymes set the ultimate standards for future development.

A recent invention, the 'electrochemical leaf', further mimics nature by channelling electrical energy into enzyme cascades (production lines) that are trapped and crowded within the nanopores of a conducting metal oxide electrode material. Such simple nanoconfinement, now so easily energized, produces a massive increase in rates of biocatalysis with exquisite control of complex chemistry.

Armstrong has also demonstrated the attachment of enzymes to semiconductor nanoparticles to harness sunlight and convert H_2O into H_2 or CO_2 into CO. Enzymes are so efficient that the performance of these solar fuel-forming systems is limited by the abilities of the semiconducting systems to capture sunlight and transfer electrons, allowing focus to shift, strange as it seems, away from catalysis itself.

Professor Peter Edwards, Dr Tiancun Xiao, and Dr Zhaoxi Zhang founded a spin out company called Oxford Sustainable Fuels in 2018. The company aims to reduce the environmental impact of plastics by utilising the low energy process, pyrolysis. Pyrolysis thermally decomposes plastics as well as other waste materials such as tyres and biomass, and through Oxford Sustainable Fuels' unique purification and stabilisation technology, converts the waste into high quality transportation fuels and chemicals. In essence, this process creates valuable products from materials that would have otherwise been disposed of in landfill sites and incineration or end up polluting our oceans.

Professor Kylie Vincent's research explores the fact that hydrogen holds great promise as a clean renewable fuel for the future with the only waste product being water. However it is not easy and cheap to release the enormous amount of energy stored in hydrogen in a controlled way for use as a fuel. Current methods involve using platinum which is very expensive and a limited resource.

Vincent's work is inspired by enzymes found in bacteria which are able to efficiently use hydrogen as a fuel. She has used infra-red spectroscopy to look inside the enzyme to understand how they do this, revealing details of how the hydrogen molecule is split at a metal site containing nickel and iron. Once the process is fully understood, simpler catalysts can be built containing these cheaper metals to model the chemistry that happens in the enzymes, taking us a step closer to the reality of affordable vehicles running on hydrogen as a clean renewable fuel.

Looking inside Banana-shaped liquid crystals

Carla Fernández-Rico.

Carla Fernández-Rico, 3rd year DPhil student in the Oxford Colloid Group supervised by Professor Roel Dullens, describes the development of a new system of micrometre sized banana-shaped particles. With these 'bananas' the researchers experimentally confirm the existence of the so-called 'splay-bend nematic' liquid crystal phase, which was predicted 40 years ago, but had remained elusive until now. These results provide the cornerstone for the further development of new banana-shaped liquid crystals.

Liquid crystals are a fascinating state of matter that we encounter in our everyday life. For example, the cell membranes in our bodies are in a liquid crystalline state - and so are the functional materials used in displays of TVs and computers. The reason this state of matter is a cornerstone of both living and technological materials is inherent to its unique properties: it shows order in a preferred direction, like a solid, but it also flows, like a liquid, and as such, it easily responds to external stimuli such as electric fields.

The *shape* of the liquid crystal forming building blocks, which are typically elongated molecules, has an enormous impact on the way they pack into liquid crystals. While simple rod-like molecules form just five liquid crystal phases, banana-shaped molecules form more than fifty phases. These 'banana phases' were discovered 20 years ago and have since then initiated a true 'banana-mania' in the field of liquid crystals. The fact that even a small molecular curvature results in a new library of banana phases is not only fascinating from a fundamental point of view, but also from an industrial perspective, as they can switch their orientation under electric fields at ultra-fast speeds, making them ideal candidates for new highly responsive displays.

Fig. 1. Scanning electron microscopy image of the colloidal bananas. Note the false colouring emphasizes the shape of the particles. The scale bar is 5 micrometers.

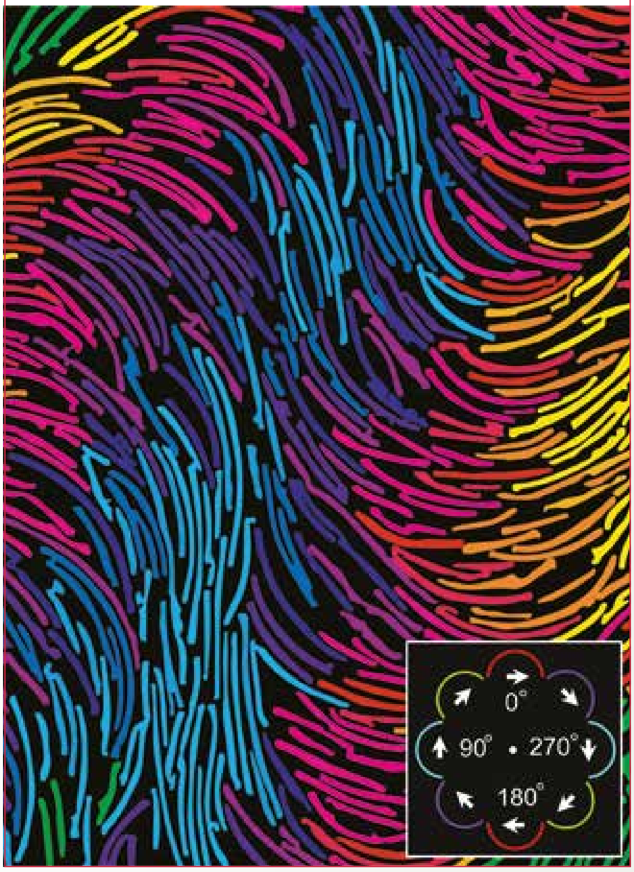


Fig.2: Bananas in the splay-bend nematic phase colored according to the particle orientation as indicated by the white arrows in the inset.

Fig.3: Confocal microscopy image of the splay-bend nematic phase. Note the wavy nature of this phase arises from the banana-shape of the particles when packing close together. The scale bar is 10 micrometers.

Despite the importance of banana phases, to date nobody has managed to look inside them and directly visualize the way the banana particles pack or move. This is largely due to the fact that molecular systems are extremely small and move very fast, making their direct imaging extremely challenging even when using the most advanced microscopes.

Carla Fernández-Rico and co-workers used colloidal bananas and optical microscopy to study and visualize, for the first time, the inner details of banana-shaped liquid crystals with single particle resolution.

Using image analysis techniques, they directly determined the positions and orientations of the banana-shaped particles, which enabled the identification of a range of different banana phases (see Fig.2). Moreover, with their colloidal bananas they experimentally confirmed the existence of the so-called splay-bend nematic LC phase (see Fig.3), which was predicted 40 years ago, but had remained elusive until now.

Publication: C. Fernández-Rico et al, (2020) Science 21 Aug 2020: Vol. 369, Issue 6506, pp. 950-955. DOI: 10.1126/science.abb4536.

The Dullens/Aarts group. Professor Dirk Aarts is seated in the front row, 3rd from left, next to Professor Roel Dullens (front row, 4th from left).

Lab in a van: The Chemystery Machine

The new van outside the teaching labs.

Jennie Botham, CTL Lab Technician, writes about an exciting new resource allowing us to take the joys of chemistry to more and more young people.

Thousands of young people from around the UK and abroad visit the Department of Chemistry each year. Many take part in practical workshops in the new Chemistry Teaching Laboratory (CTL) working with Department staff and our ambassadors, who are drawn mainly from our undergraduate and graduate community. Additionally, outreach teams go out to schools to deliver practical workshops, lecture-demonstrations and academic and career talks. The purpose of our outreach work is to inspire young people, their parents, guardians and teachers about the role of chemistry in their lives and in society, increasing the understanding of chemistry as a vibrant, relevant and 'living' science. We aim to encourage young people to aspire to study chemistry post-18, and, by working to support young people, the teaching staff and technicians who work with them, help them to attain the qualifications required to open up opportunities in the chemical sciences.

Our ability to visit schools has, until now, been limited by the expense of hiring taxis or vans and this has, by necessity, limited the distance the teams are able to travel. A planned period of closure of the CTL due to construction work associated with the new Life and Mind Building provided an opportunity to expand our portfolio of outreach activities based in schools and in order to facilitate the programme, the Department has recently taken delivery of a large van, which has already proved invaluable with local visits to schools.

The van has six seats and a generous cargo area so can transport the whole team and all of the chemicals and equipment needed.

A variety of portable workshops and two new lecture-demonstrations which highlight Oxford Chemistry research have been developed that are safe for use in a school environment and age appropriate. The equipment for the activities is packed into boxes that are easily transportable and quickly replenished when back at the department. Supported by department staff, trained ambassadors deliver the activities, developing their own communication and presentation skills, in line with the Vitae Researcher Development Framework.

Covid-19 has interrupted the planned delivery of face-to-face workshops and lectures further afield, but we hope to be back on the road as soon as it is safe and prudent so to do. In the meantime, the team have been developing workshops and talks for online delivery. This included a new Chiral Chemistry resource which brings in the main protease of SARS-CoV-2, an area of active research in the department. Additionally, our UNIQ programme moved online, with a whole array of video lectures, live panels, interactive seminars, workshops and a new kitchen chemistry practical looking at turmeric as both indicator and dye. Whilst the online resources have been welcomed by school students and teachers, we are looking forward to the return to in-person events as soon as possible. The work of the outreach team is generously supported by the Department as well as through alumni donations and sponsorship.

The Chemistry Teaching Laboratory (CTL).

Award for practical chemistry course

The Chemistry Teaching Laboratory team have been awarded one of the inaugural Vice-Chancellor's Education Awards, recognising new and innovative approaches to teaching within the University. The prize was awarded for the design and implementation of an integrated practical course.

For many years the undergraduate inorganic, organic, and physical lab work took place in separate buildings. In designing a new course the team focused on interdisciplinary approaches to solving problems, drawing techniques from the whole discipline of chemistry as well as biochemistry and physics. The purpose-built Chemistry Teaching Laboratory, opened in October 2018, facilitates this novel approach to teaching practical chemistry.

Inspiring the next generation

Chemistry has never been more relevant to our lives, yet school students can struggle to look beyond the list of facts and the (usually dead) scientists portrayed in their textbooks. A new strand in our outreach work has been the development of a series of career and research talks given by our wonderful DPhil ambassadors. Through sharing their own personal stories of study and academic ambition, as well as explaining their research and its relevance, they have been changing the perception of the chemical sciences and Oxford Chemistry. School groups have the opportunity to ask questions about further study, and the underlying chemistry and research.

With the move to online outreach delivery, these talks are being recorded and are being offered as a super-curricular series for post-16 state school pupils, entitled *Ask a Research Chemist*.

Conscious that attitudes to science and chemistry form early on in a young person's school career, the department is also delivering an *Ask a Chemist* series for school students from primary to secondary and their teachers. This monthly online Q&A is designed to complement the recent RSC careers campaign 'Chemistry: Making the Difference.' We are keen to hear from all those who have been connected with Oxford Chemistry and who would be prepared to take questions about their careers. Please contact outreach@chem.ox.ac.uk if you would like to be involved.

Supporting students for 40 years

Jennie Botham, BSc (Hons), RSciTech.

In July, Lab Technician Jennie Botham celebrated 40 years in the Department of Chemistry. Jennie started work in the ICL teaching labs in 1980, soon after she finished her A levels. Jennie says: "I chose to study chemistry because I enjoyed it at school. I had a very good teacher who made it fun and I seemed to be able to understand it fairly easily. I chose to become a lab technician because it seemed like an interesting job when I finished school. I started straight after A levels as a trainee and I was able to learn on the job doing day release to college."

Jennie studied alongside her work to obtain her degree in chemistry, and became a Registered Science Technician through the Royal Society of Chemistry. Over the past 40 years thousands of students have benefited from her guidance and expertise.
Now working in the CTL, Jennie spends most of her time supporting the undergraduates, providing chemicals, troubleshooting equipment and explaining unfamiliar techniques. In the vacations she tries out new practical experiments, stock takes, and orders consumable items.

Jennie says: "The most exciting thing about my work is seeing how the undergraduates develop. They start off very unsure about their practical work and it is great to see them become more confident. When they go on to become researchers and academics it is very satisfying to think that I may have played a part in encouraging them to do the best they can."

Inform, Inspire, Engage

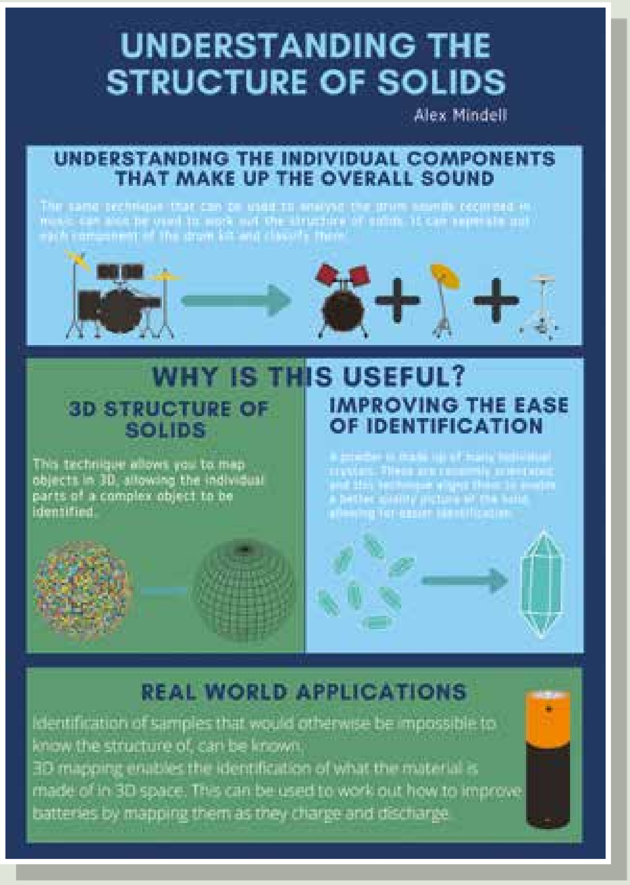
Jess Fleming (Lincoln 2016) writes about a project to help students communicate their research.

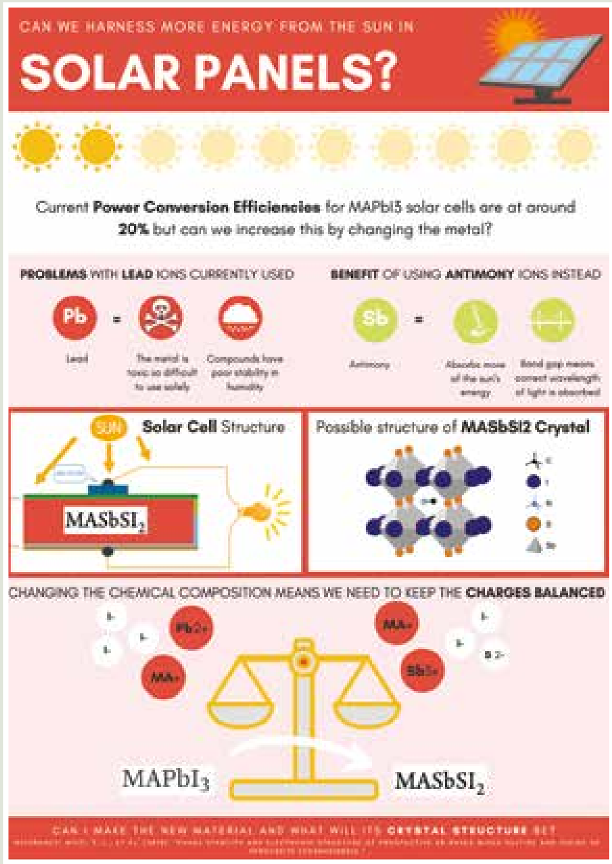
What links birds, drum kits and interstellar gas clouds? All featured in the department's infographics project, launched for the first time this academic year.

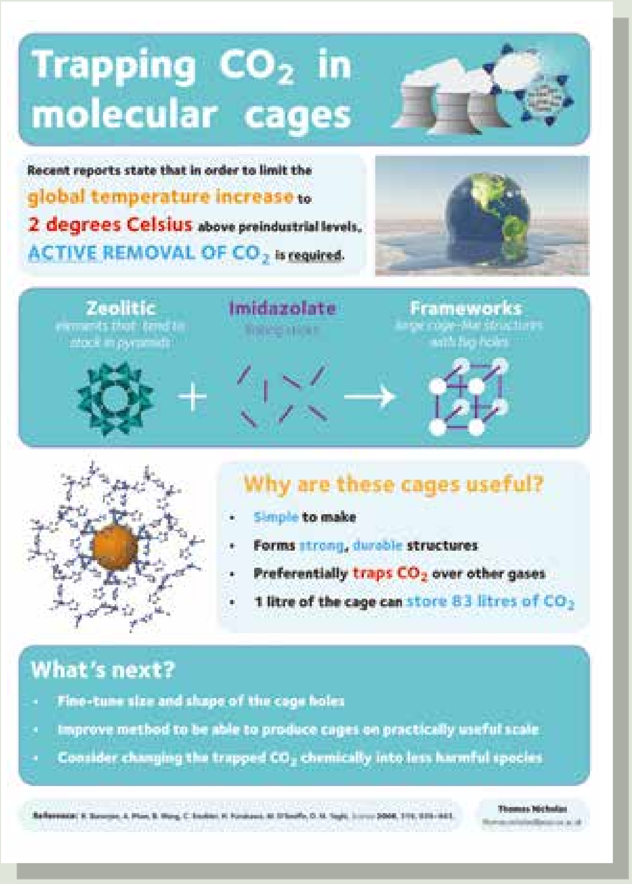
In October last year, 20 Part II students were brought together with the challenge of using this novel format to communicate their research to a wider audience. After some initial training in science communication, the students had two weeks to produce an infographic to be shared with their peers in a Q&A session at the Chemistry Teaching Laboratory.

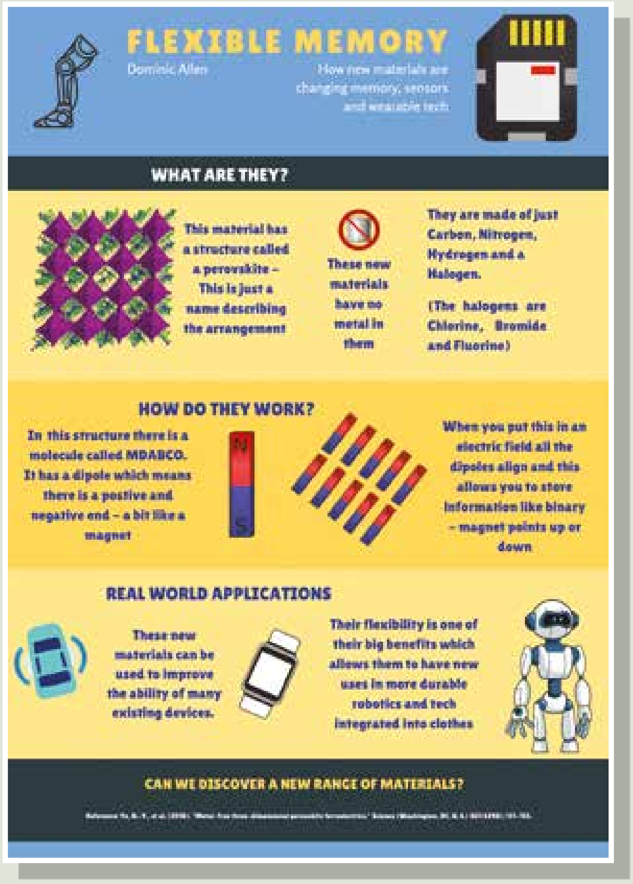
The word itself gives a clue to its function: infographic = information + graphics. An infographic is a combination of charts, images and minimal text designed to communicate a complex idea in an accessible and engaging manner. A well-known example is Compound Interest, run by Andy Brunning, which features an extensive library covering the chemistry in everything from porridge to nail polish.

Unfortunately, the typical format of a journal article is hardly conducive to public engagement. Instead, the "inverted triangle" approach is encouraged: start with the findings, move onto the method then briefly cover the background. Text should be concise and replaced with simple diagrams wherever possible. The number one rule? Be ruthless! It's time to decide what really matters.









Simplifying your science can be a lot harder than it sounds. Randall Monroe's book "Thing Explainer" uses only the 1000 most common English words to describe topics including chemistry's periodic table. In his version, fluorine becomes "green burning air that kills" and sulphur is "smelly yellow rocks"! Whilst it wasn't necessary to go quite this far, eliminating the jargon is key to a successful infographic.

The students' creations have now become part of the department's wider outreach work. They were displayed at the department's annual alumni reception at the Royal Society of Chemistry (RSC) and have been used in wider training activities. Given that a recent RSC survey found roughly half the public don't feel confident discussing chemistry, clearly outreach work is as important as ever. It prevents disinformation, inspires the next generation and boosts funding for research.

The participants themselves also benefited from being challenged to think about their research in a new way and really understand the fundamentals of it. A diverse mix of groups were brought together to share their science and become more confident communicators, hopefully inspired to do more public engagement work in the future. One participant said "the infographic writing helped me better understand my Part II research by making me summarise and present it as simply as possible to explain it to a non-scientist. It was also a helpful insight into scientific communication that stood me in good stead to start the huge task of writing a thesis".

The project is currently at the pilot stage, organised by Richard Cooper, Martin Galpin and Saskia O'Sullivan with a view to expanding it further next year. See the images for some examples of the students' output so far.

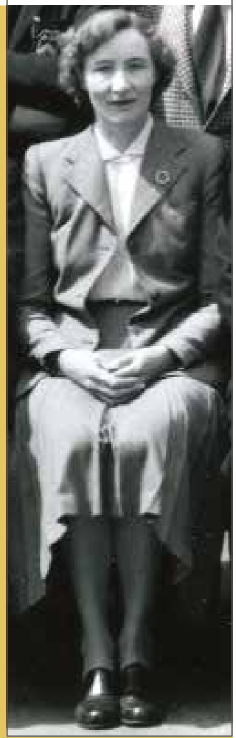
Find out more or have a go:

https://www.compoundchem.com/

Thing Explainer **by Randall Moore**

https://www.rsc.org/campaigning-outreach/outreach/public-attitudes-chemistry/

Pioneering Women Chemists at Oxford



Muriel Tomlinson in 1956.

In 2020 the University marked one hundred years since women were awarded Oxford degrees. Women had studied at Oxford since the 1870s, but were only admitted as full members of the University in 1920. Oxford Chemistry alumna Judith Mirzoeff (St Hilda's, 1956) remembers pioneering Oxford women chemists Muriel Tomlinson and Margaret Christie, and describes her own experience of studying chemistry at Oxford in the 1950s.

Exactly 60 years ago, I handed in my Part II thesis, which did little to elucidate the decomposition of polythionates, and left Oxford.

I shall never forget the thrill of my first day four years earlier – freedom at last, even though we were still minors and college rules were quite parental. Coming from a girls' school I was used to clever women, but was nevertheless relieved that the other freshers in St Hilda's were not too daunting. There were only a handful of girls in our chemistry year, perhaps 10% of the couple of hundred students. Our days were well defined, morning lectures, afternoons in the lab. One elderly Fellow could be relied on to give women A grades for their practical work. I'm afraid we made sure to seek him out.

Laboratory work with my personal tutor, the redoubtable Dr Muriel Tomlinson, in the organic Dyson Perrins, was a different experience. She would stalk the benches looking for sloppy practice and smeary glassware. When the culprit, usually male, protested that a flask was clean inside, "How do you know?" she would retort. The only mistake of mine that went uncorrected was a careless misspelling of phthalic acid throughout an essay.

Miss Tomlinson was a tall figure usually wearing a blue tweed suit (skirt not trousers then of course), with a pearl brooch on the lapel. She has related that she had been attracted to chemistry at school because the word conjured up a delightful blue colour for her. This colour-thinking or synesthesia is a rare condition, which may have inspired her choice of tweed.

She had been a brilliant student at Somerville, doing Part I in two years and getting a first. She was made a fellow of St Hilda's in 1946 and worked in the DP with Robert Robinson, on indoles and carbazoles. She was the only woman there at the time. We could not use her student text, Introduction to the Chemistry of Benzenoid Compounds, not published until 1971 (and still listed by Amazon). Despite her formidable aspect she was kind and helpful if students had family or financial problems.

We knew little of her outside interests, although I remember her buying a handsome mahogany table for her sitting room, and taking care of the strip of college garden edging the Cherwell. She was also said to drive to the opera at Glyndebourne with her friend Helen Gardner, the English don. They would find a handy barn on the way to Sussex where they could change into their evening dresses.

In 1958, St Hilda's acquired an inorganic chemist from Cambridge, the Scotswoman Margaret Christie. She was a gentle unflappable soul and it was with her that I did my Part II. One afternoon, sucking up 25ml of copper sulphate solution into a pipette, I lost concentration and got a mouthful. I washed out the bitter taste and thought no more of it until I was very sick in the middle of the night. Such an accident would be impossible now, I imagine. I realised that practical research was not for me and went off to edit abstracts and then became a science writer. I believe I was the only applicant for my first job, at the Zinc Development Association (motto:Think Zinc). Touring the brilliant new integrated undergraduate labs last year, many of us thought that we might like to start again and perhaps make different choices.

Judith Mirzoeff (Topper) 1956-60

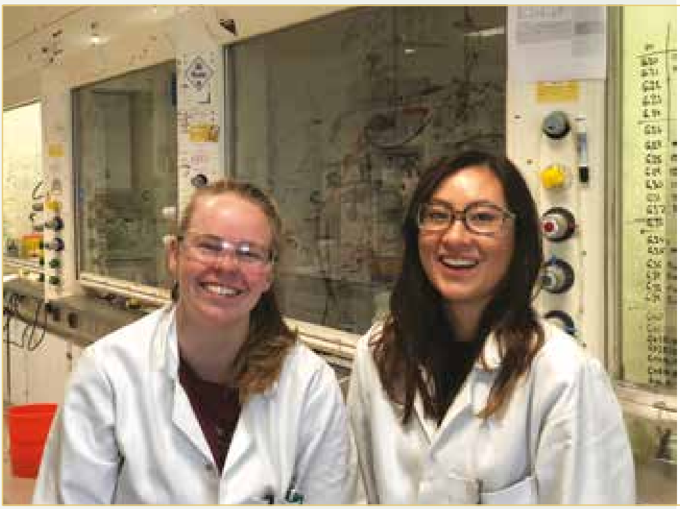
Oxford Women in Chemistry

This year, **Oxford Women in Chemistry** (OxWiChem) was founded by a group of DPhil students. The aim of our initiative is to celebrate and promote the work of women in chemistry, and encourage diversity and inclusion within the department. OxWiChem has three main goals: to promote the research and achievements of female chemists, to encourage an inclusive community within in the department, and to highlight the array of career opportunities available to graduate chemists.

Our inaugural seminar saw the department's own Professor Dame Carol Robinson give an inspirational and motivating talk about her career to a brimming audience! She captivated the audience by taking them through her unique career journey to academia, from leaving school at 16 to becoming the first female Professor of Chemistry at Cambridge, and later Oxford, and finally her current role as President of the Royal Society of Chemistry.

The OxWiChem inaugural seminar with Professor Dame Carol Robinson.

Since the inaugural seminar, we have coordinated various events for the department, notably hosting an IUPAC Global Women's breakfast event for the academic, administrative, technical staff and undergraduate and postgraduate students. We have forged strong links with chemical industry and recently hosted a virtual interactive workshop on implicit bias, run by Dr Rebecca Ruck, Executive Director of Process Research and Development, Merck. Keen to promote a variety of chemical careers, OxWiChem will be hosting a panel of female scientists from Pfizer later this year.



OxWiChem representatives Kathryn Leslie and Daniella Cheang.

One of the ways OxWiChem have been celebrating the achievements of women in the department and highlighting varying career-paths, has been through our twitter profile series. In this series, we feature profiles of women both currently working in the department or from part of our extensive alumni community. If you would like to read some of the profiles you can find them by searching **#OxWiChemProfiles on twitter.**

OxWiChem ultimately strives to form a supportive community, therefore we would love to hear from our alumni members, working across an array of sectors. If you are interested in taking part in our profile series or other initiatives, please get in touch with our President, Daniella Cheang, at our email address **oxwichem@chem.ox.ac.uk**.

If you would like to know more about us and what we are doing, please visit our website **http://www.oxwichem.co.uk**

2019 Ox WiChem OXFORD WOMEN IN CHEMISTRY

From the PCL to Pyongyang

Oxford Chemistry alumnus Professor Ian Wells (Worcester 1965) describes his extraordinary career.

I really enjoyed my chemistry studies at Oxford (1965-69) - although I was most comfortable with physical chemistry, better at analysis than synthesis and much preferred spending time at a laboratory bench to studying for exams! My tutor and mentor was Dr John Danby, and I especially recall one tutorial when he demonstrated how to decode a puzzle using a perspex rod.* My 'part two' was in his PCL mass spectrometry research group working on a new monopole radio-frequency mass spectrometer which had been built by the technical staff in the basement. This was a wonderful introduction to problem solving and 'getting things to work' which I have been able to draw on ever since.

After graduating I started my career as an industrial chemist in electrochemistry and photochemistry. In 1976 I joined the NHS as a clinical scientist - my wife Helen had made a similar move the previous year into NHS administration - as we both wanted to take relevant skills overseas to a needy country at some point in the future.

Getting a continuous flow analyser to work properly.

NHS Clinical Biochemistry laboratories in the 1970s employed both chemists and biochemists and almost all the assays were developed in-house. My early work was setting up and running assays, mainly using spectrophotometry, and included getting a new continuous flow analyser to work properly! This involved teaching myself Wang Basic to re-write the computer programme used to convert the analog output into results and led to my first conference paper.

In 1980 I moved from Epsom to the Guildford Hospitals and laboratory computing gradually took over most of my time. I was also able to study on day release for a PhD in the medical applications of Artificial Intelligence (AI) at the local University of Surrey where I was its first ever computer science student. As analysers became smarter and were able to calculate their own results my focus changed to interfacing (not as easy as it sounds in those days!), networking and developing clinical laboratory information systems using advanced software tools. I was fortunate to be a pioneer in this new field and was able to publish a number of papers and lecture at conferences in the UK, Europe and the US.

In the mid-1990s I moved to the Medical Physics department to lead a medical computing section developing clinical databases and setting up large scale cluster computing and storage systems for digital images. I was also invited back to the University of Surrey as a part-time lecturer in Artificial Intelligence where I was able to draw on both my PhD research and my experience in medical decision making. I was subsequently appointed a Visiting Professor in 2005 and then an Emeritus Professor in 2014.

My wife and I both retired at the end of 2011 after working for almost 70 years between us in the NHS and, as the gap year had not been

Ian and his wife Helen walking on the Antarctic mainland in February 2013.

Ian and Helen at Pyongyang Friendship Hospital.

invented when we graduated, we decided to take a 'senior version' and indulge our passion for travelling to remote places. Our goal was 'pole to pole' and we duly crossed both 80ºN, reaching Moffen Island which is 'the end of the earth' for Europe and Asia, and 68ºS after negotiating Drake's Passage and walking on the Antarctic mainland. In addition to polar bears and penguins the third 'P' for the year was Pyongyang, the capital of DPR (North) Korea, where I had been invited to give a series of lectures on AI at the English-speaking Pyongyang University of Science and Technology (PUST).

Despite the practical challenges, we did not hesitate when we were invited to join the long term staff at PUST and to use our skills to help the people of this needy but hauntingly beautiful and friendly country. Initially we were both lecturing, and then in 2015 we were invited to become directors of the new medical school being established on the PUST campus. This was a wonderful opportunity to put our NHS experience to good use, visit local hospitals and attend weekly UN Development Programme meetings.

We worked at PUST for six years until we retired (again!) in 2018, and later that year three PUST graduate students came to study at the University of Surrey for six months. Shortly before they returned home they spent a memorable day in Oxford which included a tour of the new Chemistry Teaching Laboratories – they later said this was one of the highlights of their time here. The DPRK authorities are keen for more graduate and research students to spend time in the UK and we are hoping that some may indeed find suitable placements at Oxford Chemistry.

Looking back over the years I never strayed too far from chemistry, although my work as a clinical scientist moved from performing assays to devising systems for the storage, distribution and interpretation of the results. One of my responsibilities at PUST was setting up a small clinical laboratory on the campus – so my career actually came full circle and ended, where it began, with practical bench chemistry!

Professor Ian Wells

Ian lecturing to third year science undergraduates at PUST.

* *I still use this example in my AI lectures - so here is your challenge: what is the problem and the solution? The clues are in the text and you need to use capital letters and colours for the problem.*

The Centenary of the DPhil

Thank you to all those who have responded to the Department's Centenary Campaign to celebrate one century since the completion of the first DPhil in Oxford Chemistry. We have heard from alumni all over the world, with stories of their time in Oxford, advice for current and future students, and wonderful tributes to supervisors for all the support and guidance they provided. We are also extremely grateful for the generous donations that alumni have been making, which will help us proactively support the next generation of DPhil students in the Department.

Given the nature of chemistry research, every Oxford Chemistry student has a unique experience. One thing that unites all those who have studied here over the past century is resilience. From working tirelessly to repeat experiments in the quest for replicable data, to the long hours in the lab and the challenges of publishing papers, chemists certainly don't give up at the first hurdle.

Earlier this year, however, Oxford Chemistry students were tested in a new way – with the temporary closure of the laboratory buildings. They showed (and continue to show) great resilience in response to this unprecedented challenge.

They have managed to keep driving forward important work and (in the case of Part II and DPhil students) have continued to fulfil their roles as crucial members of their groups. They are using their creativity and curiosity in new ways to push boundaries with their research. They are using chemistry to help address major global challenges, such as COVID-19, food security, antimicrobial resistance, the

critical need for more sustainable energy, the plastic waste crisis, and many more. They are engaging with the public to shine a light on the vast potential of chemistry research. They are fuelling dialogue to catalyse equality and diversity in research settings. Like their predecessors, today's Oxford Chemistry students really are shaping our future, in the Department and far beyond.

There is always difficulty associated with finding funding for students, something that is truer this year than ever before. We are very grateful to all the members of our alumni community who have made generous contributions to our Centenary Fund so far, which will enable us to support outstanding students and their research during this period of uncertainty and upheaval.

While some challenges may still lie ahead, we have no doubt that our current and incoming students will have a successful academic year. As a Department we will do everything we can to facilitate this. We hope to celebrate the centenary with you in person at some point in the future, and look forward to sharing with you updates on some of the students who benefit from our Centenary Fund over the course of the coming academic year

Will you share your story?

Please do get in touch to share memories of Oxford Chemistry or offer your words of wisdom to today's students – we would be delighted to hear from you. We'd also love to see any photos you might have from your time in the Department.

Will you help shape the future for Oxford Chemistry students? Will you make a gift towards our Centenary Campaign to help support outstanding students and their research? You can make a gift online at **development.chem.ox.ac.uk/centenary-campaign**, or get in touch using the details below. You can also return the enclosed form, but please note with current restrictions there may be a delay in processing gifts made by mail. We are extremely grateful for all donations, which make a real impact to the lives of Oxford Chemistry students. There are many other ways to support students as well – perhaps you'd be interesting in mentoring, offering an internship. Please contact us to learn more.

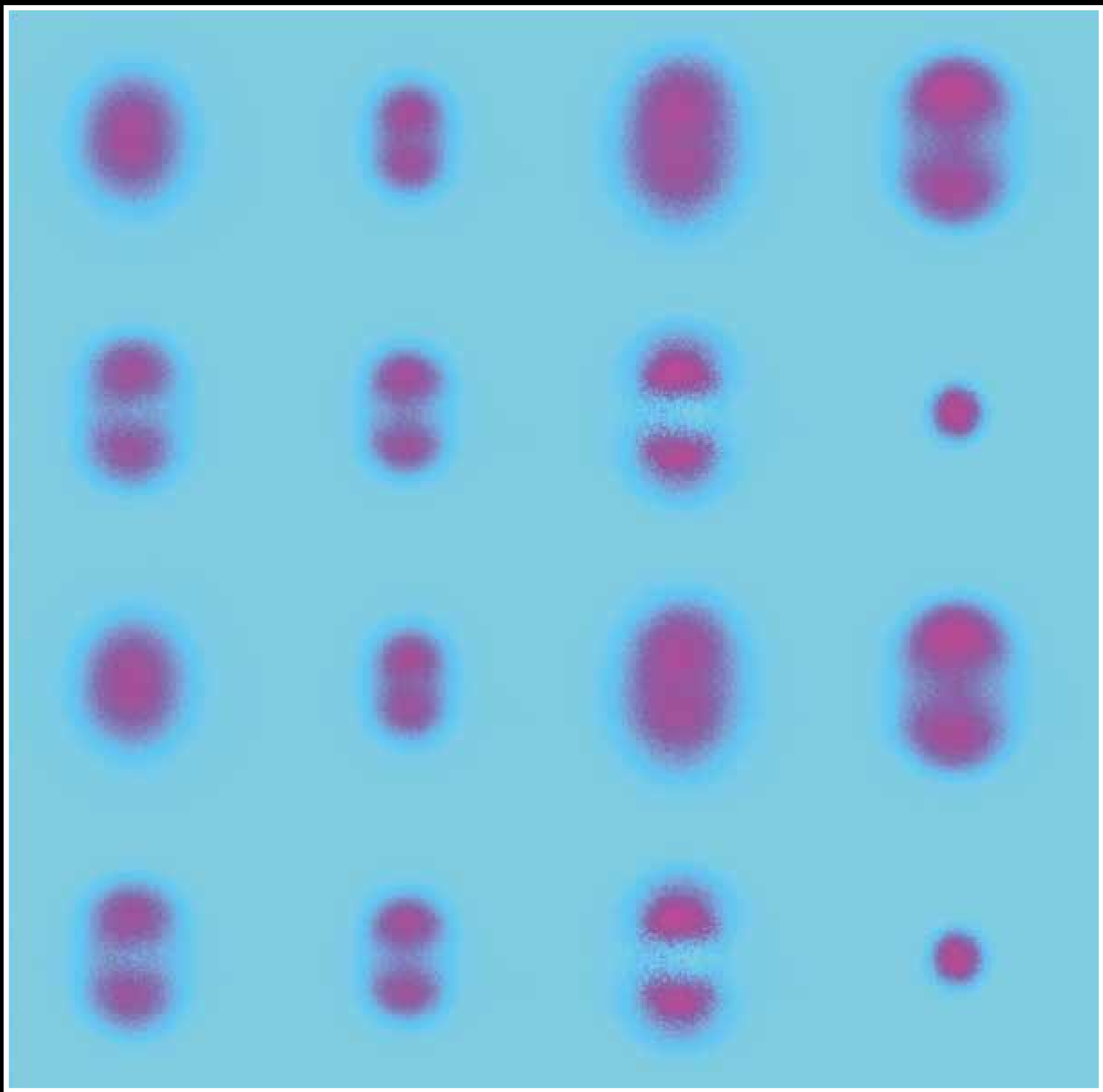
To share your memories or to support Oxford Chemistry students, please contact Jane Rice in Chemistry's Development & Alumni Relations Office:

jane.rice@chem.ox.ac.uk

+44(0)1865 275 093

Physical & Theoretical Chemistry Laboratory,
South Parks Road, Oxford OX1 3QZ;
or by using the enclosed form.

Results from Divya Popat's research in Claire Vallance's group: velocity-map images of the scattering distributions for the products of dimethylformamide photolysis at 193 nm.



Contact us

www.chem.ox.ac.uk

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

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