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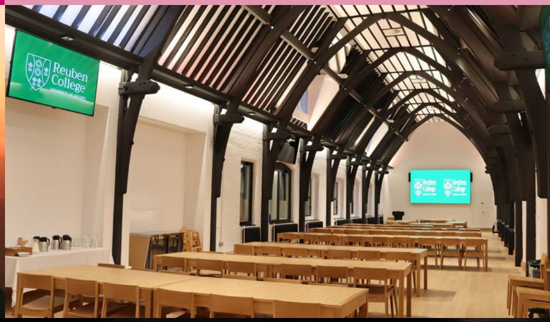


Periodic

Magazine of the Department of Chemistry

Counting electrons for catalyst screening *p.6*

UNIVERSITY OF OXFORD

DEPARTMENT OF CHEMISTRY

Issue 12
2024 – 25

From the Head of Department

It is a pleasure to welcome you to another edition of Periodic, and to introduce you to some of the developments in the Department over the past year. It has been a privilege to have had a ring side seat as we've watched the year unfold, and I hope you'll share our excitement in the way things are going.

The staff, students and alumni in the Department have continued to uphold Oxford's tradition of excellence in many ways: you'll find some of their stories in this issue, and can rest assured that they are only the tip of a large iceberg. Our academics and researchers have continued to produce world class research, publishing around 500 papers a year, and contributing a quarter of the University's patent filings. It has been a year of individual and collective achievement with a clutch of prizes and awards to staff and students highlighted later in this issue.

Since the last issue of Periodic, we've welcomed a number of new staff to the department, broadening our repertoire and bringing strength in new areas. Profs Matthew Fuchter, Anna Regoutz and Yimon Aye have joined the department as new tutorial fellows, while Dr Daniel Congrave has recently arrived on a Royal Society University Research Fellowship. We've also seen a familiar face move into a new role. Prof Charlotte Williams has been appointed as statutory Professor of Inorganic Chemistry, while also leading the new national hub for sustainable chemistry and materials manufacturing. This has coincided with the end of her term as Associate Head of Department for Research, and Prof Andrew Goodwin has stepped into the role.

Chemistry has the power to explain the world around us, and to change it for the better. We believe that harnessing that power requires us to extend the understanding of fundamental chemical principles to the point where they can be exploited properly. If we are to do that, we need to train the coming generations of chemists to assess information, explore the unknown, and exercise their own creativity. As I type this, Nobel Prizes are being awarded for machine learning and artificial intelligence. The coming cohorts of our graduates will face ways of working that my own generation did not have to worry about, but we intend to ensure they are well prepared. It is already clear that automation and machine learning will need people who can define the problem, understand the output, and deploy their own creativity. Our aim is to nurture these skills, and to give opportunities to the best candidates. We're privileged to have been awarded two new Centres for Doctoral Training this year: the Inorganic Materials for Advanced

Professor Stephen Faulkner

Manufacturing Centre for Doctoral Training welcomed its first cohort this year, while that in Chemical Synthesis for a Healthy Planet is recruiting its first cohort to start in October 2025.

These are some of our early steps in addressing the challenges that face society. In a time of economic stress and limited resources, the time is ripe for chemists to personalise medicine and diagnosis, and to reinvent the chemical industry – switching the feedstocks away from fossil fuels and developing methods that can use simple compounds (including CO_2) as raw materials. I hope that I'll be able to tell you more about this next time I write.

We're always delighted to hear from members of the Oxford Chemistry family. It has been a pleasure to meet many of you this year at events in Oxford and elsewhere.

I hope that you'll enjoy reading this issue. ■

Contents

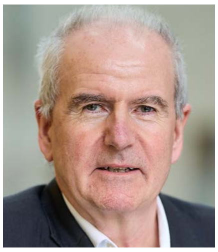
News and achievements

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

Four chemists from Oxford University have won prizes from the Royal Society of Chemistry this year, in recognition of their brilliance in research and innovation. The awards are among the oldest and most prestigious research prizes in the world, having recognised excellence in the chemical sciences for more than 150 years.

Prof Harry Anderson received the Pedler Prize for his work directed towards creating molecular compounds with unprecedented properties, and changing their molecular architectures to achieve desired characteristics. A particular interest is in large organic molecules that allow the flow of electrons over distances of several nanometres.

Prof Robert Hoye was awarded the Beilby Prize for research at the interface of chemistry, materials science, and engineering. His work focuses on developing new light-sensitive materials for renewable energy applications and healthcare imaging technologies. This year Prof Hoye was also awarded a Senior Research Fellowship by the Royal Academy of Engineering.



Prof Dermot O'Hare received the John B Goodenough Prize for his work towards finding solutions to global issues relating to energy, zero carbon and the circular economy. His group has five strategic research themes: circular economy, carbon dioxide management, green hydrogen, low carbon feedstocks, and materials for environmental sustainability.

Prof Angela Russell received the Jeremy Knowles Award, for outstanding contributions made by a mid-career scientist working at the chemistry and life science interface. Professor Russell's research seeks to develop an effective drug to treat children with the fatal muscle-wasting disease Duchenne muscular dystrophy (DMD) through increasing the levels of utrophin, a muscle protein.

Prof Dame Carol Robinson FRS received the Lifetime Achievement Award from the European Patent Office. The award recognises Professor Robinson's ground-breaking work in mass spectrometry, advancing drug discovery, and personalised medicine.

Prof Simon Aldridge FRS was elected Fellow of the Royal Society. He said: "I'm extremely happy that the group's work has been recognised in this way by the Royal Society – all the more so, given the fundamental nature of much of the science that we do. Most importantly, it is recognition of the dedication and inspiration of the exceptional students and co-workers with whom I have had the privilege to work over the past 25 years."

Prof Véronique Gouverneur FRS received the Davy Medal in this year's prizes from the Royal Society. She was also among four Oxford researchers awarded major European Research Council Advanced Grants this year. Prof Gouverneur will use this to develop ground-breaking new methods for fluorine chemistry that will convert naturally occurring fluorspar into critically needed fluorine-containing molecules.

The recipients of the inaugural SCGC–First awards were announced, marking a significant milestone in Oxford University's collaboration with SCG Chemicals Public Company Limited. Recipients included Profs Grant Ritchie and Dermot O'Hare (photo in previous column) for a pilot programme on the interaction of cold atmospheric plasma with size-selected catalyst precursors for plasma enhanced catalysis, and Prof Edman Tsang who will investigate efficient ammonia synthesis at mild conditions over tailored oxide catalysts.

Prof Fernanda Duarte was one of the finalists in this year's Blavatnik Awards for Young Scientists in the UK. The prestigious awards celebrate the past accomplishments and future potential of the UK's most innovative young scientists and engineers.

Prof Darren Dixon was announced as the 2024 recipient of the Charles Rees Award for excellence in the field of heterocyclic chemistry, awarded by the Heterocyclic and Synthesis Group of the RSC. He received this award for his "innovative and creative work on structurally complex heterocyclic alkaloid natural product synthesis".

Profs Ludmilla Steier and Yujia Qing both received European Research Council starting grants in late 2023. Prof Steier's work is on next-generation photocatalysts that efficiently synthesise energy-dense chemicals with sunlight. Prof Qing aims to establish a general method to identify protein variants containing different patterns of post-translational modifications.

Dr Craig Campbell, Departmental Lecturer in Practical Chemistry, was awarded a Mathematical, Physical and Life Sciences (MPLS) Divisonal Teaching Award. Craig was described in his citation as "a truly exceptional teacher, who cannot do enough for his students". Dr Alan Roth, a Visiting Lecturer in Chemistry, also received an award for his Scientific Entrepreneurship Course.

Prof Hagan Bayley FRS was awarded the Buchanan Medal in the 2023 Royal Society prizes. The award recognises Prof Bayley's role in founding the highly successful biotech company Oxford Nanopore.

Nenad Vranješ, former manager of the Department's electronics workshop, was awarded an Honorary MA by the Vice-Chancellor. Nenad retired in July 2022 after 44 years of service to the Department of Chemistry.

Dr Clare Rees–Zimmerman, a Junior Research Fellow in Dirk Aarts' research group, was awarded the 2023 Katharine Burr Blodgett Award for best PhD thesis in colloid and interface science. Her PhD thesis investigated the microscale motion of particles dispersed in fluid, addressing the need to make functional materials more sustainable by using less of the expensive components while still delivering the required properties.

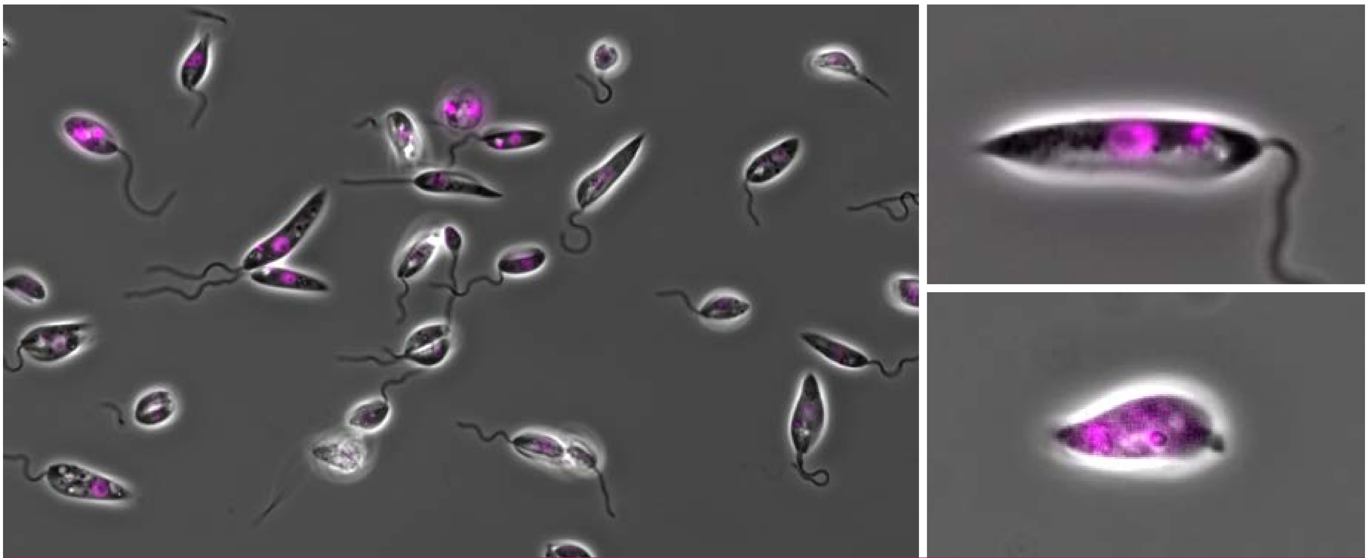
Veronika Juraskova (Duarte group) and Jan Christoph Thiele (Kukura group) received Schmidt AI in Science Fellowships. The programme aims to accelerate the next scientific revolution by supporting talented postdoctoral scholars to apply artificial intelligence techniques across the natural sciences, engineering and mathematics.

Aleksy Kwiatkowski, Anna Miller, and Matthew Southern, three graduate students from the Department, were awarded Industrial Fellowships by the Royal Commission for the Exhibition of 1851. Industrial Fellowships are awarded to graduates with the potential to make an outstanding contribution to industry, for research supported by a company, leading to a patent, product or process improvement and a postgraduate award.

The Department's master glassblower, Terri Adams, was featured in BBC Two's *David and Jay's Touring Toolshed* earlier this year. As well as showcasing some of her scientific glassware, Terri was able to show the team her artistic projects, including a cricketer sculpture and a breathtaking plasma illuminated dragon. ■

New research

Frederica Butler reports on some of the latest stories from the Department



Microscope images of Leishmania parasites, with the cell nucleus and kinetoplast (mitochondrial DNA) stained in purple. The zoomed in images show examples of parasites before (top) and after (bottom) treatment.

Developing effective antiparasitic drugs

Oxford team synthesises alkaloids as potential treatments for neglected tropical diseases

doi.org/10.1021/jacsau.4c00007

Visceral leishmaniasis and Chagas disease, both classified by the World Health Organisation as neglected tropical diseases, affect millions of people worldwide and are fatal if not treated properly. Unfortunately, existing treatments have limited effectiveness and are highly toxic toward healthy cells. Couple this with a lack of approved vaccines, as well as the emergence of drug resistance, and the urgent need for safe and effective new drug candidates for both diseases is clear.

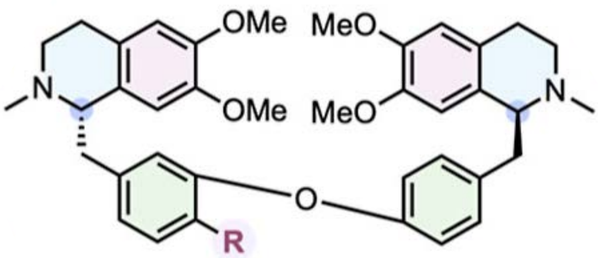
DPhil researchers Ana Sozanschi and Hannah Asiki from Ed Anderson's group, in collaboration with the Butantan Institute in Brazil and Oxford's Nuffield Department of Medicine, have synthesised a series of alkaloids in the benzyltetrahydroisoquinoline (BI) family as potential drug candidates against the parasites responsible for visceral leishmaniasis and Chagas disease. Excitingly, three of the synthesised alkaloids meet the Drugs for Neglected Diseases initiative criteria for a 'hit' against Chagas disease.

The researchers report in a study published in *JACS Au* the synthesis of 14 BIs and 12 (bis)benzyltetrahydroisoquinolines (BBIs). They screened these compounds for biological activity against forms of the relevant parasites that live inside, and outside, cells.

The amount of each compound required to kill 50% of the parasites (known as the IC50 value) was compared to the toxicity towards healthy cells (CC50 value). For an ideal drug candidate, the selectivity index – ratio of CC50/IC50 – should be as high as possible, meaning that the compound is potent against the target parasite (low IC50) while not harming healthy cells (high CC50).

Achieving a high selectivity index (a value above 10) is notoriously difficult, and none of the BIs or BBIs tested were suitable against Visceral leishmaniasis. However, three of the compounds could be classified as hits against Chagas disease, showing a selectivity index above 10. In addition, the three successful compounds had relatively short synthesis procedures, with fewer than 8 steps, and were active at concentrations below 10 micromolar.

The researchers conducted preliminary studies to understand the mechanism of action of the most promising alkaloids on a related



Example of the class of BBI alkaloids that the team synthesised in this study.

parasite, which is responsible for a more common form of leishmaniasis. Light microscopy also revealed a change in the shape of the parasite cells when they were treated with the alkaloid. Further investigations revealed that these changes were due to cell cycle interference and incorrectly replicated organelles.

"Natural products are well-recognised as sources of new medicines, but the relationship between their structures and bioactivity properties, and their mechanisms of action, are often unknown" commented Prof Ed Anderson. "We are excited to contribute to potential treatments of these debilitating diseases not only with the BI family, but also other natural products that can be readily accessed and varied through chemical synthesis."

The team's study provides a basis for the development of new, and much needed, antiparasitic agents against diseases such as leishmaniasis and Chagas. Further work will focus on examining how the most promising alkaloids interact in the body, as well as gaining a deeper understanding of their mechanism of action. ■

As easy as counting to ten

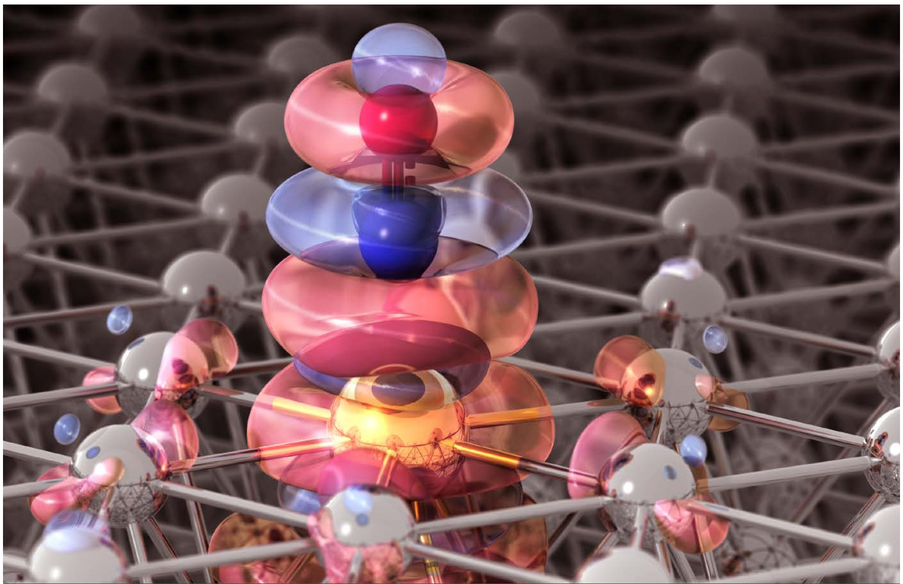
Counting electrons for rapid alloy catalyst screening

doi.org/10.1038/s41557-023-01424-6

Single-atom alloys (SAAs) are made by embedding a dopant, like rhodium, into a host metal such as copper at ultra-high dilution. SAAs can catalyse challenging reactions relevant to sustainable chemicals and fuels manufacturing much more effectively than single metals. Over the past decade, the Stamatakis group has worked closely with colleagues in UCL, Cambridge, and Tufts University (USA) to predict and demonstrate these materials' catalytic properties.

In a recent study published in *Nature Chemistry*, the team analysed large datasets and found that adsorption energy trends on SAAs follow a "10-electron-count" rule. This rule not only explains the origin of their catalytic activity but can also be used for rapid computational screening of promising SAA catalysts for future chemical transformations.

The 10-electron-count rule uses an intuitive molecular orbital (MO) approach to predict the adsorption strength between an adsorbate, which could be atomic (such as H, O and N) or molecular (such as CO and NO), and the metal dopant on the SAA. The team use computational methods to show that the adsorbate-dopant interaction is strongest when the number of valence electrons on the metal dopant and the number of valence electrons on the adsorbate that interact with this dopant, sum to ten. This electron count corresponds to filling all the bonding and non-bonding orbitals, without filling any of the antibonding orbitals, in the MO diagram for the system.



NO molecule adsorbed onto a single atom alloy surface, with electron density shown in cyan and blue.

Using the 10-electron-count rule could help to develop a more targeted approach to designing better catalysts for various important chemical processes, such as ammonia synthesis. The team used their rule to predict that rhenium would be the most promising dopant in a gold-based SAA catalyst for reducing nitrogen to ammonia. This conclusion is in line with predictions from much more expensive and demanding machine-learning studies.

"While we have previously generated lots of data on the catalytic behaviour of SAAs, physical chemistry-based explanations were lacking. We are very excited to report such a simple and elegant principle explaining SAA reactivity" says Prof Michail Stamatakis.

This intuitive and simple rule can be used to establish a clear guide, for both theoreticians and experimentalists, to support the design of more efficient catalysts for industrially relevant processes, without the need for expensive and complex simulations. ■

Molecular sensors

A dynamic and selective optical chloride ion detector

🗎 doi.org/10.1002/chem.202400952

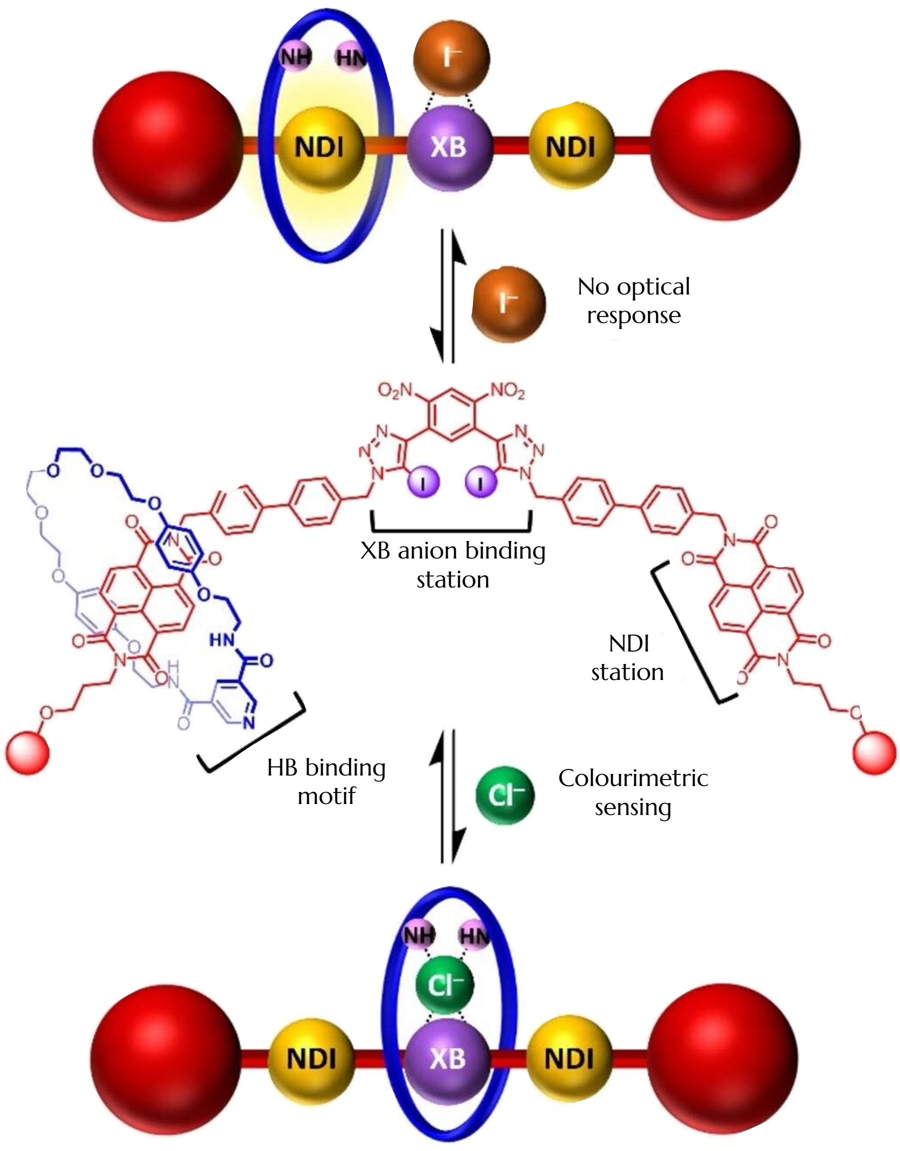
The ability to selectively detect different anions is pertinent to a wide range of environmental, medicinal and industrial applications. In particular, the development of sensors capable of distinguishing between chemically similar halide ions, such as chloride and iodide, is desirable due to the critical role played by these ions in different aspects of human health.

Researchers in Paul Beer's group have been developing 'mechanically interlocked molecules' that are strategically designed to change conformation in response to certain external stimuli.

In a recent study published in *Chemistry: A European Journal*, the researchers report a mechanically interlocked molecule capable of selective optical sensing of chloride ions over iodide ions.

The molecule of interest is a 'rotaxane', which contains a central axle threaded through a cyclic molecule (macrocycle), and stoppers on each end to prevent dethreading of the macrocycle. The rotaxane synthesised in this work contains various stations along the axle – two peripheral naphthalene diimide (NDI) stations, where the macrocycle resides, and a halogen-binding (XB) station in the middle.

The researchers examined the response of the rotaxane to addition of anions using ^{1}H-nuclear magnetic resonance (NMR) spectroscopy. When chloride ions were added to a solution of the rotaxane, the NMR response indicated that both the macrocycle and axle components participate in chloride binding, whereas iodide ions appear to interact only with the axle binding groups. The ultraviolet/visible light spectrum of the bare rotaxane contained a characteristic absorption band at 450 nm, which significantly decreased in intensity when chloride ions were added, with no change observed with iodide ions.



Representation of the rotaxane as a selective optical sensor for chloride over iodide anions. Adding iodide ions has no effect, whereas chloride ions shift the position of the macrocycle along the central axle, detectable by spectroscopy.

Analysis of the spectra implies a movement in the position of the macrocycle from the NDI station to the XB station on addition of chloride ions, forming an interlocked cavity around the XB station with chloride encapsulated at the centre. Iodide ions, however, are too large to fit in this cavity, so the macrocycle remains at the NDI station and no chemical or optical responses are observed.

Hui Min Tay, the lead researcher on this study, says "in the Beer group, we use our understanding of seemingly simple intermolecular interactions like hydrogen bonding and halogen bonding to construct sophisticated molecular machines with potential applications in ion recognition and sensing. It is an exciting field of research that combines scientific investigation and creative molecule design."

This work illustrates the potential of mechanically interlocked systems for anion recognition and sensing. The mechanical bond effect and the dynamism unique to these systems is cleverly exploited to distinguish between chemically similar ions. ■

Hydrogen fuel from seawater

Developing efficient catalysts to generate clean power from our oceans

doi.org/10.1038/s41929-023-01069-1

When hydrogen combusts it releases a great deal of energy, producing only water as a byproduct. As such, hydrogen shows promise as a clean fuel to support a global shift towards sustainable energy and net zero emissions.

To achieve this, it is important that the hydrogen we consume is produced in a climate neutral manner. One option is to use catalysis to convert water back into hydrogen and oxygen, powered by sunlight.

Researchers in the Edman Tsang group at the University of Oxford, in collaboration with teams in China, Hong Kong, the Diamond Light Source and the Department of Physics, have been investigating robust photocatalysts that can use heat and sunlight to split seawater into hydrogen and oxygen.

A recent publication in *Nature Catalysis* details their titanium dioxide (TiO_2) photocatalyst, doped with nitrogen and platinum nanoparticles, which shows improved catalytic activity for the splitting of seawater, relative to freshwater. This result is particularly exciting when you consider that the vast majority of Earth's water is found in seas and oceans, with freshwater supplies becoming depleted worldwide.

At elevated temperatures, the team's catalyst successfully promotes the splitting of natural seawater – sourced from Bournemouth pier – as well as a range of artificial compositions that replicate water from locations such as Lop Nor in China, the Great Salt Lake and the Dead Sea. The highest catalytic activity (measured by quantity of hydrogen released per gram of catalyst per hour) was recorded for the saltiest (or most electrolyte-rich) water from the Dead Sea.

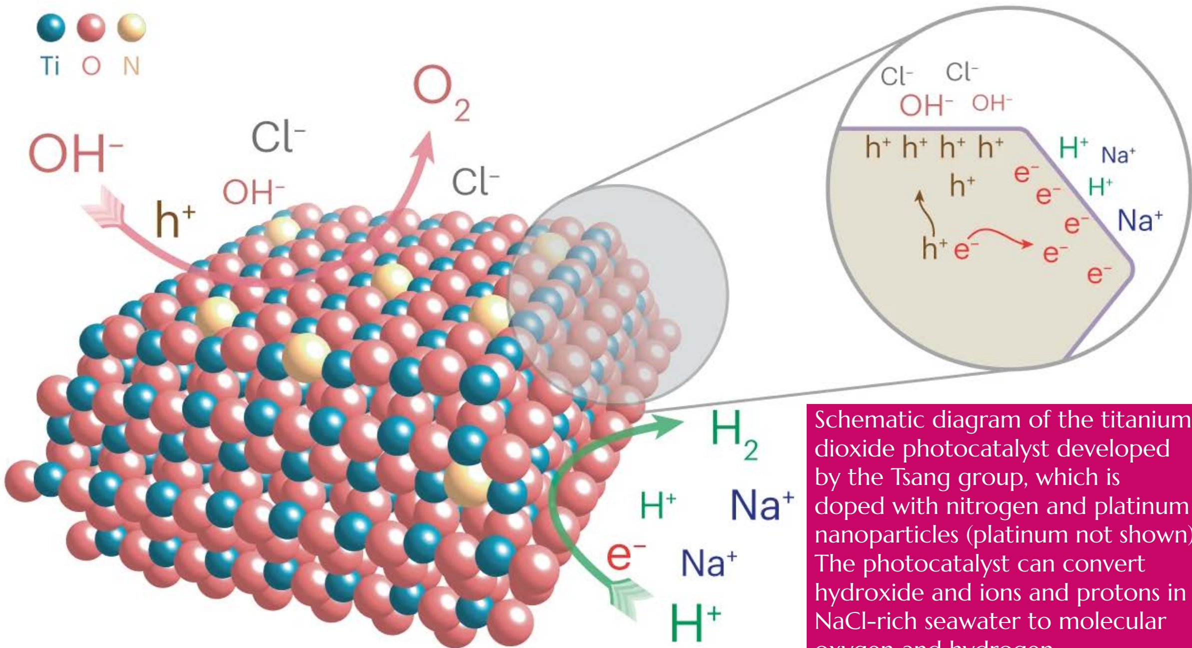
"We anticipate a potentially more efficient scenario for the future practical application of this system, wherein heat is provided by concentrated solar light rather than an external electrical heating device," said Prof Edman Tsang.

"The development of a larger solar heating system is also underway, and we are trying to recycle the heat stored in the superheated water as well," added Yiyang Li, one of the researchers on this study.

TiO_2 photocatalysts work by absorbing light to generate charge carriers (negatively charged electrons and positively charged electron-holes). These light-generated charge carriers promote reactions on the catalyst surface that enable water splitting to occur. However, charge carriers can also recombine, releasing energy as heat or light, which reduces catalytic efficiency.

In the recent report, the Tsang group researchers use a range of spectroscopic and imaging techniques to suggest that the high sodium and chloride ion content in seawater suppresses undesirable charge carrier recombination. The sodium and chloride ions polarise the surfaces of the photocatalyst particles, helping to separate charge carriers via electrostatic interactions in an effect referred to as electrolyte-assisted charge polarisation.

Excitingly, the 20% solar-to-hydrogen conversion efficiency achieved by the reported photocatalyst for artificial Dead Sea water far exceeds the minimum goal set by the United States Department of Energy for practical application of these systems (which is 10%). This study therefore represents a significant development in the field of green hydrogen generation from photocatalytic water splitting. ■



Schematic diagram of the titanium dioxide photocatalyst developed by the Tsang group, which is doped with nitrogen and platinum nanoparticles (platinum not shown). The photocatalyst can convert hydroxide and ions and protons in NaCl-rich seawater to molecular oxygen and hydrogen.

Profile: Professor Meera Mehta

Meera Mehta was born and raised in Toronto, Canada. She completed her undergraduate studies at McMaster University and a PhD at the University of Toronto before coming to Oxford in January 2018 to undertake postdoctoral work with Professor Jose Goicoechea. Meera moved to the University of Manchester in January 2020 to become lecturer in Inorganic Chemistry and establish her independent research career. She returned to Oxford in January 2024 as associate professor and leads a young, dynamic research group.

How would you describe your research?

We're interested in finding applications for sustainable elements in catalysis. Usually when we perform catalysis to manufacture goods like plastics, fertilizers, pharmaceuticals and so on, the catalysts used are expensive transition metals and noble metals, such as platinum, palladium and iridium. That is not sustainable – not only because these metals are not highly abundant in the earth's crust, but also because there are geopolitical issues around how they are sourced, due to where they're located. As these resources become less available, the costs associated with mining them – both fiscal and environmental – are only getting worse and worse.

So, part of what my research group in doing is building catalysts that allow us to make everyday commodities using highly-abundant elements like aluminium, phosphorus and boron. The particular types of transformations I'm interested in are reactions where we can recycle greenhouse gases into something useful. We're taking sustainable catalysts and performing reactions with greenhouse gases to convert things like carbon dioxide into either clean fuel sources, or into C-1 building blocks that allow us to make everyday molecules.

So you can use these catalysts to turn carbon dioxide into something useful?

Yes, that's right. There are basically two avenues in CO_2 chemistry: one is capture – but the problem with capture is that the sheer amount of CO_2 we would have to capture and store would not be sustainable. The other avenue is to convert carbon dioxide into something useful. If we can convert it back into a potential fuel source or something that we can do chemistry with, then it's a way to try and close the carbon cycle. Of course, there still many problems – how to make the process economic, how to obtain reasonable turnovers, how to get things to operate in the real-world environment – and all these will need to be solved. What my group focuses on is the fundamental research that provides proof of concept.

What's next for you and your group?

We're continuing to work with greenhouse gases. One of our first projects was converting CO_2 to a methanol surrogate, and we're also thinking about how we could convert CO_2 to higher-chain carbon products. We're also looking at how we could recycle non-CO_2 greenhouse gases like carbon monoxide and N_2O. How could they be recycled, and how could we do that selectively, i.e. how can you make sure you're only reacting one greenhouse gas in the presence of others? We're looking at all these questions.

We're also looking at how we take what we've learned from cluster chemistry to better design heterogeneous catalysts, which are the kind of catalysts that tend to be favoured by industry when making bulk commodities. Whereas homogeneous catalysts are in solution – in the same phase as everything else – heterogeneous catalysts are outside of that phase. Heterogeneous catalysts are easier to separate, they're more robust, and they're recyclable, so industry has a preference for them, but the problem with heterogeneous catalysts is that they're often difficult to smart design because a lot of the time we don't know their mechanism of action, so they can be difficult to study. I am interested in knowing about the catalysis of clusters but also in understanding the mechanisms of how these clusters do what they do, to provide insight into how we build better heterogeneous catalysts.

So now as a group we're pursuing two main avenues – expanding into heterogeneous catalysis and thinking about other transformations too.

How does it feel to be back in Oxford, and what do you like most about being here?

It's great to be back. I think the best thing about being here is that you're just surrounded by some of the most thoughtful minds – people who are really on top of their game, and people who really want to spend time on taking on interesting problems. For me, that is what's so inspiring to be around every day. ■

New professors

We were delighted to welcome three new members of academic staff this Michaelmas

Yimon Aye

Yimon joined us from the École Polytechnique Fédérale de Lausanne, with a research programme focused on understanding reactive small-molecule-driven cellular communication processes. Her work is of relevance to human health, and she and her team are working to develop novel therapeutic and technological interventions.

Yimon said: "Personally, coming to Oxford marks a homecoming after 20 years. I am ready to take on new research directions, new challenges/risks/opportunities, and do everything I can to give back, which gives me an enormous sense of personal fulfilment beyond scientific and pedagogical aspirations."

Matt Fuchter

Matt Fuchter joined us from Imperial College London. His research uses chemical synthesis and physical science innovation to invent new methods, molecules and materials to advance chemistry-led modern science.

Key themes in the Fuchter group's research are: the development of photoswitchable molecules and materials; chiral materials for technological applications; and the science of drug discovery.

Matt said: "As a highly collaborative scientist I am really excited about all the new partnerships that will develop with other researchers at Oxford."

Anna Regoutz

Anna joined us from UCL. She leads an interdisciplinary team of experimentalists with expertise in thin film synthesis, surface and interface chemistry, and X-ray photoelectron spectroscopy. Her research covers four key areas: Hard X-ray Photoelectron Spectroscopy; sol-gel methods for thin films; materials and interfaces in power electronics; inorganic materials for biosensors.

Anna said: "I am excited to meet the students and colleagues in the Department of Chemistry who make it such an inspiring workplace, and I look forward to contributing to the strong solid state and materials chemistry community." ■

Inorganic Materials for Advanced Manufacturing

This new doctoral training centre, known as IMAT, builds on the success of the current OxICFM programme (Oxford Inorganic Chemistry for Future Manufacturing). IMAT will focus on designing, synthesising and characterising inorganic materials, from batteries and solar cells to catalysts and polymers. It will equip scientists with the tools to address critical societal challenges in the manufacturing sector.

A strong industrial component throughout the taught elements of the course, internships in industry, and a doctoral research project in a field of interest, will mean the training is relevant to a range of different business sectors and sizes.

Prof Simon Aldridge FRS, IMAT Director, said:

“The new CDT in Inorganic Materials for Advanced Manufacturing offers a fantastic opportunity for students who are interested in the fields of inorganic chemistry and materials science to obtain a world-class training delivered by a team of leading academic and industrial experts.”

Chemical Synthesis for a Healthy Planet

CSHP aims to address some of the most serious challenges facing humanity over the coming decades, including the rising needs for clean energy, food, medicines and materials. Most chemical production processes are highly energy intensive, requiring fossil fuels and rare metals and producing colossal amounts of waste.

Synthetic chemists trained through CSHP will learn cutting edge chemical synthesis, while embedding circular and sustainable chemistry into their work. Students’ doctoral projects will develop innovative, sustainable chemical strategies within pharmaceuticals, agrochemicals, and materials chemistry contexts.

Prof Michael Willis, who leads the CSHP programme, said:

“The new CDT in Chemical Synthesis for a Healthy Planet is a ground-breaking programme that will target the training of synthetic chemists in cutting edge chemical synthesis, while intrinsically embedding circularity. It will revolutionise the training of the future synthetic chemistry workforce, equipping UK industry with the skills in sustainable chemical innovation that it urgently needs.”

Making our chemical future

Training the next generation of chemistry researchers

In March this year, two new doctoral training centres based at Oxford Chemistry were announced by the UK’s Engineering and Physical Sciences Research Council (EPSRC). These two programmes focus on training doctoral scientists to design and synthesise the materials and chemicals humanity needs in order to secure a healthy, sustainable future.

IMAT is a joint endeavour run by Oxford’s Departments of Chemistry and Materials, including a team of over 60 academics from a range of disciplines and 19 companies and national facilities. CSHP is a collaboration between Oxford’s Department of Chemistry and the University of York’s Green Chemistry Centre of Excellence, with partnerships with a wide range of small and medium-sized enterprises. Applications to both programmes are currently open. For more information, see imatcdt.chem.ox.ac.uk and cshp-cdt.chem.ox.ac.uk. ■

New method detects fake vaccines

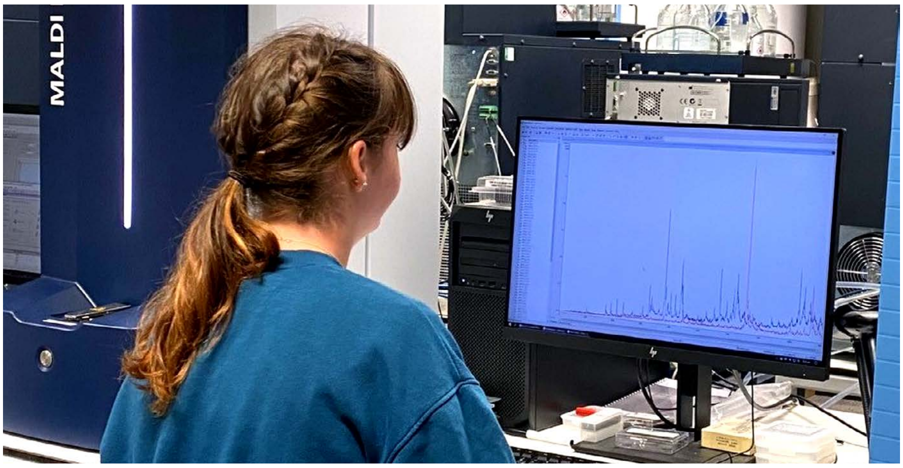
An Oxford team has developed a novel method for vaccine authenticity screening. The first of its kind method, which uses machine learning, was developed by a collaborative team of chemists, biochemists and medics.

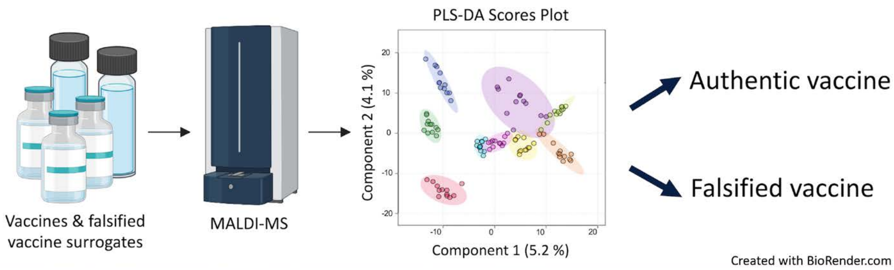
The team's method uses clinical mass spectrometers already present in hospitals, making the approach feasible for global supply chain monitoring. Their discovery offers an effective solution to the rise in substandard and counterfeit vaccines threatening public health, proving effective in differentiating between a range of authentic and 'faked' vaccines previously found to have entered supply chains.

The global population is increasingly reliant on vaccines to maintain population health, with billions of doses used annually in immunisation programs worldwide. The vast majority of vaccines are of excellent quality. However, a rise in substandard and falsified vaccines threatens global public health. Besides failing to treat the disease for which they were intended, these can have serious health consequences, including reduced confidence in vaccines and, ultimately, death. Unfortunately, there is currently no global infrastructure in place to monitor supply chains using screening methods developed to identify ineffective vaccines.

In this new study, researchers developed and validated a method that is able to distinguish authentic and falsified vaccines using instruments developed for identifying bacteria in hospital microbiology laboratories.

Prof James McCullagh, study co-leader and Professor of Biological Chemistry in the Department of Chemistry said: "This method is the culmination of a number of years of collaborative research that has brought together scientists from across the university (in Chemistry, Biochemistry and the Nuffield Department of Medicine) with outside partners including at the Rutherford Appleton Laboratory at Harwell and the University of Huddersfield. Rebecca Clarke (former Part II student) and John Walsby-Tickle (Mass Spectrometry Services Manager) both played key roles in the method's development in the Department of Chemistry.





"We are thrilled to see the method's effectiveness and its potential for deployment into real-world vaccine authenticity screening. This is an important milestone for our Vaccine Identity Evaluation (VIE) consortium which focuses on the development and evaluation of innovative devices for detecting falsified and substandard vaccines, supported by multiple research partners including the World Health Organisation, medicine regulatory authorities and vaccine manufacturers."

The method is based on matrix-assisted laser desorption/ionisation-mass spectrometry (MALDI-MS), a technique used to identify the components of a sample by giving the constituent molecules a charge, and then separating them. The MALDI-MS analysis is then combined with open-source machine learning. This provides a reliable multi-component model which can differentiate authentic and falsified vaccines, and is not reliant on a single marker or chemical constituent.

The method successfully distinguished between a range of genuine vaccines – including for influenza (flu), hepatitis B virus, and meningococcal disease – and solutions commonly used in falsified vaccines, such as sodium chloride. The results provide a proof-of-concept method that could be scaled up to address the urgent need for global vaccine supply chain screening. ■

Read more: doi.org/10.1038/s41541-024-00946-5

PERIODically

Charlie Simms introduces the new series of the Oxford chemistry student podcast about periods

You have been standing on your feet for six hours; the solvents are making your head hurt; you feel dizzy – and then, you get your period.

People who have periods can feel like their environment has not been made to include them, and nowhere is this truer than in the lab. Menstrual health is often overlooked, and stigma around periods stifles conversation.

PERIODically is a podcast, now in its second series, written and produced by chemistry students at the University of Oxford. Our aim is to understand the impact of menstrual health on our lives as chemists, and reduce stigma around periods. Can we decrease taboo and increase belonging through discussion?

On PERIODically we discuss our own experiences with periods whilst studying chemistry, and in the first series we focused on the impact of menstrual health on labs, tutorials and undergraduate experiences.

We found that those with periods and period-related conditions found it harder to work long hours in labs, attend tutorials and study comfortably whilst on their period. Research by one of our team, MChem student Lottie Oliver, considered students' experiences of the laboratory. In this, she found statistical differences between the frequency of physical hindrance experienced in the lab for students with periods, compared to those without. Students detailed how their experience changed during their period: increased sensory sensitivity, pain and lack of emotional resilience. We hope her initial research will inspire further study in this area.

Another member of our team, MChem student Sofia Olendraru, recently headed a campaign for free, easy to access period products. This was a success; now free period products are supplied in all female and disabled toilets around the Department of Chemistry. With these supplies on hand, worries around leakages, unexpected bleeding and finances have been lessened – a fantastic first step towards menstrual equity.

After the first series of the podcast was released, we soon realised that chemists across the world recognised and related to our experiences. We heard from many who experience conditions such as endometriosis, polycystic ovarian syndrome or perimenopause; the first series had only scratched the tip of the iceberg.

PERIODically

The Oxford Chemistry Period Podcast

Visit linktr.ee/periodically_ox, or scan the QR code, to find out more and listen to the podcast.

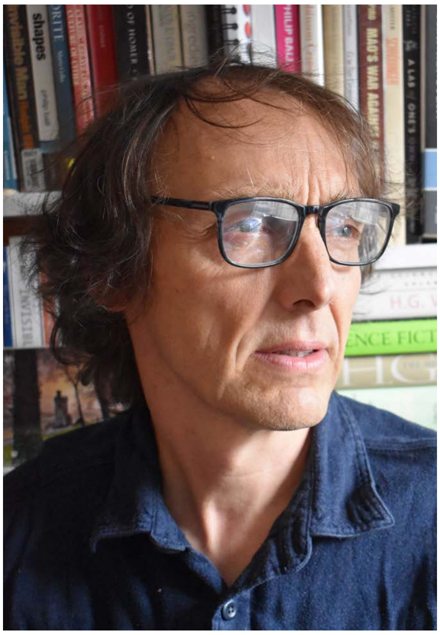
In series two, we've invited guests from undergraduates all the way up to senior lecturers to talk about their widely varying experiences with menstrual and reproductive health. We highlight the structural difficulties for those who menstruate at all points in their career as chemists, emphasising the need for change in our field.

PERIODically has had thousands of downloads in over 50 countries, and what we are most proud of is the platform we provide for stories about reproductive and menstrual health. So, we challenge you: have a listen to the podcast. Use the experiences of us and our guests when making decisions in your institutions. Think actively about including those with periods. We believe that in doing this we can create a better environment for those who menstruate, and especially chemists. ■

Some of the PERIODically team: Manami Imada, Sofia Olendraru, Charlie Simms, Lottie Oliver, Josie Sams and Felicity Smith (left to right).

How Life Works

Oxford Chemistry alumnus Philip Ball (Merton, 1979) is one of the UK's best-known science writers. He is the author of many popular books on science, covering topics including the nature of water, the discovery of the elements, and the history of experimental science. After completing his chemistry degree at Oxford and a PhD in physics at Bristol, Philip worked as an editor at Nature for over 20 years and contributed to national and international newspapers and journals, including Prospect magazine, The Guardian, Chemistry World and The New York Times. He talks with Periodic about his latest book, How Life Works.



You did your undergraduate degree in chemistry at Oxford. As someone who writes about science, what did you take from your time in Oxford?

It was a long time ago! To be honest, at that stage I imagined (vaguely) going into a life in science. But I enjoyed writing up my Part II thesis in chemistry, and also later my PhD thesis (in physics), and only then did it begin to occur to me that there might be some way of combining my interest in science with my passion for writing. One of the nicest aspects of having studied at Oxford was reconnecting, in my later career, with some of the brilliant people who were my tutors and lecturers, such as Peter Atkins, Tony Cheetham, and John Rowlinson.

What prompted the idea for this book and what made you decide to write it?

Over the course of the past three decades I have become concerned about the stories we tell about biology: about the matter of how life works. I am constantly astonished and deeply impressed at how biologists wrestle from the messy and capricious stuff of life any insights at all into what living matter is and how it sustains itself. But in comparison to the ingenuity and virtuosity that goes into such research, the narratives that seem to percolate into the public arena – about genes, cells, evolution, and us – have struck me as increasingly and perhaps even dangerously simplistic and out of kilter with what we now know.

I was motivated to put this down on paper after spending the summer of 2019 as a visitor in the Department of Systems Biology at Harvard Medical School. There I learnt that the conventional narratives in biology were even more outdated than I'd appreciated. I felt it was time to try to explain the current state of play in our understanding of what genes do and don't do, why cells do the things they do, and what makes life such a special and unusual state of matter. When I started writing the book, I admit that I did not have a clear idea of how, or even whether, the latest scientific understanding might translate into anything like a coherent picture. Readers will have to judge for themselves whether my book finds one!

You write that you think a recalibration in biology is long overdue. Why is now the right time for a 'New Biology', and how would you envisage this happening?

One reason why now is the right time is a negative one: we have come to see that the Human Genome Project, despite its immense value for basic research, has not delivered on its promises either of providing lots of new cures or of revealing how life works.

But there is a more positive reason too why now is the right time to speak of a new biology. Research in molecular and cell biology has made astonishing strides in the past two decades or so, in part thanks to powerful new experimental techniques. It has revealed that many aspects of biology are not quite as we thought: a circumstance often said to have shown that the way life works is more complicated than we thought. That is true, but I think we have reached a point where it is not simply an accumulation of ever more details. Rather, we can start to see some common themes emerging. In particular, life's molecular processes – especially for complex, multicellular beings like us – seem to be less a matter of the precise unfolding of some plan or blueprint via well-defined pathways of information flow, and more a matter of interactions among molecules that are fuzzy, collective, contextual, and able to improvise and innovate. To my mind, life looks less computational and more cognitive.

I think that one of the most important enablers of a shift in narrative will be a switch from a focus on the gene to a focus on the cell. This has been remarked on by many leading biologists, including the Nobel laureate Paul Nurse. Of course genes are absolutely central to any understanding of how life works, but they are not alive themselves and have no agency. I don't think an understanding of life can ever flow upwards from the level of the gene. It has to start with something that is genuinely alive and agential, and the cell is the smallest unit that satisfies those criteria.

You say that in retrospect it should have been obvious all along that evolvable systems must involve some kind of agency. Do we need to look for a theory of agency in biology?

I think we do, but I'm aware that not everyone agrees! Some find agency too mysterious and woolly a notion, and certainly there is no commonly agreed definition of it. To me, however, it refers to the capacity that seems to set living organisms apart from non-living matter: namely, the ability to manipulate or transform itself and its surroundings in ways that facilitate the attainment of some self-defined goal (such as self-preservation, self-sustenance, and reproduction). It has always been recognized that living things are goal-directed (even if the process by which they arise and change, evolution, is not). A theory of agency should supply a way to understand that characteristic, in a way that does not need to invoke anything mystical or vitalistic.

You believe we are at the beginning of a profound rethinking of how life works. What are the most important questions we need to ask now?

There are so many! Many of them are somewhat technical, for example:

- What are the roles of disorder in protein structure?
- How does the three-dimensional structure of chromatin influence gene expression?
- What are the roles of noncoding RNA molecules?
- Why does nature make such extensive use of the collective aggregates of biomolecules called condensates?
- How are cell fates determined, and how malleable are they?

However, these issues seem to me to be interwoven into a wider question about how causes of outcomes at the level of whole organisms – including manifestations of disease – become spread across many levels of space and time in biology. How are they integrated, and how autonomous are they? There are also profound questions about how all this newly emerging knowledge might impact our understanding of how evolution works. I don't think it is going to undermine Darwinism or anything, but the conventional thinking – the Modern Synthesis – might well need some tweaking.

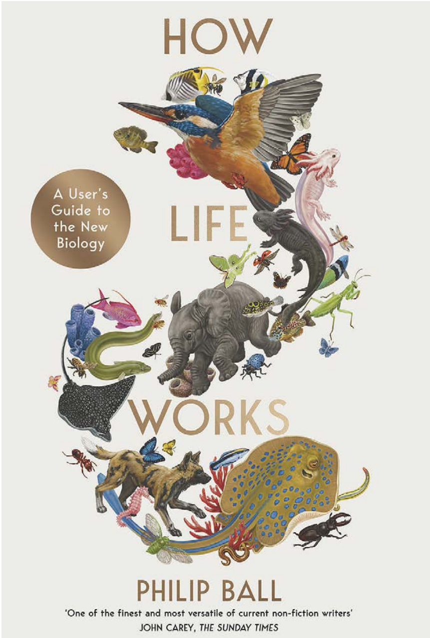
You've written extensively on chemistry: in your view, what is the relationship between chemistry and "How Life Works"?

Chemistry is at the heart of it! But it's an unfamiliar kind of chemistry. I had become accustomed to thinking of all the crucial chemistry of life as a matter of well-specified interactions governed by molecular recognition. It turns out that much of it is not like that! Instead, biomolecules seem often to work combinatorially, in groups, making use of lots of rather weak and often somewhat unspecific interactions. One of the issues that intrigues me is whether we can learn from these biological principles in the way we design complex artificial molecular systems for supramolecular chemistry, polymer chemistry, and so on.

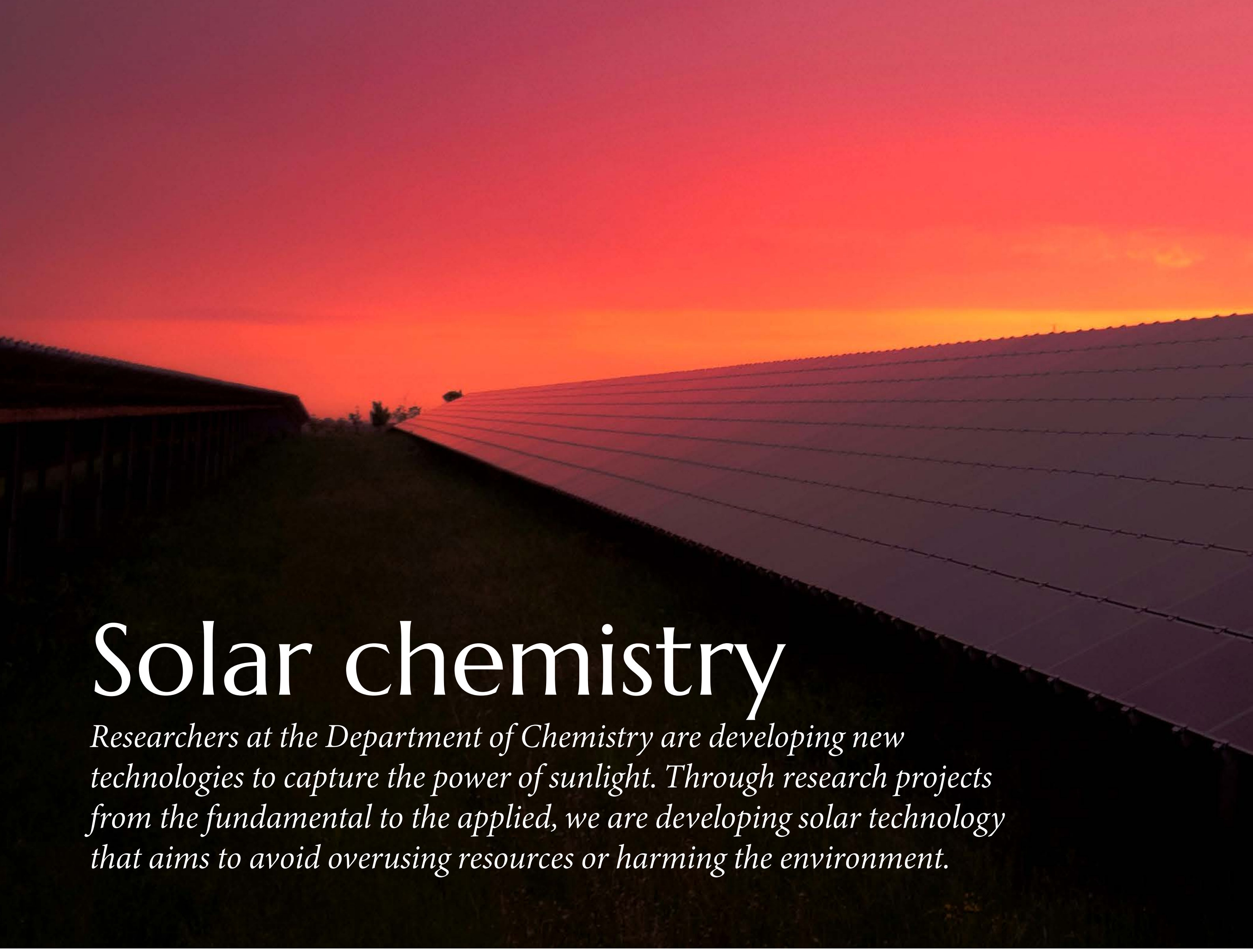
Clearly there is much more to be explored on the topic of how life works. Will you continue to write about this, and/or are you working on other projects?

I have a possibly unfortunate tendency to rush on to the next project once I have finished writing a book. But this time I am trying to resist that, because I feel there is so much more to be said about the issues raised in *How Life Works*. It seems to have become part of a wider move to re-evaluate the way we think and talk about life. So I will be mining this seam for some time to come, I hope.

Having said that, I am working on the next projects too. One of them is a short and highly illustrated history of alchemy, which will look glorious and has been fun to write. ■



How Life Works is published by Picador and available now.



Solar chemistry

Researchers at the Department of Chemistry are developing new technologies to capture the power of sunlight. Through research projects from the fundamental to the applied, we are developing solar technology that aims to avoid overusing resources or harming the environment.

The sun sustains life on Earth as we know it, whether it's the food we eat, the fuels we burn, or the electricity we produce. The finite supplies of fossil fuels that power much of modern life derive their energy from organic molecules formed over millennia, ultimately from prehistoric plants that used photosynthesis to trap sunlight's energy.

Even high tech renewable power sources like solar panels and wind turbines are powered by the sun's radiation. In the case of a solar panel the link to the sun is obvious, whereas for wind power the energy comes via global climate patterns, caused by the sun's heating and cooling of the atmosphere.

It is difficult (though not impossible: for example nuclear fission, and geothermal heat) to think of methods of generating power that *don't* rely on the massive nuclear fusion reactor at the centre of our solar system – the sun.

In the face of climate change and depleting fossil fuel stocks, one of today's technological challenges is to find new, sustainable ways to harness the sun's power.

Solar fuels

One way to capture the sun's power is to use sunlight to catalyse the making of fuels from abundant chemicals, such as water and carbon dioxide. The resulting solar fuels are a way to reuse two of the main byproducts of fuel combustion, including the potent greenhouse gas carbon dioxide.

Sometimes termed artificial photosynthesis, the idea is to design catalysts that absorb photons of sunlight and can then speed up a reaction to make fuels or other useful chemicals. Several teams in Oxford Chemistry are working on designing and testing new catalysts for these types of solar fuel reactions – you can read about Edman Tsang's work in this area on p.8.

Ludmilla Steier's research group is developing a range of photocatalysts for the efficient and stable production of high-value fuels and chemicals from solar energy. She uses a technique known as atomic layer deposition, whereby gas particles react with a surface one layer at a time to build up a highly controlled thin-film structure. Her group can control growth of their materials at the atomic scale to achieve defined, effective catalysts.

The work of Iain McCulloch's group in this area focuses on organic semiconductor photocatalysts. Clever optimisation of the energy levels and properties of these materials aims to improve their efficiency and open up new routes for fuel generation from carbon dioxide, a well-known greenhouse gas.

The team has been developing ring-shaped polymer catalysts, which can be tuned to use sunlight to chemically transform carbon dioxide into useful chemicals such as hydrogen, methanol, and syngas (a mixture of hydrogen and methane).

New photovoltaics

As well as photocatalysts for fuels, the McCulloch group is also working on developing new solar cells. Conventional photovoltaic cells use crystalline silicon to generate an electric current from sunlight. New organic solar cell materials are capable of absorbing more photons and generating larger cell voltages than conventional photovoltaics.

In 2022, McCulloch received a Royal Society prize for his work, saying at the time that the "climate crisis and the protection of our environment is one of the biggest societal issues facing us right now, and chemistry has a role to play in offering new alternatives and solutions. Our research in solar energy and solar fuels can help to move these technologies firmly into the mainstream, eliminating our dependency on fossil fuels."

Claudia Tait's work in electron paramagnetic resonance (EPR) aims to understand the fundamental physical processes at the basis of converting solar energy into electricity. Solar electricity generation relies on separating electrons, and Tait's group uses EPR spectroscopy to probe the interactions of unpaired electrons with other nearby electrons and nuclei. This provides a detailed picture of the molecular environment of the species involved in the photovoltaic process. The hope is that this theoretical understanding will help us to design and optimise better photovoltaic cells in the years to come.

Energy cycle

New materials will be required at all stages of solar electricity generation and storage. Robert Hoye's research vision is to develop a new generation of energy materials that will help us to develop high-performing devices for clean energy conversion at all stages of the power cycle.

Recent studies in the Hoye group have, for instance, considered using bismuth compounds to generate solar fuels, and developing new halide perovskite photovoltaics. Through careful control over bulk properties and interfaces, his team assemble complex structures to derive functionality from new materials, including applications in photovoltaic and photoelectrochemical cells.

Prof Hoye was also recently involved in writing a report describing a roadmap for using photovoltaics for sustainable energy conversion: you can read more in the *Journal of Physics: Energy*.

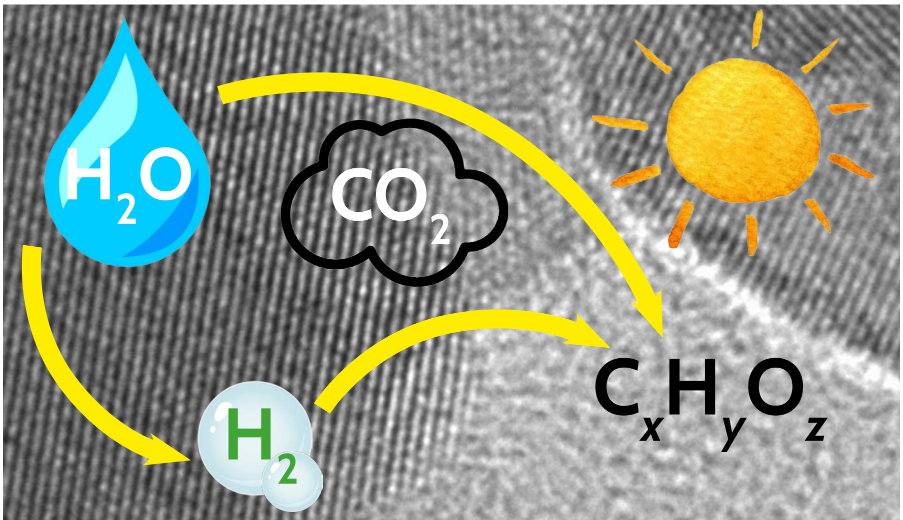
Fundamental science

Volker Deringer's team uses advanced machine learning methods to model disorder in amorphous systems, unravelling the structures of simple chemicals like phosphorous and calcium carbonate, whose atomic-level structure has eluded chemists for decades. Some of his recent work has focused on structural and electronic transitions in disordered silicon, the material from which most solar cells are currently made. Deringer emphasises that the team's work is "purely driven by curiosity – we aim to create the most realistic models of amorphous structures, and we aim to understand the subtle rules that guide their formation."

Indeed, Oxford has a long history of pushing the boundaries of fundamental research, which often leads to unexpected technological advances. A famous example of this in the energy sector is the early work on lithium-ion batteries, which relied on fundamental solid-state research in Oxford's Inorganic Chemistry Laboratory.

Batteries for the future

A national grid based on solar energy will require a way to store power – after all, demand doesn't stop just because the sun sets. Research in the groups of Oxford's solid state chemists, such as Michael Hayward and Simon Clarke, is focused on the synthesis and characterisation of new solid-state compounds which might be used as the energy storage materials of the future. ■



Work in Ludmilla Steier's research group focuses on desiging, characterising and testing new catalysts to produce high-value carbon-neutral fuels and other chemicals from solar energy.

Leading in sustainable chemistry

Professor Charlotte Williams OBE FRS has been appointed to the Professorship of Inorganic Chemistry, one of Oxford's five statutory chairs in Chemistry

Prof Williams is an expert in catalysis, sustainable chemistry and polymer materials. All of the polymers her team develops are designed to be renewably sourced, with structures managed from the atomic to the macroscopic length-scale for their target applications. The team also considers the end-life management of the polymers, to allow for recycling or degradation depending on their application.

A major area of interest for Prof Williams is carbon dioxide chemistry. Her team have discovered high performance catalysts that allow CO_2 to be transformed into oxygenated polymers. Williams' catalysts feature two metal centres, often acting better together to maximise carbon dioxide uptake at low pressures and produce useful polymers and materials. She specialises in understanding how carbon dioxide is incorporated into the polymer, applying spectroscopy, kinetics and computational methods to provide theories that explain catalytic synergy and carbon dioxide chemistry. The CO_2-derived polymers show significantly reduced greenhouse gas emissions, and are useful for applications including home insulation and other long-lasting consumer products.

She has also researched a new type of self-switchable catalysis, whereby a single catalyst selectively enchains mixtures of monomers and is switched between different catalytic cycles on demand. The switches are triggered by the presence or absence of key monomers, like carbon dioxide or cyclic anhydrides. Highly sequence-selective copolymers can be formed using this method. She remains especially interested in developing other forms of switchable and selective catalysts that work using raw material or impure mixtures, since these are often found in both natural and industrial systems.

Making polymers is only part of the picture. Prof Williams' team are just as interested in the process of unravelling polymers back to useable monomers. Her team have been developing low-temperature recycling catalysts that reverse the polymerisation process, often starting from a polymer chain end, so as to selectively produce pure monomers. The team have so far discovered low temperature recycling routes that work for different types of polyesters and polycarbonates, including recovery of the monomers from waste plastic packaging being used in the cafeteria of Oxford's Chemistry Research Laboratory.

Much of Prof Williams' work is driven by catalysis using earth-abundant metals, such as sodium, potassium, magnesium and iron. These highly abundant elements also come at a lower cost than other metals.

Prof Williams pays particular credit to the research teams she has worked with over her career, including her past advisors, mentors, academic collaborators, industry partners, and, most of all, to her current and past research team.

"The reason I come into the lab every day is to work with such a talented and committed research team who have the energy and enthusiasm to try to solve complex scientific questions. Not only is it great fun, but seeing them develop their independence, scientific confidence and careers is one of the most rewarding parts of the job."

Throughout her career Prof Williams has worked closely with industrial partners. She founded, and still serves as Chief Scientific Officer, at Econic Technologies, a UK company that sells catalysts and processes globally, enabling carbon dioxide utilization. She will head up the new SCHEMA sustainable chemicals and materials manufacturing hub (see below), which is focused on transforming the way chemicals and polymers are designed, made and recycled.

In her view, we need even more scientists and engineers to propose creative and distinctive approaches to chemical production, polymerisation and recycling. She says:

"Only with enough focus on transformative discovery science can we hope to answer the environmental and societal questions surrounding the most sustainable ways to make and use our future materials."

Prof Williams served as Associate Head of Department (Research) in the Department of Chemistry from 2020 to 2024, and prior to her time in Oxford she was a professor, and head of materials chemistry, at Imperial College London. She has also worked at the University of Cambridge, and the University of Minnesota, and her degree and PhD are from Imperial College London.

The previous Professors of Inorganic Chemistry at Oxford were Peter Edwards, Malcolm Green, John Goodenough (also Nobel Laureate in 2019), and the first holder of the chair, John Stuart Anderson. ■

SCHEMA: a new sustainable chemicals and manufacturing research hub

The University of Oxford is leading a major UK government investment in research to improve the sustainability of chemical and polymer production

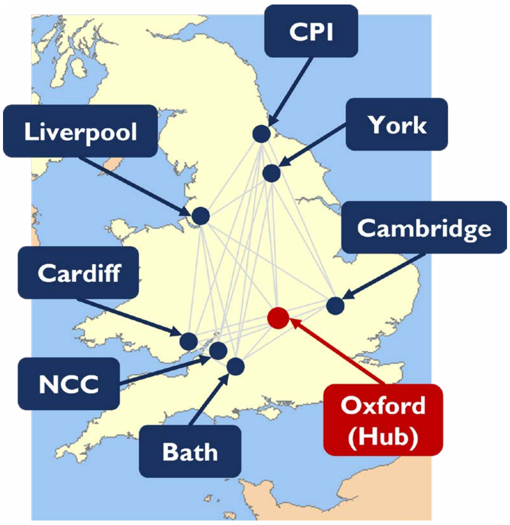
The Sustainable Chemicals and Materials Manufacturing Hub (SCHEMA) will bring together researchers from across the UK working with a large consortium of commercial, technology translation and civic partners. The hub has been funded by £13.75 million from the Engineering and Physical Sciences Research Council (EPSRC) and leverages a further £22 million in funding from its partners.

SCHEMA is one of five new manufacturing research hubs supported by EPSRC, which aim to address a wide range of challenges in commercialising early-stage research within different manufacturing sectors.

The SCHEMA hub is led by Professor Charlotte Williams OBE FRS from the Department of Chemistry, and will involve academics from Chemistry, Engineering, Materials Science, Computation, Environmental Economics, and Law at the Universities of Oxford, Bath, Liverpool, Cardiff, York and Cambridge.

Professor Williams said: "It is imperative that the chemical industry reaches net zero emissions and sustainability as so many essential downstream industries depend upon it. Our hub will be well placed to tackle this difficult challenge by bringing together a very wide range of academic expertise with companies from across the supply chain."

The research focuses on transforming the way chemicals and polymers are designed, made, and recycled. This includes supporting the transition away from the use of virgin petrochemicals and redesigning processes and materials to increase recycling rates. A key focus will be to design processes that can produce chemicals and polymers from renewable raw materials such as biomass, carbon dioxide, and even industrial wastes, and integrating renewable energy into the process engineering. This will build upon the University Oxford's research on transforming carbon dioxide and biomass wastes into plastics, elastics, adhesives, and coatings.



The research teams will work across the fields of sustainable chemistry, process engineering, polymer materials science, and digital technologies. A key aim is to leverage recent developments in computation and information technology to design future materials that are both functional and fully sustainable, embedding principles of circular economy and end-of-life management.

Professor Jim Naismith, Head of the Mathematical, Physical and Life Sciences Division at Oxford, said: "Finding new ways to sustainably make things is a challenge of our age. It is quite right that the University plays its part. The SCHEMA hub is a collaborative venture engaging academia, industry, and policymakers. The hub will rethink and reformulate chemical production, making it not just environmentally friendly, but an engine of innovation and progress for generations to come."

Within SCHEMA, researchers will work with a range of partners including businesses, catapults, professional societies, and international academic partners to tackle the shared materials design and sustainability challenges of important end-use sectors. These partnerships will enable sustainable chemicals and polymers to be designed for immediate use within key sectors including electronics, transportation, energy generation and storage, construction, and fast-moving consumer goods.

Professor Williams said: "Supply chain partnerships are at the heart of SCHEMA. Our success will also rely on strong advocacy and engagement. Our prior success working with major national and international bodies will be used to support joined-up policy, legislative, and economic environments for the technologies developed in SCHEMA."

At launch, the team are supported by 25 companies from across the supply chain, representing polymer and material end-users.

The hub seeks to ensure that the UK remains at the forefront of major international efforts to transition to sustainable chemical manufacturing. The research program will train a new generation of postdoctoral and early career researchers to take on leadership roles in UK sustainable chemical manufacturing.

Professor Charlotte Deane, EPSRC Executive Chair, and a professor in Oxford University's Department of Statistics, said: "Given the scale and importance of the UK's manufacturing sector, we must ensure that it is able to benefit fully from advances made across the research and innovation ecosystem. With their focus on innovation and sustainability the advances made by the hubs will benefit specific sectors, the wider manufacturing sector and economy, as well the environment."

Chemical manufacturing is crucial to the UK's economy. It is the UK's second largest manufacturing industry, directly employing over 140,000 people and delivering turnover exceeding £75 bn per year. However, there is an urgent need for this industry to tackle the environmental impact from both manufacturing and its products. Greenhouse gas emissions from the global sector are significant, with it currently accounting for approximately 5–6% of emissions, which is 2–3 times larger than the global airline industry. Coupled with this are the challenges of raw material being sourced from fossil fuel extraction and refining, pollution in water and soil, and globally low rates of polymer recycling.

The academics working in SCHEMA have strong track records in commercial partnership and entrepreneurship. For example, Prof Kylie Vincent, the hub's champion for equality, diversity and inclusion, is a founder of HydRegen, which applies innovative chemo-enzymatic processes to make chemicals. The hub is strongly integrated with high-tech and growth SMEs as well as multinationals. It builds upon the successful partnerships established in the Oxford and Bath-led Innovation Centre for Applied Sustainable Technologies. ■

The SCHEMA team, gathered in Oxford this September for a launch meeting.

Oxford Chemistry Outreach

Innovating to support science education in schools

Puzzle boxes

Pupils pit their wits against cryptic chemical clues

Problem-solving, teamwork, resilience, numeracy, creativity – just a few of the skills that students develop during their time on the MChem course at Oxford.

How can we convey these skills to school students? Enter the Oxford Chemistry puzzle boxes! Working against the clock, teams of school students solve a set of chemistry puzzles to reveal secret codes and unlock a mystery box.

Puzzle boxes are offered to groups during taster days or residential visits to an Oxford college, and can be requested by schools when organising trips. They are delivered by our Outreach Ambassadors (Oxford Chemistry students).

DPhil student Dori Szalay says: "Successfully completing our amazing puzzle boxes requires a very different skill set from students than what they're used to in school. The same is true for us as ambassadors!

"After just the first workshop, you quickly realise that often you help the most by not giving students the answer. Seeing the joy and sense of accomplishment on their faces after they solve my cryptic clue and, eventually, the puzzle is priceless."

Since the programme's inception in late 2021, we have worked with nearly 5000 young people.

Dr Hugh Munro, tutor for access at Wadham College, says: "The puzzle box sessions delivered by the Chemistry Department are always a highlight of school visits to Wadham. The teachers frequently comment on the excellent pitch of the content, and it's always brilliant to see how the groups take on a challenge which is very different to the teaching they're used to in school.

"The teams delivering the sessions are exceptional, and ably support the groups whilst also subtly showing what it's like to study at the university too."

> *I learnt how to problem solve with multiple concepts in chemistry.*
>
> Student

Read on for an introduction to the three sets of puzzles developed by the Outreach team.

Lab Lurker

Year 12 (16–17-year-olds)

Students find out more about eight research groups at Oxford Chemistry as they perform microscale redox, electrolysis and precipitation reactions, all to determine the next target location of a lab saboteur.

Poison Puzzle

Year 10–11 (14–16-year-olds)

Poison Puzzle is a race against time to access the antidote to an (imaginary!) arsenic poisoning. The problems standing in their way cover topics such as atom economy, indicators, chemical structures, hydrophobic coatings, chromatography and polymers.

Graffiti Game

Year 9 (13-year-olds)

Preventing damage to Oxford Museums by a misguided undergraduate is the goal of this puzzle box, where students consider non-Newtonian fluids, balance equations, investigate solvents, undertake a microscale titration, explore photochromic paints and inspect fossil evidence. ■

If you would like to support our work with young people visiting Oxford, please visit bit.ly/OxChemSupport

Building Bridges

Exploring forensic chemistry with novel primary school activities

Building Bridges

Building Bridges is an enrichment programme for school students launched in 2022 that aims to boost their motivation, engagement and academic belonging. The project is a partnership between the University of Oxford and other higher education and third sector providers.

This year's enrichment theme, titled 'Into the Blue', focuses on heritage science, taking a closer look at blue pigments and the role of analytical chemistry. Working with school teachers and researchers at the Ashmolean Museum, School of Archaeology and Faculty of English, Oxford Chemistry produced a scheme of work consisting of seven numbered 'Bridges' – activities dedicated to particular learning objectives.

'They excelled ... we saw a different side to them in that environment.'

Year 6 teacher

One of the new activities is *Death in a Victorian Drawing Room,* an hour long workshop. This exciting activity has been delivered 29 times over the last year to around 850 school children by a dedicated team of Oxford Chemistry staff and students.

Participants solve a fictional unexplained death from the Victorian era. Using portable infrared (IR) and ultraviolet (UV) spectrometers that are brought to their classrooms, and data from Shimadzu liquid chromatography mass spectrometry and atomic absorption spectroscopy simulations, pupils work to determine key pieces of information such as the amount of lead and opioid drugs in the victim's blood.

Using IR/UV kits with 9–11-year-olds is very unusual, and the team are particularly proud of this aspect of the project. Its resounding success can be simply summed up by one student who proudly presented themselves at an activity station and declared: "This is the best fun!"

From their evidence, the students draw conclusions and determine further lines of enquiry to pursue beyond the session. The twist to the workshop is that the participants are not given a definitive answer at its conclusion. This allows students to hold competing evidence-based explanations, and encourages them to debate their positions and determine their next steps in the investigation.

'[They] had a great time carrying out experiments to solve the mystery and loved getting hands-on with the equipment and running their own UV-vis and IR spectra. Thanks for a brilliant session.

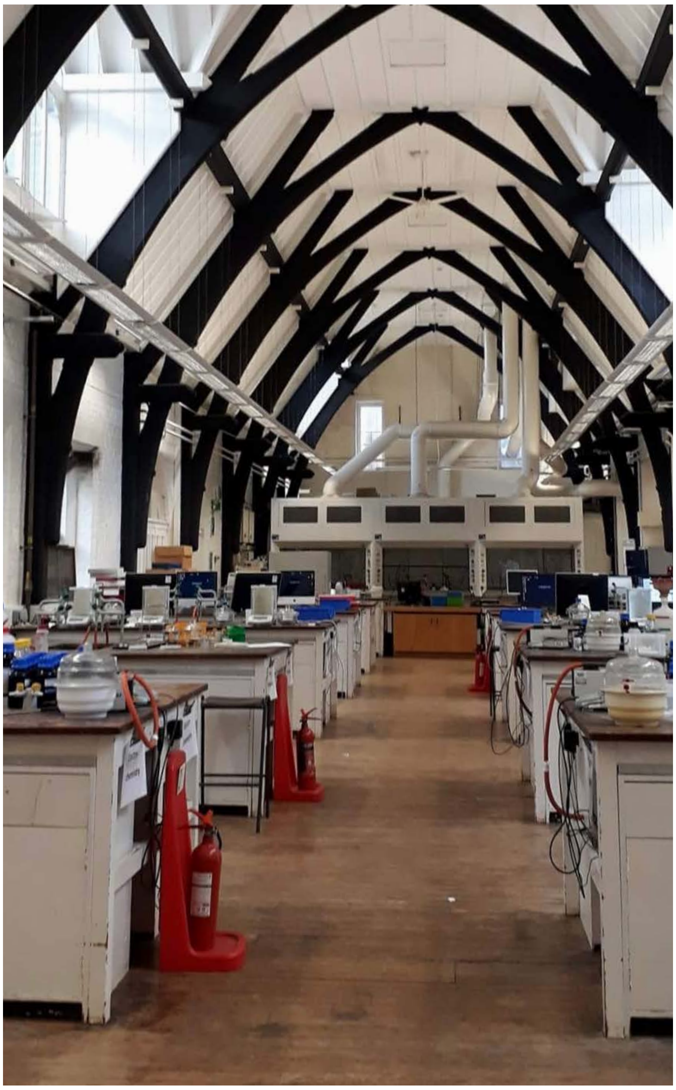
Supervising adult

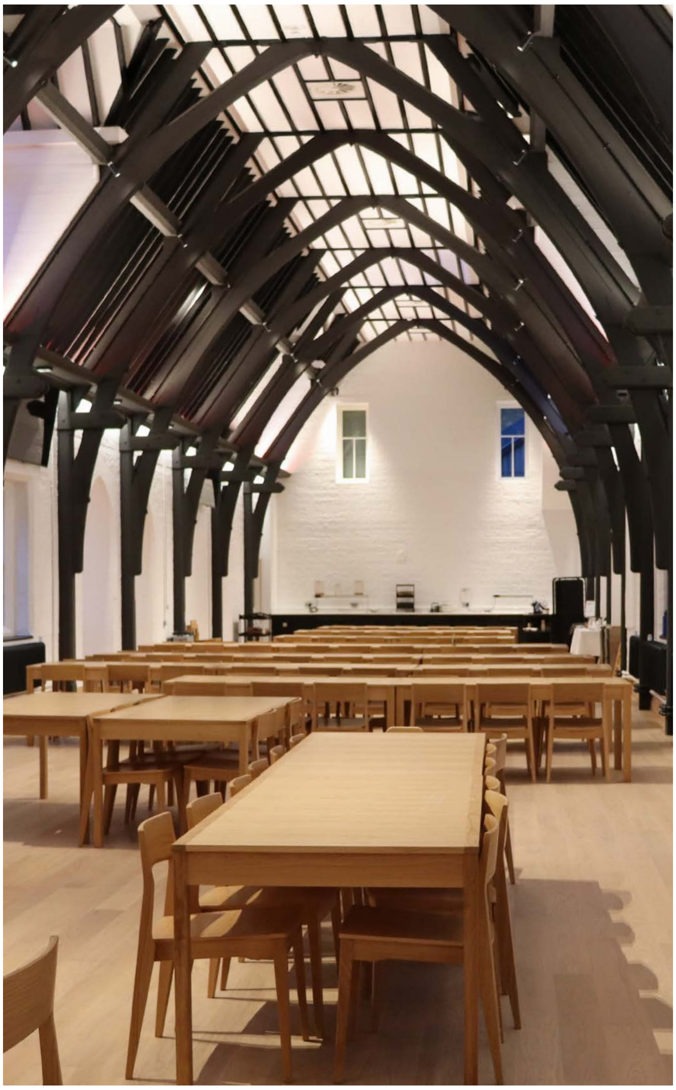
The exercises provide an excellent opportunity to consider how scientific research progresses, whereby justified conclusions lead to additional investigations. ■

You can find more information about the Building Bridges Partnership Project at bit.ly/OxBB

In with the new

Peek inside the former ICL teaching lab, now home to Oxford's newest college





The golden rule in the lab – *no eating!* – is familiar to any chemist. But it has been broken now in the former ICL teaching lab, now home to Reuben College's dining hall.

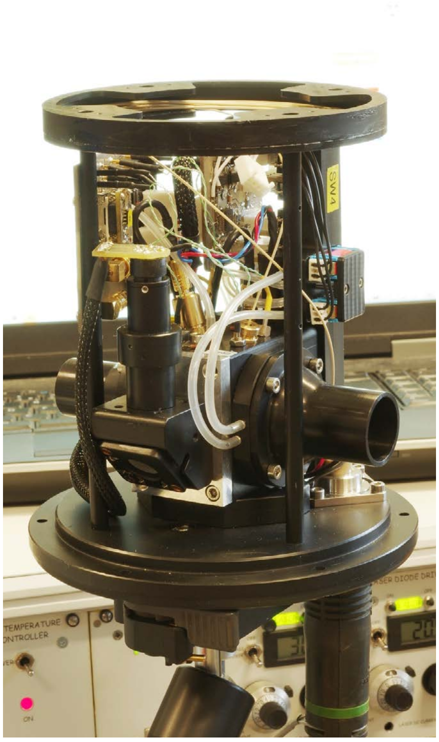
Established in 2019, Reuben is Oxford's 39th college and is dedicated to graduate study with a focus on interdisciplinary research. Reuben is housed in parts of what were the Inorganic Chemistry Laboratory and the Radcliffe Science Library – both of which still occupy other sections of the buildings. The former inorganic teaching laboratory is now the dining hall, and the servery is where the old prep room used to be.

Senior Teaching Lab Technician Jennie Botham, who worked in the ICL Teaching Laboratory for many years, said "Working in the old Teaching Lab and interacting with so many different people there – from undergraduates to a Nobel Laureate – was always an interesting experience." On a few occasions Jennie also helped various film crews set up scenes in the lab when it was used as a set for programmes including the BBC's *One Show*, and the 1997 film *The Saint*. ■

Senior Teaching Lab Technician Jennie Botham, demonstrating in today's Chemistry Teaching Laboratory, which opened in 2018.

Designing new diagnostic tools for lung disease

Some of the most interesting and innovative work happening in the Department of Chemistry brings together the skills of people from many different disciplines



For more than a decade, scientists in Prof Grant Ritchie's group have been collaborating with colleagues in Oxford's Department of Physiology, Anatomy, and Genetics to develop a laser gas analyser (LGA). This new research tool non-invasively measures the concentrations and flow of breath gases, allowing clinicians to track these as a patient breathes and accurately assess how efficiently the lungs are functioning. This information is important when investigating both healthy lungs and respiratory diseases such as chronic obstructive pulmonary disease (COPD), asthma, cystic fibrosis (CF) and long COVID.

This long-term multidisciplinary project has resulted in the design and build of seven LGAs, five of which are currently being used at hospitals around the UK for research studies. Consulting engineer with the Ritchie group, John Couper, described some of the design challenges, and how he has worked with colleagues to solve them.

John says: "I've been working on this project for several years now, though I'm not a chemist. I always describe myself as a physicist, doing engineering on a physiology project, in a chemistry department!

When I began work on this, the group had built a benchtop prototype of the LGA to test the basic spectroscopic techniques. What they wanted was to build a portable device that could be used in hospitals to measure breath gas exchange.

From an engineering point of view the requirements were that the device would be safe, portable and robust enough to be moved around hospitals. We also had to think

about how to protect the machines and the patients in terms of the design and materials. The interface between the users and the device is via standard medical bacterial and viral filters.

We've now built seven of these devices – more than originally planned. A basic three-gas model measures carbon dioxide, oxygen and water vapour. Then there's a five-gas model which can also measure tracer gases like methane and acetylene.

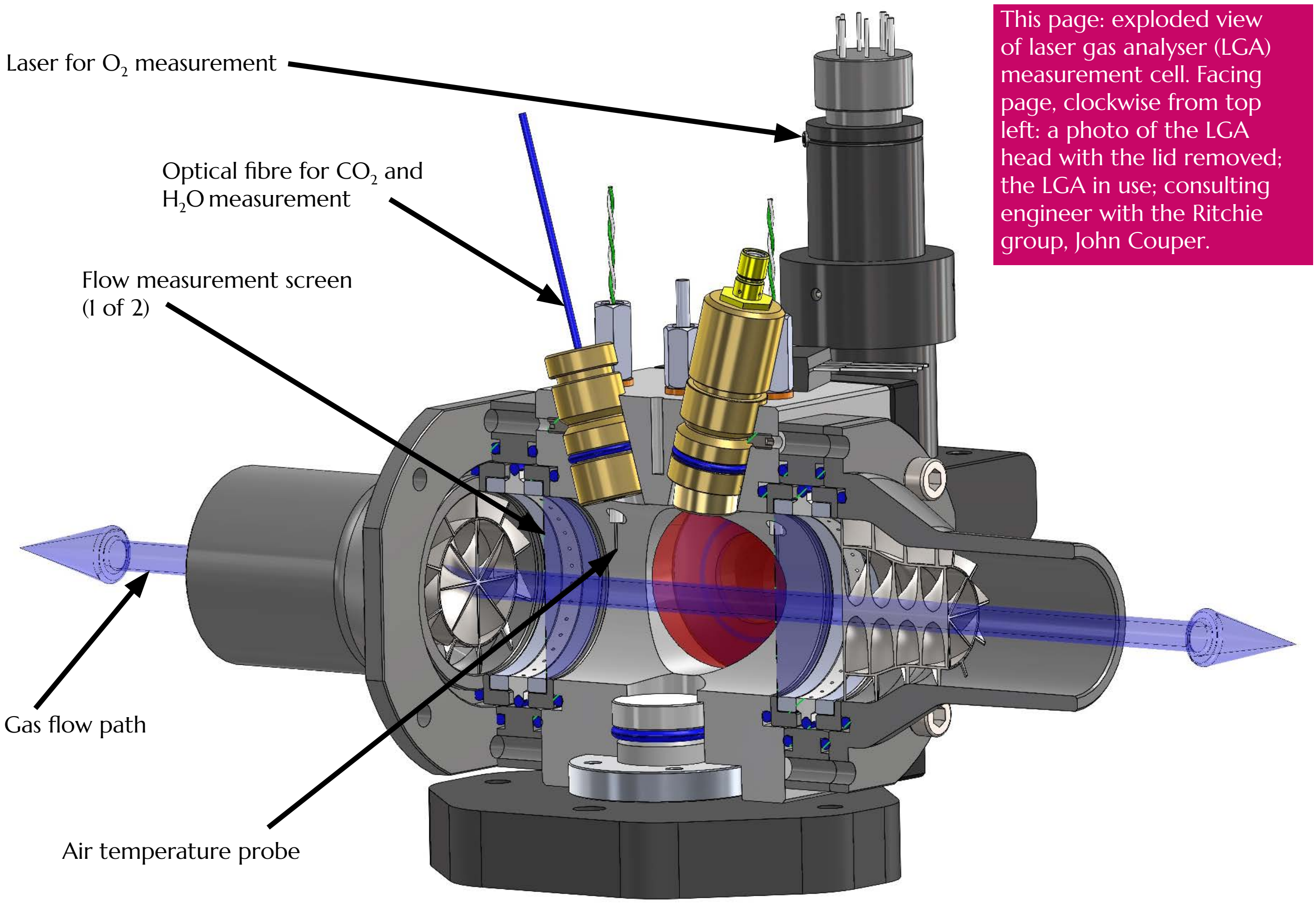
The gases are measured by spectroscopy – essentially, we have a laser for each gas that we're measuring, and each is measured 100 times a second. We take the resulting spectrum and do a fit, and from that we get the number density of each gas. When combined with flow data, the integrated quantity of each gas flowing is calculated.

We don't measure all the gases by the same method. The absorption of the oxygen is very low at the wavelength we're using, so we have to use a long path length. This is a challenge; the device is only 24 mm inside. So, we use a cavity-enhanced measurement with high reflectivity mirrors both sides of the path, which greatly increases the effective path length. For CO_2 and water, the laser outputs are combined into one path and measured by direct absorption with the laser beam passing twice across the device giving a path length of about 50 mm. For all the gas measurements, each laser is scanned through the absorption line and the data analysed to obtain the number density. When we need to measure tracer gases it's a bit more complicated and so we build in a Herriott cell – a multipath cell where we can fit in a path length of around about 0.6 metre.

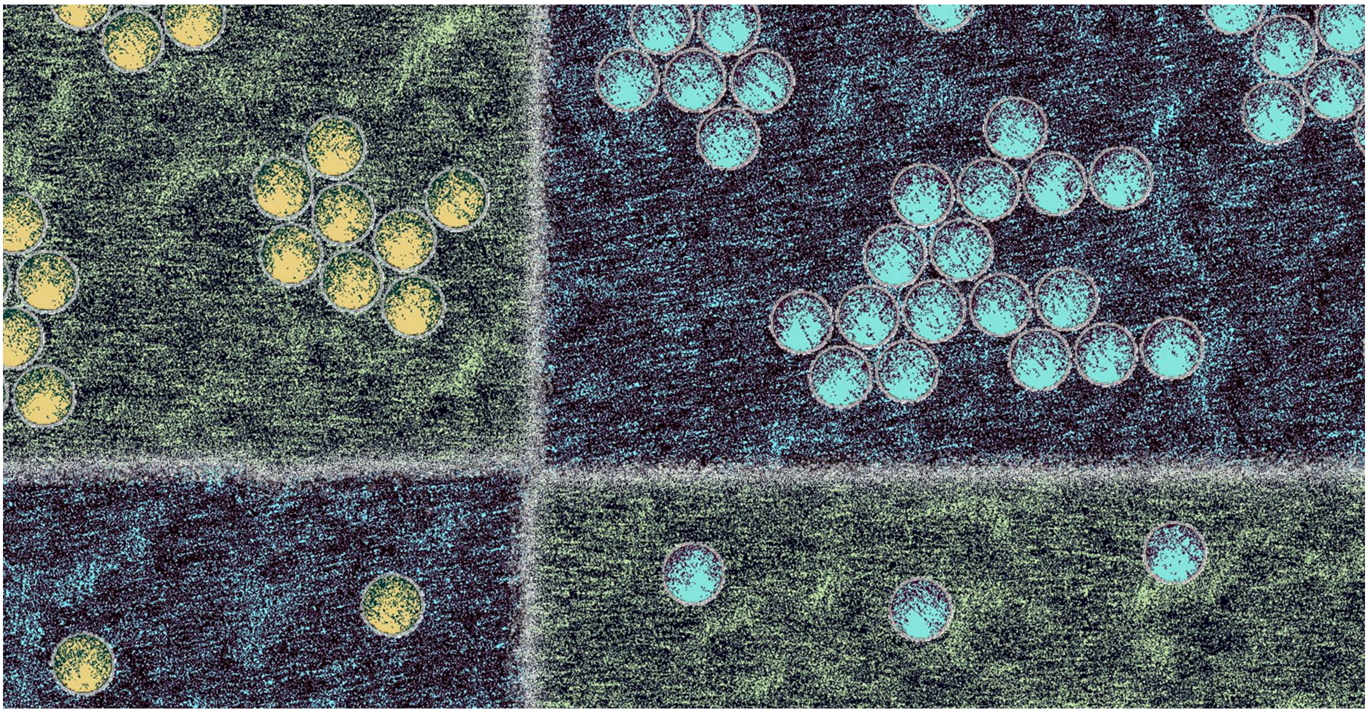
We have also designed a smaller five-gas device for use in paediatric medicine. This was a challenge, because we had to have a smaller internal volume than the adult devices – they are about 50ml inside, and the paediatric device needed to be less than a third of that. So, we scaled everything down, and the mechanical structure had to change quite a lot.

My engineering involvement is in the design of the device's head – the part with the optics in, and the breathing path. I do the engineering design and drawings – I tend to think in terms of the fine detail. This project is still evolving, with changes to design and data analysis giving performance improvements. I am not involved in the software development work though for the data acquisition and analysis; that's just magic! The custom electronics for the LGA were developed by the team in Chemistry's electronics workshop, with most mechanical parts made in the mechanical workshop. The LGA design has been a true team project.

It's been lovely to be a part of something that has involved the expertise of many talented colleagues, and the results have outperformed my expectations. Seeing the progress through from the early stages to its current real-world use has been a joy. I think it is the most satisfying project I have worked on." ■



This page: exploded view of laser gas analyser (LGA) measurement cell. Facing page, clockwise from top left: a photo of the LGA head with the lid removed; the LGA in use; consulting engineer with the Ritchie group, John Couper.



It’s not only opposites that attract

Oxford Chemistry study shows like-charged particles can come together

“Opposites charges attract; like charges repel” is a fundamental principle of physics. But a study published earlier this year in *Nature Nanotechnology* has demonstrated that similarly charged particles in solution can, in fact, attract each other over long distances. Just as surprisingly, the team found that the effect is different for positively and negatively charged particles, depending on the solvent.

Led by Prof Madhavi Krishnan, the team found that in water negatively charged particles attract each other at large separations whereas positively charged particles repel. The reverse was true for solvents such as alcohols. These findings are surprising because they seem to contradict the central electromagnetic principle that the force between charges of the same sign is repulsive at all separations.

Using a theory of interparticle interactions that considers the structure of the solvent at the interface, the team established that for negatively charged particles in water there is an attractive force that outweighs electrostatic repulsion at large separations, leading to cluster formation. For positively charged particles in water this solvent-driven interaction is always repulsive, and no clusters form.

Besides overturning long-held beliefs, these results have immediate implications for a range of processes that involve interparticle and intermolecular interactions across various length-scales, including self-assembly, crystallisation, and phase separation.

The team tracked negatively charged silica microparticles suspended in water using bright-field microscopy and found that the particles attracted each other to form hexagonally arranged clusters. Positively charged aminated silica particles, however, did not form clusters in water.

This effect was pH dependent: the team were able to control the formation (or not) of clusters for negatively charged particles by varying the pH. No matter the pH, the positively charged particles did not form clusters.

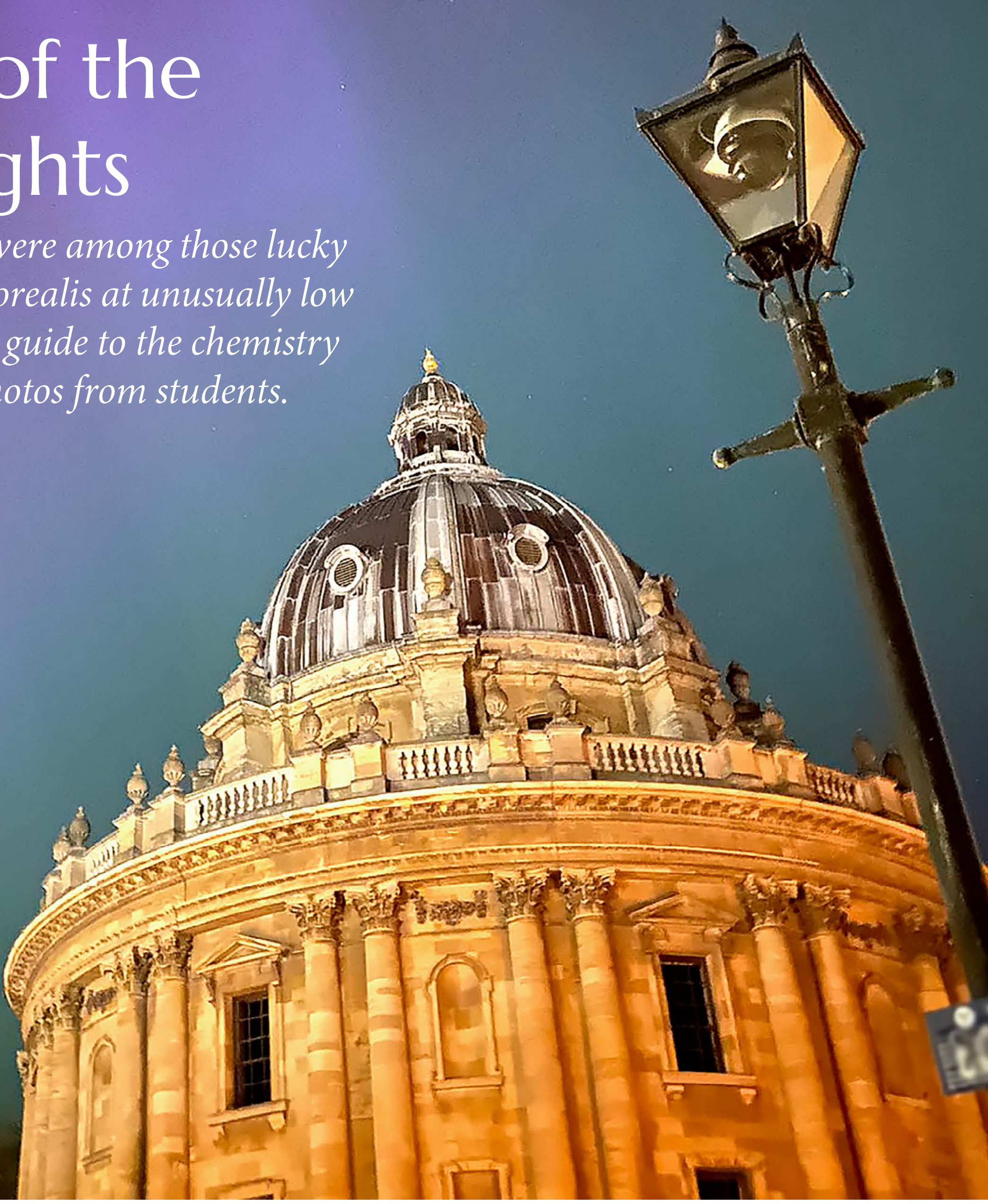
Naturally, they wondered whether the effect on charged particles could be switched, such that the positively charged particles form clusters and the negatively charged do not. This is exactly what they observed by changing the solvent to alcohols, such as ethanol, which has different interface behaviour to water. Now the positively charged aminated silica particles formed hexagonal clusters, whereas negatively charged silica did not.

According to the researchers, this study implies a fundamental re-calibration in understanding that will influence the way we think about areas such as pathological malfunction associated with molecular aggregation in human disease, or stability of pharmaceutical and fine chemical products. ■

Read more: Wang, S *et al.* A charge-dependent long-ranged force drives tailored assembly of matter in solution. *Nat. Nanotechnol.* **19** 485–493 (2024). doi.org/10.1038/s41565-024-01621-5

Chemistry of the northern lights

In 2024, Oxford residents were among those lucky enough to see the aurora borealis at unusually low latitudes. Here's our handy guide to the chemistry behind the colours, with photos from students.



What is the aurora?

Aurora borealis, also known as the northern lights, is caused by solar winds. Streams of high energy particles shoot from the sun towards Earth at supersonic speeds and disturb the patterns of the Earth's magnetic field.

Although most particles in the solar wind are deflected by the Earth's magnetic field, some are trapped and accelerated along the field lines towards the North or South Pole until they hit the atmosphere, causing the bright lights of the aurora.

Usually, auroras are only visible near the geomagnetic poles. In the north this means that aurora borealis is typically constrained to arctic regions. But, during periods of particularly intense solar activity as in mid-May this year, the strong solar wind can cause the aurora to be visible further south.

Why those colours?

Tall, waving curtains of green, blue, pink and purple light stretch for hundreds of kilometres through the night sky on nights when the aurora is visible. What causes the colours?

When the accelerated electrons hit gas atoms and molecules in the Earth's atmosphere, they provide a burst of energy that jolts them into high energy states. These atoms and molecules then relax down to their usual form, and in doing so they release light via a similar mechanism to a glowing neon discharge lamp.

The array of coloured light we see mostly corresponds to different energy gaps for oxygen and nitrogen in our atmosphere. For instance, oxygen atoms more than 60 miles high in the atmosphere generate the dominant green light. Even higher, above 150 miles, the oxygen atoms collide more infrequently and have time to undergo a slow transition that gives off red light. Lower in the atmosphere, excited nitrogen molecules can also emit blue and red light. The mixture of all of these reds, greens and blues leads to the dazzling array of colours seen in Oxford in 2024. ■

The Jamie Ferguson Chemistry Innovation Awards

The winners of this year's awards were announced in June by Oxford University Innovation (OUI) and the Departments of Chemistry and Materials

Now in their third year, the awards were created to honour the memory of Dr Jamie Ferguson who sadly lost his life during the Covid pandemic. Jamie was Deputy Head for Physical Sciences at OUI, and his guidance and passion helped Chemistry to become one of the most commercially engaged departments at Oxford.

The winning entries for 2024 highlighted some innovative concepts, and showed exceptional creativity and inventiveness. They included ideas such as cleaner hydrogen use in chemical production, an agrochemical for improving crop resilience to floods, advancements in materials for safer and more efficient batteries, and the development of new medical treatments using 3D printing.

The winners each received a £500 cash prize, a trophy in recognition of their achievement, and support from OUI to advance their idea towards commercial success.

Cath Spence, one of the judges from OUI, said: "It has been an honour to again judge this year's Jamie Ferguson Innovation Awards and witness the remarkable ingenuity of the participants. The winning projects, from sustainable hydrogen use to flood-resilient agrochemicals and advancements in battery safety, are not only groundbreaking but also have the potential to create real-world impact.

"We are excited to support these innovators as they take their ideas from concept to commercial reality."

Mairi Gibbs, Oxford University Innovation CEO, said: "OUI is very proud to celebrate the innovative achievements of this year's winners of the Jamie Ferguson Innovation Awards. Each of these projects demonstrates the impact potential of Oxford research and showcases the incredible talent and dedication of our community.

"Jamie's legacy of creativity and passion for science continues to inspire us, and these awards are a testament to his enduring impact on Oxford University Innovation and the Department of Chemistry."

The four winners – Alex Evans, Maya Landis, Rebecca Latter and Jorin Riexinger – explain their ideas across the page.

Alexander Evans, Maya Landis, Rebecca Latter and Jorin Riexinger, winners of the 2024 Jamie awards.

Maya Landis

Vincent group DPhil student

Hydro-green-ation: towards cleaner use of hydrogen in chemical synthesis

Today's methods for the hydrogenation of nitro-groups to amines, one of the most important processes in chemical industry, suffer from low selectivity and require elevated pressures of hydrogen gas. I presented a novel catalyst with high selectivity in the presence of a wide range of sensitive functional groups, that is able to produce amines at atmospheric pressure, room temperature, and in aqueous conditions – if applied, this innovation could help shift hydrogenation chemistry towards greater environmental sustainability.

Rebecca Latter

Flashman group DPhil student

An agrochemical promoting flood resilience – for when crops are out of their depth

Flooding is a major cause of crop losses globally and a problem that is being exacerbated by climate change. This threatens food security and is a source of instability in agricultural businesses. My PhD research has focused on an enzyme called plant cysteine oxidase which plays a key role in coordinating flooding adaptations in plants. We have been investigating whether inhibition of this enzyme prior to flooding, through the use of a chemical treatment, may promote plant flood tolerance. Following the identification of some small molecule inhibitors and some successful experiments in a model plant species, *Arabidopsis thaliana*, this was the idea that I presented at the Jamies.

Alexander Evans

O'Hare group researcher

Leading the charge: revolutionising battery safety and efficiency with next generation materials

Since their inception, the separator, a crucial component preventing short circuits in batteries, has not attracted proportionate attention compared to electrode and electrolyte components, despite its significant role in ionic mobility and safety functionality. Through technology that I have developed we can optimise the bottleneck in battery technology; offering the opportunity to develop a step change by using functional polypropylenes as the separator. Our patented flame retardant polypropylenes based on phosphorous bound moieties are self-extinguishing materials which can work to shut down battery fires at the point of ignition. Furthermore, we have recently incorporated and are actively evaluating bound carboxylates that will boost battery efficiency, translating to shorter charging times, an aspect fundamental to the electrification of the transport sector.

Jorin Riexinger

Bayley group DPhil student

A 3D-printed therapeutic platform

Synthetic tissues are soft and biocompatible structures composed of hundreds of compartments (volumes typically in the range of picolitres), resembling properties of natural tissues, such as communication. One way to form synthetic tissues is through 3D-printing, whereby the compartments are positioned in a lipid-containing oil, forming droplet interface bilayers (DIB) between compartments. DIB-based synthetic tissues can sense, store, process and transmit electrical and chemical signals in a patterned manner. Furthermore, compartments can contain living cells for the purpose of tissue engineering. Recent advancements in creating DIB-based synthetic tissues render them suitable as a versatile platform for therapeutic purposes. ■

Waynflete inaugural lecture

In January of this year Prof Véronique Gouverneur FRS gave her inaugural lecture as Waynflete Professor of Chemistry

Prof Gouverneur's lecture, delivered at the Examination Schools on January 19, was titled *Rethinking fluorine chemistry with global challenges in mind.*

She described her group's research, which is focused on fluorine chemistry, with an extensive research programme aimed at developing novel synthetic methodologies for the preparation of fluorinated targets.

Fluorine can be highly advantageous in pharmaceutical and agrochemical compounds as its presence can dramatically alter chemical and biological properties.

Prof Gouverneur became the Waynflete Professor in 2022. Previous Waynflete Professors include William Henry Perkin Jr. (the first head of the Dyson Perrins laboratory), Sir Robert Robinson, Sir Jack Baldwin, and most recently Steve Davies.

On her appointment to this statutory professorship, Prof Gouverneur said: "In Oxford, organic chemistry has been championed by illustrious Waynflete Professors, faculty members, and their teams: a glorious past. So, I am thrilled to take on the Waynflete Professorship.

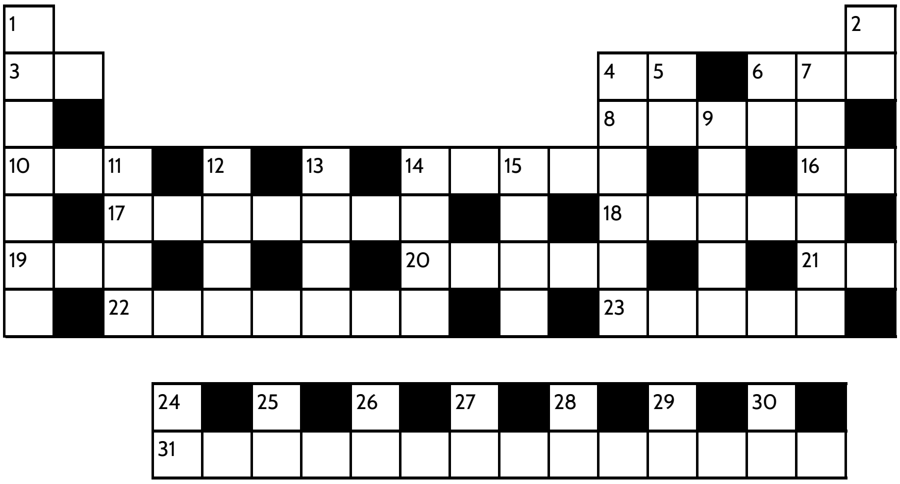
"I am convinced that our future is bright with the best of organic chemistry yet to come, and profound changes and unexpected advances ahead of us – most likely at the interface with other disciplines." ■

Chemistry puzzles

Solutions to the puzzles may be obtained by emailing chemistry-news@chem.ox.ac.uk

Periodic table crossword

Bonus once completed: how many of the 14 single-letter chemical element symbols can be found in their correct position in the periodic table?



Across

3 Abbreviation for Latin phrase "year of the Lord" (2)
4 Anything but 3 (2)
6 Frequently (3)
8 Temporary failure (5)
10 Goat child (3)
14 Each (5)
16 California city (2)
17 Gave in (7)
18 Musical notation for all players (5)
19 Musical style originating in Jamaica (3)
20 Snow shelter (5)
21 Negative (2)
22 Pencil brand with museum in Keswick (7)
23 Enclosed bundle of axons (5)
31 Expressing something that is not the case (14)

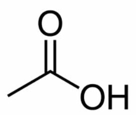
Down

1 Advocating warlike policies (7)
2 Towards (2)
4 Enid _____, children's author (6)
5 Metal in limestone (2)
6 Makers of Explorers and Landrangers (abbr.) (2)
7 Relating to Jellicles, perhaps (6)
9 _____ Mannion MP, Secretary of State for Social Affairs and Citizenship in *The Thick of It* (5)
11 A sociologically significant pairing, such as spouses or siblings (4)
12 Swerve suddenly (4)
13 Side (4)
14 Adjust, especially text (4)
15 Moray, conger, electric (4)
24 First predominantly artificial element (2)
25 Major constituent of brass and bronze (2)
26 Formerly the heaviest halogen, until tennessine was discovered in 2010 (2)
27 Transition metal used for shiny electroplating (2)
28 Alkaline earth metal used as a radiocontrast agent (2)
29 Silvery precious metal (2)
30 Metal that melts at 30°C (2)

Find the pairs

Can you match the common name for these chemicals to their molecular structures?

1 Paracetamol
2 Caffeine
3 Vitamin C
4 Teflon
5 Vinegar
6 Soap
7 Polyester
8 TNT

A


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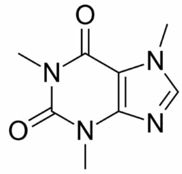

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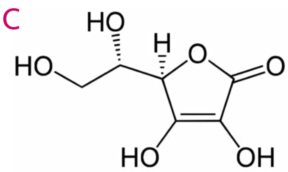

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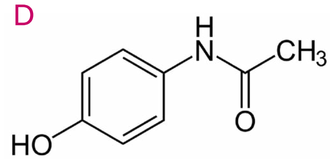

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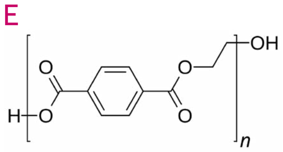

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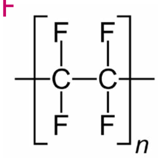

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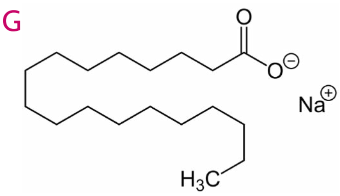

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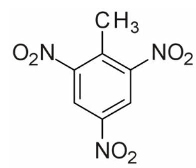

Imaging nanoparticles

Holography measures the phase and amplitude of light, and can be used to image nanoscale objects such as single molecules. Scientists from the Kukura group at Oxford Chemistry have demonstrated detection of the ultra-weak light scattering from single proteins using optical holography. The images above show the phase of the light scattered by single gold nano particles, amd the inset image shows a simulated ideal phase image of scattering particles. Read more about this study, which was recently published in Nature Photonics: doi.org/10.1038/s41566-024-01405-2

Contact us

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