Chemistry Update

Newsletter 335, 31 August 2021

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Calendar of Events

Online Open Day
Date: Sunday 19 September
Time: 10am—4pm

Seminar
Developing and implementing inclusive and anti-racist pedagogy for courses, laboratories and degree programs
Speaker: Dr Grace Lasker, University of Washington, Bothell
Date: Thursday 23 September
Time: 3pm—4pm
Location: Virtual

Date of Next Issue:
24 September 2021

Dr Glenn Hurst Awarded National Teaching Fellowship

Glenn Hurst has been recognised with a prestigious Advance HE 2021 National Teaching Fellowships in recognition of his remarkable contributions to higher education teaching and pedagogy.

Dr Glenn Hurst is an Associate Professor in the Department of Chemistry and Green Chemistry Centre of Excellence at the University of York, and in receiving the Fellowship becomes one of the youngest academics in the UK to be recognised in this way.

He uses holistic, systems-thinking approaches to equip the scientists, engineers and policymakers of tomorrow with the knowledge and skills to address complex and interdisciplinary global problems. His approach allows students to transition from a surface-level reductionist approach to a deep understanding of subject matter by identifying key thematic connections across disciplines.

Indeed, Glenn is internationally renowned for his work in incorporating Green Chemistry into curricula. His unique approach involves a strong degree of contextualisation, blended with the engagement of students through the integration of innovative technology-enhanced learning methodologies and social media. In this way, he is able to train students to work in teams and prepare them to solve grand challenges as outlined by the United Nations Sustainable Development Goals.

In terms of sharing best practice, Glenn regularly publishes his work with students undertaking education-based research projects and is often invited to talk at international meetings. He regularly facilitates and delivers continuing professional development training in education for colleagues in York and beyond and he chairs the University's Learning and Teaching Forum, which nurtures and shares creativity and good practice in learning and teaching across the institution.

Reflecting on his award Glenn noted: "I am very grateful for the mentorship and support of colleagues together with the talented students I teach. In the future, I would like to truly transform the international Green Chemistry education community, developing transferable methodologies to implement systems thinking approaches and enhance interdisciplinary learning across a range of programmes."

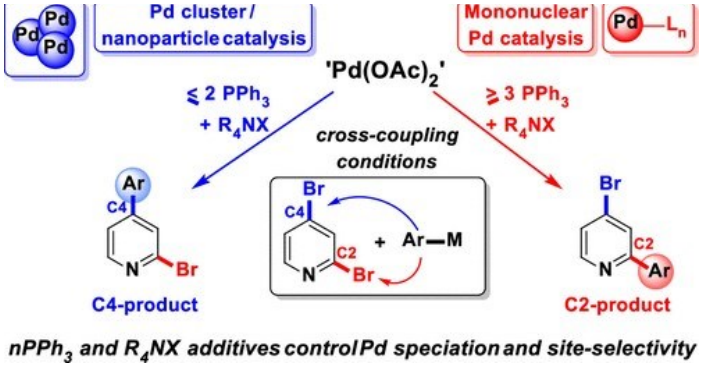
Head of Department, Professor Duncan Bruce said: "I am delighted with the news of Glenn's richly deserved National Teaching Fellowship. Three members of staff in The Department of Chemistry now hold these awards, reflecting the outstanding educators in the Department and the passion we have for providing high quality, innovative education to our students."

Glenn has previously won multiple national and international awards including the Royal Society of Chemistry (RSC) Higher Education Teaching Award 2020, American Chemical Society Award for Incorporating Sustainability into the Curriculum 2019, Educate North Teaching Excellence High Commendation 2019, Times Higher Education Most Innovative Teacher of the Year Finalist 2018 and JISC HE Social Media Superstar 2017.

The National Teaching Fellowship (NTF) Scheme is organised by Advance HE. Each year it celebrates and recognises around 50 individuals from across the UK who have made an outstanding impact on student outcomes and the teaching profession in higher education.

Switching catalyst selectivity

Recent research from the Department of Chemistry has shown that the selectivity of palladium-catalysed reactions can be dramatically switched using very small changes in reaction conditions.



Palladium-catalysed reactions are of key importance in synthetic chemistry, being widely applied in pharmaceutical and agrochemical sectors of industry. In particular, cross-coupling reactions offer a straightforward way of converting carbon-halogen bonds into new carbon-carbon bonds, building-up the complexity of molecular frameworks. However, achieving the desired selectivity in systems that have multiple halogen atoms, each of which can be a potential reaction site, can be extremely challenging.

In recent work published in *Journal of the American Chemical Society*, Professor Ian Fairlamb, working in collaboration with Dr Charlotte Willans from University of Leeds and Dr Mark Ford from Bayer AG has explored innovative ways in which the selectivity of such reactions can be controlled.

In particular, the researchers discovered that the selectivity of very well-established catalyst systems could be completely changed by making very small changes to the reaction conditions. Specifically, they found that for reactions of 2,4-dibromopyridine, the reactive site could be switched from the 2-position to the 4-position by decreasing the amount of triphenylphosphine ligand and adding a simple tetraalkylammonium salt.

Careful studies by the team led them to conclude that the small change in reaction conditions converted the catalyst from a mononuclear species with a single palladium centre (red, see Figure), to a palladium cluster (blue, see Figure). This change in catalyst speciation led to the resulting switch in reaction selectivity.

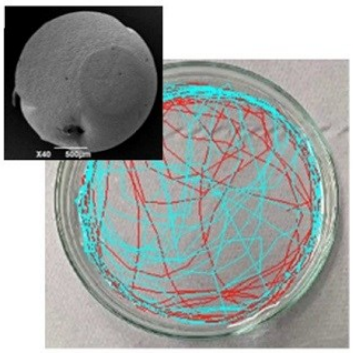
Professor Ian Fairlamb explains: “I think that in general, researchers in this area should be screening a range of palladium catalysts with different speciation – something that is rarely considered. As we show here, the results can be very interesting and potentially widen the scope of what can be achieved in this important class of reaction, generating different, unexpected products from the same starting material in a controllable way.”

He goes on to add: “General rules about palladium catalyst speciation are not so easy to develop, but we are working hard towards that goal. Furthermore, future research in Pd-catalyzed cross-coupling chemistry needs to focus on using very low palladium loadings, particularly with sustainability and cost in mind – we therefore need to do everything we can to enable catalyst systems to do more using less.”

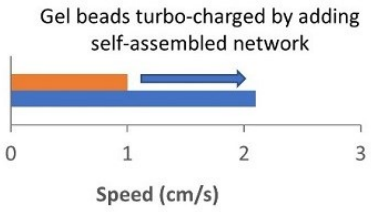
The research is published in *Journal of the American Chemical Society* and has recently been featured in *Nature Reviews Chemistry*.

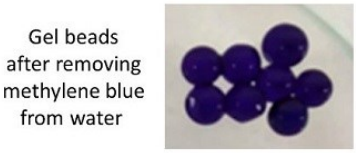
Self-propelling gel beads as highly-mobile waste collectors

Recent research from the Department of Chemistry has created gel beads that can spontaneously move when placed in water. By assembling a unique nanoscale network within the particles, the beads become turbo-charged and better able to remove a pollutant dye from the water.



Plotting the movement of different gel beads in water





Working in the research lab of Professor David K. Smith, Dr Carmen Piras fabricated innovative hybrid gel beads by mixing the well-known polymer gelator agarose with a self-assembling small molecule gelator previously developed in their lab. After soaking the hybrid gel beads in ethanol and placing them in water, she found that they spontaneously moved around in the water, as can be seen in this video.

This type of movement is actually well-known, and occurs as a result of the so-called 'Marangoni Effect' - as the ethanol diffuses out of the beads it changes the surface tension of the water. However, what surprised the researchers, was that by incorporating their own self-assembled network within the agarose beads, they could turbo charge the movement, enabling the beads to move twice as fast, and twice as far, in the first minute.

By cutting the gels into different shapes, they could control the type of movement. For example, by cutting the gel into a star-shape, it tended to spin on its own axis, rather than moving through the water like the spherical beads.

The researchers knew that their self-assembled network should be capable of binding to pollutants, like the industrial dye, methylene blue. Fascinatingly, these properties were transferred to the moving gel beads, which became much better able to remove this pollutant from water.

Dr Piras said: "We hope that in the future, self-propelling gel beads such as these may be able to remove pollution from difficult to reach areas – essentially seeking it out and collecting it like a mobile waste collector. To achieve this we would need to achieve greater control over the movement of the gel beads, and optimize the self-assembled network to maximise pollutant uptake.'

The research is published Open Access in *Chemistry – A European Journal*.

Online Department suggestion box

The online Equality and Diversity suggestion box has been extended to be a suggestion box for the whole Department. You can submit your thoughts/suggestions/ideas for general Departmental matters as well as matters relating to Equality and Diversity. You can find the Google form at this link.

Researchers identify new enzyme that infects plants - paving the way for potential disease prevention

Scientists have identified an unusual enzyme that plays a major role in the infection of plants - and have shown that disabling this enzyme effectively stops plant disease in its tracks.

Phytophthora infestans found in potato plants

By discovering previously unexplored ways in which crop pathogens break through plant cell walls, the scientists have opened up opportunities for developing effective disease control technologies.

The new research, published in *Science*, describes a family of enzymes found in a microorganism called *Phytophthora infestans*. The enzymes enable crop pathogens to degrade pectin - a key component of plant cell walls - thereby enabling the pathogens to break through the plant's defences to infect the plant.

Led by biologists and chemists from the University of York, the international team of researchers discovered the new class of enzymes that attack pectin called LPMOs. The team also showed that disabling the gene that encodes this enzyme rendered the pathogen incapable of infecting the host.

Damage

P. infestans is known to cause potato late blight, a devastating plant disease that led to widespread starvation in Europe and more than a million deaths in Ireland in the 1840s, in what became known as 'The Great Famine'. Plant infection continues to cause billions of dollars' worth of damage to global crop production each year and continues to threaten world food security.

The identification of this new gene could open up new ways of protecting crops from this important group of pathogens.

Lead author on the report, Dr Federico Sabbadin, from the Department of Biology's Centre for Novel Agricultural Products (CNAP) said: "These new enzymes appear to be important in all plant pathogenic oomycetes, and this discovery opens the way for potentially powerful strategies in crop protection".

Professor Simon McQueen-Mason, also from CNAP, remarked that the work was "the result of interdisciplinary collaborations between biologists and chemists at York along with plant pathologists at the James Hutton Institute, and genomicists at CNRS, with invaluable molecular insights from Professor Neil Bruce (CNAP) and Professors Gideon Davies and Paul Walton in the Department of Chemistry at York."

The research is part of the project *New Enzymatic Virulence Factors in Phytophthora infestans*, running from 2021 to 2025, and is supported with a £1m grant from the Biotechnology and Biological Sciences Research Council, part of UK Research and Innovation (UKRI).

The Roger J Mawby Demonstrator Awards 2020/21

Roger J Mawby was one of the founding academic staff members of the Department of Chemistry and was an inspirational teacher. Roger gave detailed and engaging lectures, frequently using chemical demonstrations to illustrate important concepts in transition metal chemistry and catalysis. In addition he gave stimulating and challenging tutorials that allowed students to develop and build their understanding of chemistry. **The Roger J Mawby Demonstrating Prize** is awarded to 5-6 students annually at a value of £150 per prize, to reflect Roger's passion for student learning.

The winners of the **The Roger J Mawby Demonstrating Prize for 2020/21 are:**

♦ **Rachel Steen**	For delivery of consistently high quality teaching, support and management of student groups in the laboratory.
♦ **Alastair Robinson**	For the development of resources to assist teaching during the pandemic and consistent high quality demonstrating.
♦ **Rosalind Booth**	For highly conscientious demonstrating, particularly in helping students link between theory and practice in the laboratory.
♦ **Chloe Howman**	For consistently high quality demonstrating, especially when supporting students who find practical work more challenging.
♦ **Nik Vagkidis**	For exceptionally diligent management of student groups in the laboratory, ensuring support to all students and helping to link the context of undergraduate practicals with research in the department.
♦ **Rebecca Donovan**	In particular recognition for efforts in the mentoring of new demonstrators and consistent high quality demonstrating.

Other GTAs nominated/shortlisted:

* Gayathri Athavan	* Amelia Gilio	* David Husbands	* Anna Patterson
* Natalia Baranska	* Chris Goult	* Molly James	* Saikiran Ravi
* Verity Barber	* Susanna Harrison	* Rachel Little	* Rajat Sharma
* Ryan Barker	* Giordaina Hartley	* David Loades	* Theo Tanner
* Conor Black	* C. Peter Howe	* Connor Murrill	* Amber Yeoman

We appreciate the work of all our GTAs during 2020/21, another challenging year.

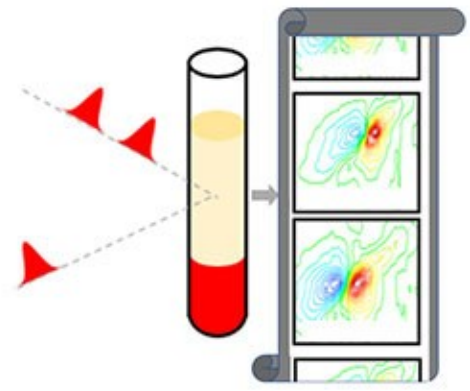
Unfortunately it is still not feasible to hold an event to celebrate this year, but we still want to let all GTAs know that their work and efforts are greatly appreciated.

Dillon group researching indoor air pollution

The Dillon group are on to their next field campaign, researching indoor air pollution. Here Catherine O'Leary and Yasmin Mueller (pictured) with Ellen Harding-Smith are comparing impacts of a selection of eco cleaning products chosen by *Which?* magazine.

York to upscale analytical technology for drug design and biomedical diagnostics

York researchers are leading a team that will receive £450k to create the world's first high throughput two-dimensional infrared (2D-IR) screening facility for the pharmaceutical and healthcare sectors.



Rapid 2D-IR analysis of proteins under physiological conditions

2D-IR spectroscopy uses state-of-the-art lasers to excite vibrations of molecules and make a sensitive 'map' of the 3D structures and intermolecular interactions of proteins and DNA.

However, water present in biological samples absorbs infrared light, obscuring signals from biomolecules. World-leading research led by the University of York, in collaboration with the Central Laser Facility, has developed a patent-pending method to suppress these water signals enabling proteins or DNA to be cleanly measured.

Principal Investigator Professor Neil Hunt, from our Department of Chemistry, explains: “This exciting new development means 2D-IR spectroscopy measurements of protein structure and dynamics can be performed in physiologically relevant solvents and biofluids, paving the way to 2D-IR use in drug design and biomedical analysis.”

To develop the project, York, in partnership with global biopharmaceutical company UCB Pharma, medical technology SME Dxcover Ltd and the STFC Central Laser Facility, has received a grant from the UK Research and Innovation Science and Technology Facilities Council (UKRI-STFC) to move 2D-IR spectroscopy from a research laboratory to industrial-scale screening tool.

Richard Taylor, Director of Molecular Spectroscopy, Protein Structure and Biophysics at UCB Biopharma, said: "UCB identified the potential of 2D-IR as a unique structural biology tool several years ago and through our long-standing collaboration with Neil and the Central Laser Facility, we have demonstrated that it is an extremely powerful technique for analysis of protein dynamics and conformational change. We are now excited by the ability to take this research further through this partnership."

The team aims to progress the commercialisation of the tool by demonstrating how it can be used for applications in the pharmaceutical and biomedical sectors.

New starters

Dr Morwan Osman, Research Associate in Mycobacterial Structural Biology
Room: B/K063; Ext: 8251; Email: morwan.osman@york.ac.uk

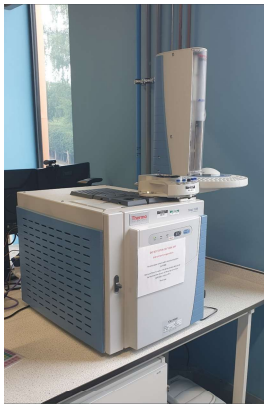
Chemistry Department Chromatography Service

Do you need access to chromatography equipment and you thought there was none available to use?

Do you have a compound that is just too tricky to separate and recover by column chromatography?

The Chromatography Service is here to help! Whether it is training on one of our instruments so that you can run routine analysis yourself, or running small batches of samples for you, the Service is here to help you develop your research with a range of instrumentation available.

Gas Chromatography (GC)



4 Thermo Trace 1300 GC's fitted with auto samplers

Analytical High Performance Liquid Chromatography (HPLC)

5 HPLC's
1 UHPLC
All have auto samplers and column ovens
Potential to carry out column cooling
Systems fitted with Diode array, variable wavelength and multi wavelength detectors
ELSD also available for detection

Preparative High Performance Liquid Chromatography (HPLC)

2 analytical/ semi prep HPLC's
All have auto samplers and column ovens
Systems fitted with Diode array detectors

There are a range of columns available for all systems to aid method development or bring your own for existing methods. Training is available for all systems.

Do you want to know more?
Contact the service on: chem-chroma@york.ac.uk