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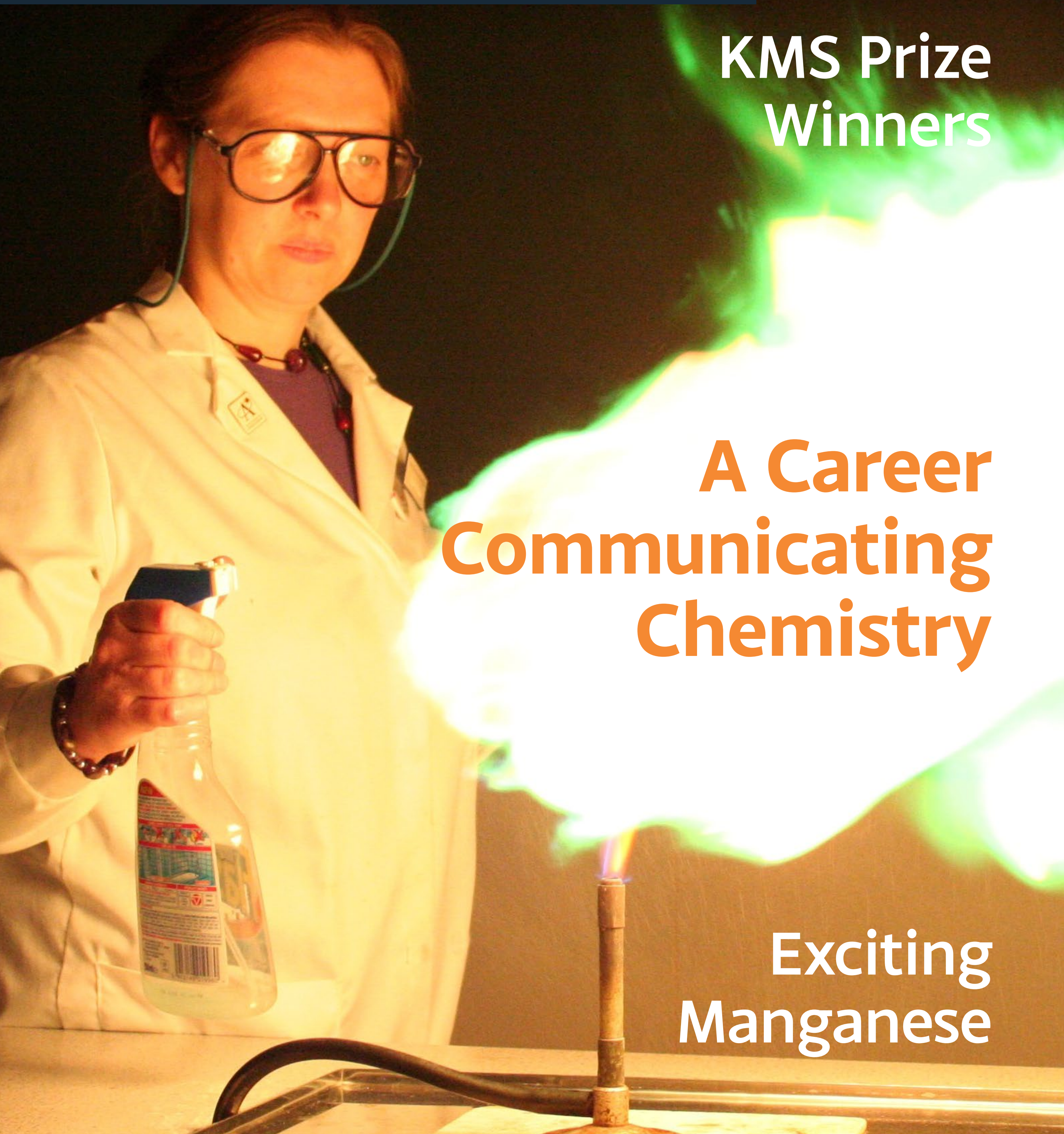
UNIVERSITY of York

ChemYork

HIGHLIGHTS FROM A LEADING UK CHEMISTRY DEPARTMENT



KMS Prize Winners

A Career Communicating Chemistry

Exciting Manganese

A chance to say 'Thank you'

PROFESSOR CAROLINE DESSENT, HEAD OF DEPARTMENT, INTRODUCES THE AUTUMN EDITION OF CHEMYORK.

Anyone who engages with the news will have learned that Universities are facing significant financial challenges. Like many institutions and businesses, inflation has hit budgets hard and geopolitics has meant that fewer international students have chosen to study overseas, reducing one of the important income streams. Our University has not been immune to these issues, so that budgets, spending and efficiencies have been somewhat unwelcome features of the last year.

In many respects, the Department of Chemistry at York entered this period well prepared. We have strong student numbers along with an exceptional profile of research grant income that combine to provide a firm foundation for our finances. However, we have still found ourselves needing to help the institution meet its budgetary goals, and this has led to some significant changes for us. Perhaps most notably, a group of our staff have chosen to retire, including a number who have worked in our department for decades. We are incredibly sad to lose all of them, and each of them has been essential to our success as a chemistry department. To give honourable mentions, we will be saying goodbye to Adrian Whitwood, Heather Fish, Julia Walton, Iman Khazul and Simon Grist from our technical staff, as well as Martin Cockett and Anne Routledge from our academic staff. Dr Annie Hodgson will also be retiring from her role as our exceptional and very long-standing schools' liaison lead. You can read more about Annie's career and exploits on page 6.

I sadly don't have the space here to write a tribute to each of these staff members, so I hope that the others on the list won't mind if I say a special thank you to one of them. Martin Cockett has been one of my Deputy Heads of Department throughout my tenure as 'HoD'. People often remark on how hard it must be being a HoD, but the job is made so much easier by having Deputies you can trust. Martin has been a steadfast pillar of sound advice, common sense and an absolutely confidential ear for me through all the challenges of the last four years. He understands the department, its history and the people who work here completely, and has striven to make this University the very best place it could be for both its students and its staff. Thank you, Martin. I've deeply appreciated what you've done as my Deputy-HoD even though I've not always found the time amidst the hurly-burly of being HoD to say it. We all very much hope you enjoy your retirement.

I've deliberately avoided saying that Martin's contributions are exceptional because all of our retirees have made exceptional contributions to our Department, whether through their technical expertise or their dedication to our students. It's certainly a feature of York Chemistry that it attracts and keeps absolutely outstanding staff who contribute so much personally to make this the special place that it is.

This issue features several excellent articles, and highlights some of our successes over the last year. We've been absolutely delighted to be awarded a new Athena SWAN Gold award, meaning that we have now been 'Gold' for a record-breaking 17 years (page 4). This year has been one when we've had great success with winning new grant funding to support PhD students. The article on page 3 highlights our two new programmes linked to training PhD students in Green and Sustainable Chemistry. This issue of ChemYork is a testimony to the fact that our department continues to thrive despite the challenges. I very much hope you enjoy reading it, and I hope you enjoy a Merry Christmas and a Happy 2025.

> "We've been absolutely delighted to be awarded a new Athena SWAN Gold award, meaning that we have now been 'Gold' for a record-breaking 17 years."

Front cover image: *One of Annie Hodgson's memorable demonstrations*

Compiled by *Duncan Bruce*

Designed by *Cookie Graphic Design*

Demonstrating Success

THE DEPARTMENT WAS DELIGHTED TO WELCOME BACK MRS GILL MAWBY TO PRESENT THIS YEAR'S ROGER J MAWBY DEMONSTRATOR AWARDS.

Dr Roger Mawby was a former, much-loved member of the academic staff of the department and a legendary and passionate teacher of our subject. After Roger died, Gill Mawby worked with us to establish annual awards in memory of her late husband to recognise the work done by our Graduate Teaching Assistants (GTAs) in supporting our undergraduates through their degree. GTAs are crucial to the teaching delivered in the Department and work in both the teaching laboratories as well as supporting workshops in Maths and Quantum Chemistry. Up to six awards are made each year to GTAs who are judged to have gone 'above and beyond' in carrying out their role.

Gill is pictured with this year's winners (L to R) Lukas Geciauskas, Stuart Smith, Oliver Stevens, Edward Cummings and Hannah Chapman and with Derek Wann who chaired the Awards Panel. (Ana Silva Terra was also a winner but was not able to be present for the photo.)

New CDTs get underway

AS REPORTED BRIEFLY IN THE STOP PRESS IN THE LAST ISSUE OF CHEMYORK, THE DEPARTMENT HAS BEEN SUCCESSFUL IN SECURING FUNDING FOR TWO OF THE NEW CENTRES FOR DOCTORAL TRAINING, FUNDED BY UKRI.

With both bids led on behalf of York by Professor Helen Sneddon, the first is Process Industries: Net Zero (PINZ) with Newcastle University and the second is Chemical Synthesis for a Healthy Planet (CSHP) awarded with the University of Oxford. Each is backed by a range of large companies as well as SMEs (the companies involved can be found on the websites) and between them, the two CDTs should result in more than 27 PhD studentships to York over 8 years.

The PINZ CDT launched in September 2024 and we have been delighted to have hosted visits from several of the companies supporting the consortium. Two York students started in the first cohort, Ben Chapman (supervised by Ian Fairlamb) and Salome Raymond (supervised by Terry Dillon and Helen Sneddon); recruitment is underway for the second cohort.

Meanwhile, the CSHP CDT is getting ready to launch in September 2025. Substantial effort went in over the summer organising networking events, at both Oxford and York, to identify potential synergies where joint projects could be envisioned, and to encourage academics to engage with the CDT both as individuals and as teams. Of the 28 projects advertised in the first round of recruitment, 8 are York led, with a further 7 Oxford-led projects also listing a York co-supervisor.

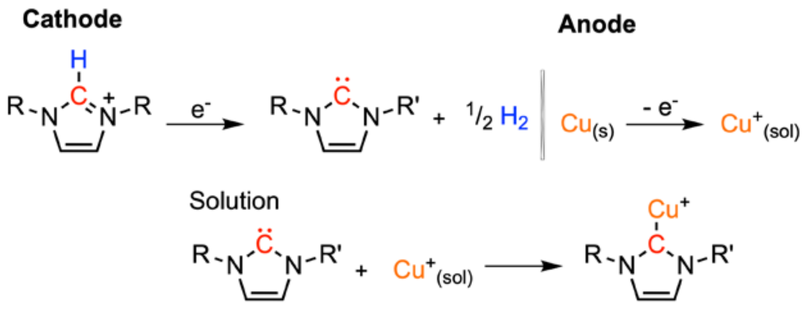
With announcements of new and renewed Doctoral Partnerships from NERC (see Stop Press), our new MSc in Data Science (page 5), previous successes with, for example, the innovative EPSRC Mobility DTP that allowed students to study for their PhD in a workplace environment and of course our long-standing MSc in Green Chemistry and Sustainable Technology, the Department is demonstrating that it is an excellent place for students to undertake postgraduate training.

PROCESS INDUSTRIES: NET ZERO
CENTRE FOR DOCTORAL TRAINING

In My Element - Copper

^{29}Cu

IN THE SECOND IN THIS NEW SERIES FEATURING COLLEAGUES AND THEIR FAVOURITE ELEMENTS, DR CHARLOTTE WILLANS, WHO JOINED THE DEPARTMENT FROM THE UNIVERSITY OF LEEDS IN 2023, GIVES US SOME NEW ANGLES ON A WELL-KNOWN ELEMENT THAT STILL HAS MANY SECRETS TO GIVE UP...

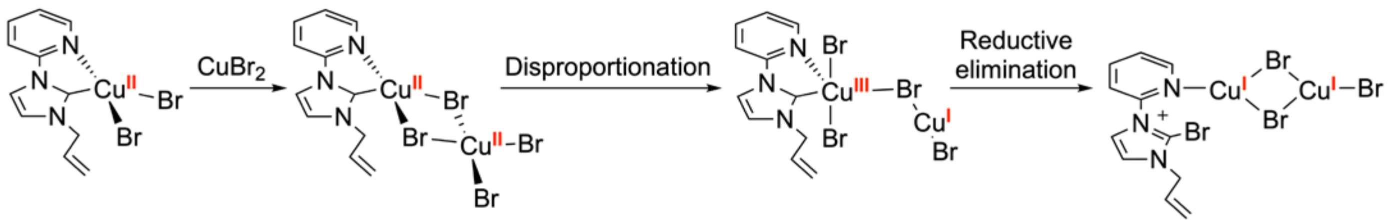


Electrochemical reactor

When I started my academic career, I was keen to focus on an area of research with sustainability in mind and catalysis using Earth-abundant base metals was becoming popular as a potentially sustainable alternative to precious-metal catalysis, particularly for industrially relevant transformations. Sitting in Group 11 just above silver (the element featured in the last edition) copper is found for example in metalloenzymes where it is responsible for transformations with no parallel in *in vitro* chemical synthesis. What then could we learn about its behaviour and how it might be tamed for greater industrial use?

Our early contributions involved electrochemical synthesis of organo-copper complexes (*Chem. Commun. 2012*, **48**, 4887), which we then translated into flow electrochemical synthesis (*Chem. Commun. 2015*, **51,** 1282). Copper can be oxidised electrochemically from a sacrificial anode, releasing ions into solution and with concomitant reduction of a ligand precursor at the cathode, the complex forms in situ. The beauty of this technique is that it uses electrons rather than harsh chemical oxidising and reducing species, and the only by-product is hydrogen so that the reaction is extremely atom efficient.

A key aspect of further developing copper in catalysis is to have a deeper understanding of how it behaves mechanistically. We have, therefore, focused on deactivation pathways with an example shown in the figure below, in which excess metal salt present in the reaction results in deactivation via disproportionation and subsequent reductive elimination (*Organometallics 2015*, **34**, 3497 and *Chem. Sci. 2017*, **8**, 7203). As copper continues to give up its secrets, new (pre-)catalysts and reaction conditions will emerge to allow it to move centre-stage in industrial processes.



Department Retains Athena SWAN Gold Award

IN THE EARLY AUTUMN, THE DEPARTMENT LEARNT THAT ITS APPLICATION TO HAVE ITS ATHENA SWAN GOLD AWARD RENEWED HAD BEEN SUCCESSFUL.

The Athena SWAN Charter is a framework that is used across the globe to support and transform gender equality within higher education (HE) and research and the Gold Award is the highest level achievable. York Chemistry was the first Department ever to be awarded Gold status in 2007 and has held the Award at that level ever since. This application, which was put together by the EDI Committee chaired by John Slattery, contains an ambitious action plan for the coming years and a more detailed account will follow in a later issue.

Data, data everywhere...

THE 2023-24 ACADEMIC YEAR SAW THE LAUNCH OF A NEW MSC PROGRAMME WITHIN THE FACULTY OF SCIENCES ON THE SUBJECT OF DATA SCIENCE, WITH CHEMISTRY TAKING A LEADING ROLE. PROFESSOR KATHRYN COWTAN HAS PLAYED A KEY ROLE IN BOTH CONCEIVING THE COURSE AND IN DELIVERING ITS CONTENT. CHEMYORK CAUGHT UP WITH HER FOR SOME REFLECTIONS ON HOW THE FIRST YEAR HAD BEEN.

Why was this a good time to launch this new degree programme?

Data science is transforming almost every area of life, including the sciences. For the whole of my career we have been solving computational problems to enable scientific progress, but in recent years the computing tools and sheer size of data sets available to us have crossed a tipping point which has made data science an indispensable tool. However, it is often the case that an individual will know their subject, but not how to manage the data or, conversely, may have all the data skills without the specialist insight into a particular problem. As such, this course represents a great opportunity to address this issue, providing a route for students to move into data science to meet both academic and commercial demand.

What are the typical backgrounds of the students who took the course?

Some students come from a background in the Natural Sciences or Medicine and are looking to add computational and data science skills to their toolbox; we teach programming from scratch to support these students. In addition, we also have students from Maths and Computing backgrounds who are looking to get experience on practical problems in the sciences. All of this is done against an interdisciplinary background to give students flexibility with their future career options.

What's the kind of material that is covered?

We teach the widely used Python programming language, starting from scratch and using practical problems rather than abstract theoretical concepts. This is followed by data analysis and machine learning techniques, as well as the tests we do to make sure that our results are meaningful. We also teach students how science works, the importance of inclusion to the scientific process, and how to read and write papers in different disciplines. Students take option modules exploring data science in two different disciplines, and perform a research project addressing a novel scientific problem.

How does all of this relate to research in Chemistry?

Despite working in the field, I was surprised at how many areas of chemistry have been touched by data science. My own work has focused on determining the structures of biological molecules, however when asking colleagues for project ideas, we got examples spanning spectroscopy, molecular properties, atmospheric chemistry, instrument development and many others.

What have been the biggest challenges in launching and then running the course?

This biggest challenge we faced in developing the course was the timescale. Given the demand for courses in this area, we developed and launched the course in only 18 months. Monumental efforts from my colleagues Dr Alan Lewis (below), Dr Conor Rankine, while the Chemistry Graduate Office were instrumental in making this possible.

What might typical jobs and careers be for graduates from the course?

Pharmaceutical and other high tech industries often offer graduate programmes as a starting point for building a career and these were one key destination we had in mind when designing the course. Other likely destinations include science, health and environmental policy, biotech and medtech, science consultancy, as well as science research.

Reaching Out

AFTER MANY YEARS OF POPULARISING CHEMISTRY TO GENERATIONS OF SCHOOLCHILDREN AND THE WIDER PUBLIC, DR ANNIE HODGSON RETIRED AT THE END OF SEPTEMBER. HERE SHE REFLECTS BACK ON THIS WORK AND SOME OF HER MORE MEMORABLE EVENTS AND AUDIENCES.

How did you first get interested in Science?

My mother was very accommodating of the home-based experiments I did with my father on her kitchen window ledge and this initial interest developed further at school in Beverley with a couple of inspirational teachers - one each in Biology and Chemistry. In particular, Mr Peace was very keen that we all developed good chemistry laboratory skills and so I've always seen the importance of the practical side of the subject.

After O- and A-levels, I went to Nottingham University to study Biology, taking Chemistry as my subsidiary in Year 1 - a choice that would ultimately prove invaluable.

How did your involvement with outreach first begin?

After my Biology degree, I took a PGCE at the University of York. In those days the Science Education Group was based in the Chemistry Department, where I enjoyed getting to know several members of staff. Armed with my qualifications I went to work as a Science and Biology teacher at Thirsk School where I really enjoyed inspiring the young people and always tried to find the 'wow factor' or 'memorable moments' in my lessons However, after four years it was clear to me that teaching was not likely to be the way I wanted to spend the rest of my working life, so I applied to join David Goodall's research group and work towards my DPhil. I arrived back in the Chemistry Department at York in October 1989 and have been here ever since!

Throughout my time in the research group, and as I began my career in the department, I sought opportunities to communicate science to the public and to young people in particular. I became involved with various University initiatives, such as trying to set up a science discovery centre in the city.

It was around this time that my long relationship with the Salters Institute began, when I organised their annual Teachers' Conference, after which York was one of two universities invited to hold one of its inaugural Salters' Chemistry Camps for GCSE students, which continued until 2015. I was the University host and ran some of the activities for the camps until sadly they came to an end.

You've popularised Chemistry to children of all ages, from the very young to those about to go on to higher education. How different are the approaches you take?

I love the challenge of communicating science to all age groups and abilities. At public science fairs, such as the Tomorrow's World Roadshow, The British Association Festivals of Science and city-centre events organised by the University of York, one minute you can be talking to a six year old, the next minute a retired science professor. The knack is to enter a dialogue to find out their level of knowledge and build upon that. Of course, public events can attract people with some strange concepts and I once had a surreal conversation in a Dublin shopping centre with an individual who informed me that the double-helix model of DNA was all wrong! Rather DNA is a nine-stranded molecule with a tenth, ethereal strand – it was hard to know where to go with that conversation!

In 2006 I was invited to deliver the Yorkshire Philosophical Society family Christmas lecture in the Tempest Anderson Hall, which was the genesis of my now famous Colourful Chemistry lecture, which I have delivered all over the country from Caithness to Dorset and Limerick to Lincolnshire. That the lectures have been memorable in the minds of the audience is perhaps reflected when out shopping and overhearing children saying to their parents, 'That's the science lady!'

My involvement with Scouting and Guiding has led me to run science events for these organisations and I obtained an RSC grant to run 'Wild about Chemistry'" to mark Chemistry Week in 2015. We had hands-on chemistry experiments in the great outdoors for 445 members of the Scout movement from Beavers to Explorers and Leaders. I have been instrumental in running day-long events for Girl Guides from across Yorkshire to encourage women into STEM subjects, but I also do things on a smaller scale. One of the most touching moments was when a five-year old Rainbow Guide said to me, "I have always dreamed of being inside a bubble, and now my dream has come true". That's the power of chemistry.

As well as taking Chemistry to the streets of York, Designer Outlet and the Centre for Early Music, you've been to CERN and Australia. Can you tell us a little bit about this international dimension?

Chemistry outreach has certainly taken me all over the world. For example, launching the Molecules for Life project, about DNA, as part of a UK delegation to Science on Stage at CERN in November 2005. Alongside the talks, shows and exhibits we had the chance to visit the Large Hadron Collider. Big science in an amazing setting.

I was honoured to be invited to accompany A-level students from the UK to attend the International Science School at the University of Sydney on two separate occasions, each time looking after five students. A real scientific highlight of these trips was being able to spend quality free time with world-leading scientists and on one visit I had lunch with Dame Jocelyn Bell Burnell (of pulsars fame) on her birthday. She gave one of the best lectures I have ever heard, and she kindly allowed us to publish an article in Chemistry Review, based on a transcript of her dynamic talk.

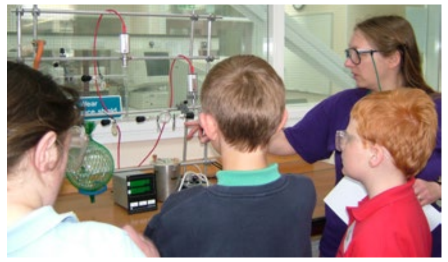
You've mentioned *Chemistry Review* which you have edited for some 28 years. How did you get involved and what happens to it now?

I took over as the editor of the A-level magazine *Chemistry Review* when founding editor John Garratt retired and my first issue was published in September 1997. My last issue marks the end of Volume 34 and will appear in April 2025.

I am delighted that the magazine will be in safe hands. Ably supported by Lisa Mayer, Andy Parsons is taking over, ensuring that *Chemistry Review* will continue to go from strength to strength, inspiring new generations of young chemists.

What's your favourite demonstration and which one goes down best with audiences?

Stolen from Paul Walton, my favourite has to be the 'fireflies', which involves a very large round-bottomed flask



filled with air and ammonia. Warm chromium(III) oxide is added to the flask, which catalyses the conversion of ammonia and oxygen to nitrogen and water. This is an exothermic reaction, so the particles of Cr_2O_3 glow red hot and float around inside the flask, looking for all the world like fireflies. Really rather beautiful.

However, the one that gets the gasp from the audience is adding dry ice to a solution of sodium hydroxide containing universal indicator and watching it bubble away, producing billows of water vapour as the colour changes gradually from purple to blue to green. The real wow moment is when the whole liquid suddenly turns yellow.

In an age where people, and especially younger people, tend to access their information online, how important do you think the kind of outreach you've practised for so long will be in the future?

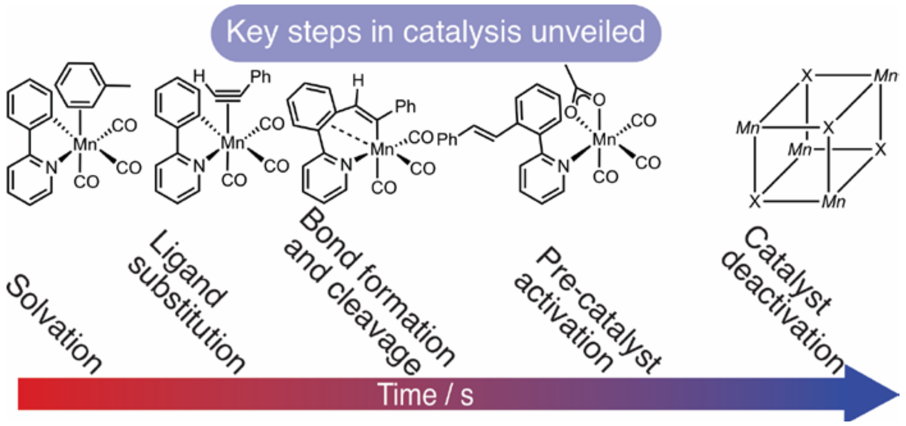
To experience hands-on experiments and demonstrations in real life makes science more tangible rather than something generated for a screen. Primary school age pupils see science as something wonderful and exciting, and my aim has always been to light a spark at a young age and then keep feeding the fire as they progress through their education.

There can be a perception that science is hard and impenetrable, but with careful thought just about any concept can be presented in a way that non-specialists can understand. As such, I believe strongly that it is important for the public to be able to meet scientists in person to understand that they are real, approachable individuals, just like them.

> "We need the next generation of science enthusiasts to take up the torch to continue inspiring young people for years to come."

Shining a light on manganese catalysis

A BROADLY BASED COLLABORATION HAS SHOWN HOW FAST INFRARED SPECTROSCOPIC METHODS HAVE LED TO A DEEP UNDERSTANDING OF CATALYTIC PATHWAYS STARTING FROM MANGANESE CARBONYLS.



As noted in the Stop Press of the last edition, earlier this year Ian Fairlamb and Jason Lynam published an overview paper in *Accounts of Chemical Research* summarising eight years of ground-breaking, published work in understanding sustainable catalytic reactions. The article detailed their studies showing how reactions catalysed by manganese, an Earth-abundant element, are able to functionalise carbon-hydrogen bonds selectively to allow carbon-carbon bond formation. The methodology allows for the step- and atom-efficient generation of compounds suitable for use in the pharmaceutical and agrochemical industries.

Their work focused on understanding how manganese compounds perform these remarkable transformations from the very fast chemical processes that govern how the compounds are activated, through to their final fate in the reaction. To study the fastest process, the team used time-resolved infra-red spectroscopy in which a sub-picosecond laser pulse activates each manganese compound, while a second pulse probes the changes that have occurred. The experiments, some of which can now also be carried out in-house using the infrared facility described on page 12 in this issue, were suggested by their Departmental colleague, Anne Duhme-Klair and were performed at the Central Laser Facility (CLF) at the Rutherford Appleton Laboratory. Some years later, Lynam and Fairlamb then realised that this method could be used in their related work on the applications of these complexes in chemical synthesis. Indeed, subsequent experiments at the CLF showed that it was possible to observe directly, for the first time, the key mechanistic steps in manganese chemistry, including the quantification of carbon-carbon bond formation.

Mechanistic catalytic work, which began in York in 2014 using infrared spectroscopy, mass spectrometry and low-temperature NMR techniques, showed that a key 7-membered intermediate acted as an pivot point for different reaction products on a timescale of seconds. That work was carried out by PhD students plus a team of MChem summer and overseas visiting students. The team further examined the pathways leading catalyst deactivation, namely manganese clusters incapable of productive catalysis and so provided insight into how future generations of active and long-lived catalyst species can be generated.

The impact of this work was recognised through the award of an RSC Horizon Prize in Physical Organic Chemistry in 2021, reflecting the multifaceted effort needed to achieve these advances and the winning team included staff at the CLF, industrial sponsors Syngenta and students from the Department. The paper is also a landmark as Fairlamb and Lynam have now published over 50 papers together as co-authors, the product of a long-standing collaboration covering aspects of synthetic and mechanistic inorganic and organic chemistry and its interface with catalysis and medicinal chemistry.

> “Through great teamwork, a comprehensive view of catalyst behaviour has been obtained by integrating studies from the picosecond timescale to those occurring over minutes and hours - a range of some sixteen orders of magnitude in time.”

ChemYork

For Excellence

FOUR FINAL-YEAR PHD STUDENTS, THIS YEAR’S WINNERS OF THE KMS PRIZE, PRESENTED ON THEIR RESEARCH AT A DEPARTMENTAL SYMPOSIUM IN OCTOBER. HERE THEY TALK ABOUT THEIR WORK AND WHAT IT MEANS TO THEM.

The Kathleen Mary Stott (KMS) Prizes are awarded competitively to up to four final-year PhD students each year. Prizewinners are selected based on the excellence of their science and their ability to communicate it alongside a broader sense of their contributions through published work, conference attendance, outreach and the like. The winners present their work at a Symposium at the beginning of the academic year in one of the Department’s highlight events.

This year’s winners give a brief account of their work.

Abby Walklett’s project is supervised jointly by Martin Fascione and Gavin Thomas in Biology.
Human cells are covered in the ubiquitous sugar, sialic acid, which is able to signal that the cell it is covering is benign and not a target for the immune system. My research focuses on its ‘evil twin’, pseudaminic acid, which is present on the surface of many pathogenic bacteria and allows them to evade attention of the body’s immune system. My work has contributed to the identification and biochemical characterisation of the first dedicated glycosyltransferase enzyme, which the bacteria use to coat their surface. Now with detailed knowledge of its structure, it becomes possible to design specific agents to inhibit its function and, because this enzyme has no mammalian equivalent, then this should be possible with no collateral damage to the organism. This research is then of direct benefit in the broader goal of tackling the crisis in antibiotic resistance.

Chloe Johnson has been working with Andy Weller and Simon Duckett.
My research has focused on single-crystal to single-crystal transformations of gold(I) phosphine complex in collaboration with Jesús Campos in Seville, Spain. The work has allowed for the isolation of the first π-acetylene complex of gold(I), which matters as alkynes are important chemical feedstocks, and π-alkyne complexes are proposed key intermediates in gold-catalysed alkyne functionalisation. Such complexes had not previously been isolated due to their instability in solution, but by synthesising the complex in the solid-state by addition of gaseous acetylene to a gold(I) phosphine precursor, we were able to prepare and characterise the new complex directly as its single crystal.

Juliet Barclay is completing her PhD with Paul McGonigal, investigating state-independent ionic conductivity.
Electrolyte design is crucial for the creation of high-efficiency electronic devices. Most utilise fluid electrolytes due to their high ionic conductivity, but these present safety issues and so solid-state electrolytes are an alternative. However, there remains a fundamental hurdle in preserving electrolyte properties across transitions between different states of matter of the same material. My research focuses on developing a series of cyclopropenium-based electrolytes which maintain the same mechanism of ionic conductivity across three states of matter: isotropic liquid, liquid crystal and crystalline solid. This is achieved by minimising ion pairing interactions between diffusely charged cations and mobile counterions, which then assemble in a stepwise manner to maintain structural flexibility into the solid state, so preventing a steep fall off in conductivity. These features are extended to give design rules which could be used to develop new electrolytes, opening up opportunities to exploit ionic conductivity in organic solids.

Sam Wilson is based in WACL under the supervision of David Carslaw, James Lee and Naomi Farren.
My research investigates how vehicles contribute to air pollution in urban areas, focusing on harmful pollutants such as nitrogen oxides (NO_x), particulate matter (PM) and ammonia. Using advanced roadside techniques and a mobile laboratory, I measure emissions under real-world conditions. These data provide valuable insights into how vehicle technology affects air quality and informs national policy. For example, I’ve evaluated the impact of the UK’s promotion of diesel fuel (2001–2015) on NO_x emissions, mapped the spatial distribution of PM in Central London, and conducted the UK’s first roadside ammonia measurements using a novel point sampling technique, developed at the University of York.

STOP PRESS

Changes at the Top - New HoD and DHoD

With Caroline coming to the end of her tenure as Head of Department, Derek Wann has very recently been announced as her successor and will assume office on 1 March next year.

In addition, Martin Cockett is retiring at the end of the calendar year and will be succeeded in his Deputy Head of Department role by Avtar Matharu.

There will be more on this story in the next edition.

New Doctoral Landscape and Doctoral Focal Awards

In addition to the new CDTs featured on page 3, Chemistry is part of the following Doctoral Awards from NERC:

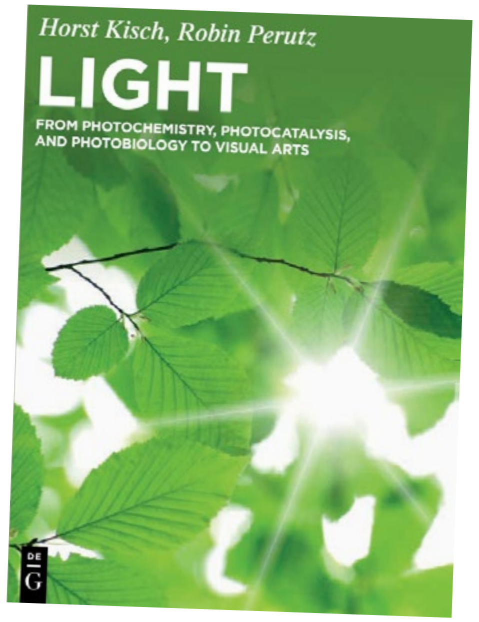
- Yorkshire Environmental Science Doctoral Training Network (YES-DTN), which involves colleagues from WACL (local coordinator Dr Pete Edwards) and partners from the University of Leeds;
- Adapting to the Challenges of a Changing Environment (ACCE+) with a number of colleagues in analytical science (local coordinator Professor Kirsty Penkman) and partners from the Universities of Liverpool and Sheffield;
- Ecosolutions involving colleagues from WACL and Green Chemistry (coordinated locally by Professor Mat Evans and Helen Sneddon) with partners from the University of Sheffield and the NERC Centre for Ecology and Hydrology

In addition, BBSRC has supported the Yorkshire Bioscience Doctoral Landscape Award (Training Award) involving colleagues drawn mainly from YSBL (local coordinator Professor Gideon Grogan) with partners from the Universities of Leeds and Sheffield.

Ecosolutions represents new investment, while the other three consortia are being funded for the third time, pointing to the success of these networks in training postgraduate students.

Seeing the Light

ROBIN PERUTZ TELLS OF THE NEW BOOK HE HAS CO-AUTHORED WITH A FRIEND FROM POSTDOC DAYS.



While light is central to our existence, sometimes we need to take a step back to recognise the many ways in which it impacts our own and other lives through photochemistry – vision, film photography, atmospheric ozone, light-driven (circadian) rhythms of waking and sleeping, photosynthesis, communication of creatures in the ocean…. Indeed, how many Nobel Prizes are relevant? Even I was surprised, 14 in the last 35 years: examples include molecular motors, light-emitting diodes, super-resolution imaging, the visual cycle and green fluorescent protein. Two more in 2023: attosecond spectroscopy and quantum dots. The central principles of photochemistry expand outwards to encompass photobiology at one side and semiconductor photocatalysis the other. In my own work on solar energy conversion, both the physics and biology are important.

Some 50 years ago, I was a postdoc in Germany and made friends with Horst Kisch. In 2021 Horst sent me a copy of his new book and a little later wrote inviting me to translate it into English and fill in a few gaps. In the event, we have added so many topics that the new English version is more than twice as long as the German original. Fortunately, Horst was wonderfully open to my suggestions and *Light: From Photochemistry, Photocatalysis, and Photobiology to Visual Art* was conceived and born, being published a couple of months ago.

Photobiology is often kept separate from photochemistry, but all the same concepts arise in biological systems: light emission, energy transfer, electron transfer, bond making and breaking. One surprise was that there is no unifying biological mechanism for chemiluminescence: the firefly, the jellyfish and the limpet all do it differently. We hope that the book will act as a bridge encouraging traffic between photophysicists, photochemists and photobiologists.

Horst's original version included a short, final chapter on the role of light in religion, philosophy and art. This chapter was by far the most taxing to translate! I took the opportunity to add photography: surely the biggest revolution driven by photochemistry. Even York Minster gets a mention.

Light: From Photochemistry, Photocatalysis, and Photobiology to Visual Arts by Horst Kisch and Robin Perutz is published by de Gruyter.

Twenty years on - where it all STEM-ed from

As part of their 20th birthday celebrations, STEM Learning has recognised the fantastic contribution made by founding director and former member of this department, Professor Sir John Holman, by naming the practical section of their state-of-the-art facilities the Sir John Holman Laboratories.

The National STEM Learning Centre in York, which is housed in its own buildings on Campus next to the Hull-York Medical School, opened in 2005 with John, who led the bid for government funding, appointed as its Founding Director. A key feature of its work is in providing the opportunity for teachers and technicians to improve their confidence in teaching practical science, health and safety and much more, which it does in its excellent laboratories.

Indeed, the practical side of science has been central to John's approach to teaching (he once observed that 'Studying science without experiments is like studying literature without books') and generations of our undergraduates will remember the demonstrations that accompanied his lectures on thermodynamics. Indeed, his famous 'screaming jelly baby' put paid to the idea that thermodynamics was anything other than the most exciting of topics!

John's influence on the teaching of Chemistry and indeed of science more widely cannot be overstated and the naming for him of STEM Learning's laboratories is a fitting tribute to his many and inspirational contributions.

Angelo's Antibiotics

WITH THE INCREASING PRESENCE OF ANTIBIOTIC-RESISTANT BACTERIA, THERE IS A PRESSING NEED TO DISCOVER TOTALLY NEW FAMILIES OF ANTIBIOTICS AND ONE SOURCE ARISES FROM THE CHEMISTRY OF METAL COMPLEXES. BUT HOW TO FIND THAT ELUSIVE NEEDLE IN THE HAYSTACK OF POSSIBLE LEADS? THIS IS THE QUESTION THAT OUR NEW ACADEMIC COLLEAGUE, DR ANGELO FREI, HAS STARTED TO ADDRESS.

Once described by his PhD Supervisor as 'a bit like an electron, all over the place' (which he describes as quite accurate), Angelo was born in the South-Eastern part of Switzerland making him one of fewer than 50,000 people speaking Romansh – the country's fourth official language. After quite an itinerant childhood (9 moves in his first 18 years), he eventually began a degree in Physics at the ETH in Zurich but quit after just one semester, instead getting by as a poker dealer in a somewhat dubious establishment. Then finding his intellectual home in Chemistry, Angelo completed his Bachelor and Masters degree at the University of Zurich, working with Gilles Glasser for his Masters thesis studying ruthenium complexes as potential photosensitisers for photodynamic therapy, sparking an interest in metal complexes for medicinal applications. He stayed at the University for his PhD with Roger Alberto, working with cyclopentadiene complexes of radioactive technetium and its congener rhenium for theranostic applications. Angelo was then on the move again with postdoctoral fellowships in Queensland (Matt Cooper and Mark Blaskovich) and with Nick Long at Imperial College, before being awarded a highly competitive Ambizione Fellowship from the Swiss National Science Foundation at the University of Bern in 2022. This enabled him to begin his independent career and he followed this with a move to a Lectureship in York earlier this year.

The main thrust of his research focuses on antimicrobial applications of transition metal complexes and, with the help of robots and machine learning, the group aims to synthesise and test more than 10,000 novel complexes in the next five years, evaluating their potential ability as antibiotics. Of course, any of these compounds could also find applications against other diseases such as malaria and fungal infections or in a range of other applications. As such, this high-throughput approach is accompanied by more detailed mechanistic studies and further development of promising candidates. When not at work Angelo enjoys spending time with his wife, his dog Bonnie, cooking, wine, (and more recently) playing padel and pickleball.

New ultrafast lasers shed light on protein structure

THE ARRIVAL OF A NEW £1M INFRARED LASER FACILITY WILL LEAD TO A STEP CHANGE IN THE ABILITY TO STUDY PROTEINS IN SOLUTION AND MUCH, MUCH MORE...

The Department has welcomed the arrival of a new state-of-the-art, ultrafast infrared laser system designed to advance our understanding of protein structure and dynamics. Research in Neil Hunt's group uses ultra-short, sub-picosecond pulses of infrared laser light to record 2D-IR spectra – essentially a two-dimensional 'fingerprint' of a molecule's vibrations. In the case of proteins, these 2D fingerprints are extremely sensitive to secondary structure, which is, in turn, linked closely to a protein's function. A major strength of 2D-IR spectroscopy is that it can be used to measure protein structure in solution at room temperature, bringing us closer to the goal of observing protein structure directly under physiological conditions.

The new laser system, funded by a £1M strategic equipment grant from EPSRC, can record a 2D-IR spectrum in around one minute using just 20 microlitres of sample, whereas previously the same spectrum might have required 30 min acquisition time! Perhaps most importantly, the use of pulsed lasers allows 2D-IR to suppress strong absorptions from water that overlap strongly with protein signals, allowing 2D-IR to 'see through' the solvent, akin to seeing the needles in the proverbial haystack.

The design of the instrument was first introduced by the UK's Central Laser Facility, based at the Rutherford Appleton Laboratory near Didcot, with whom Neil's group has collaborated for many years. The grant to build the instrument in York is part of a UKRI strategy to roll-out world-leading technology to UK Universities as the national facilities move on to their next stage of development. As such, the York 2D-IR instrument is available for wide use by academics and industry, and has already played host to collaborative research with academics from Sheffield to Stellenbosch and with several pharmaceutical companies.

The ability to measure protein structure in solution quickly with only small amounts of material has opened up a number of new projects. For example, 2D fingerprints of proteins are very sensitive to the binding of small molecules, meaning that there is a role for 2D-IR in drug design. Thus, it fits into a niche between high-throughput screening methods such as surface plasmon resonance, which miss out on structural information and very high resolution, but lower throughput methods like X-ray crystallography, which need low temperatures and solid-phase samples.

Measuring structure-specific protein fingerprints also creates opportunities for 2D-IR in protein analysis, whether as a tool to confirm that proteins are folded correctly or to ensure that synthetic proteins match their biological target and are unaffected by storage or transport. The instrument has also been used to study structures of novel cyclic peptides designed to combat antimicrobial resistance with colleagues from South Africa.

The ability to measure 2D-IR fingerprints also means that it is possible to unravel contributions from mixtures of proteins, leading to applications in the analysis of biofluids such as blood serum. The human bloodstream contains a large number of proteins the type and concentrations of which fluctuate with a great many factors, from metabolism to the presence of disease. No current technology is able to provide a snapshot of the protein profile of a blood sample quickly yet 2D-IR screening has shown the potential to play a future role in early detection of cancers.

However, the potential of 2D-IR extends beyond the study of proteins and is being exploited by others in the department, among them being Jason Lynam and Ian Fairlamb who are interested in photo-initiated catalysis using manganese carbonyls as featured on page 8.

"The opportunity to have instrumentation like this at our fingertips has revolutionised our research, allowing us to explore a wide range of exciting new projects"