Chemistry Update

Newsletter 330, 26 March 2021

Inside this Issue

Calendar of Events

MolMat Seminar
Speaker: Professor José Mascarenas, CiQUS, USC
Date: Friday 16 April
Time: 9am—10am
Location: Virtual (Zoom)

Organic Seminar
Speakers: Dr Susannah Coote, Lancaster University and Professor Peter O'Brien, University of York
Date: Wednesday 28 April
Time: 9am—10.30am
Location: Virtual

Academic Mental Health Seminar
Speaker: Dr Zoë Ayres, Hach
Date: Wednesday 28 April
Time: 12pm—1pm
Location: Virtual

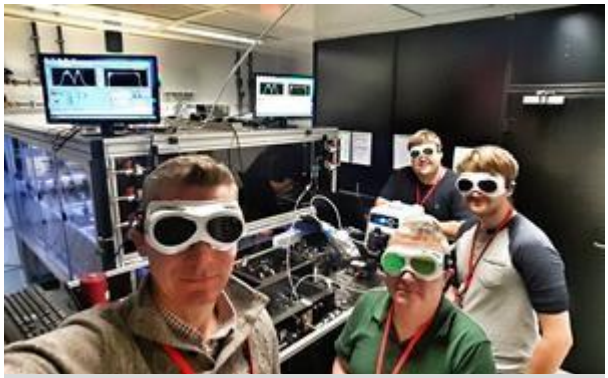
Date of Next Issue:
30 April 2021

Taking mechanistic snapshots of important synthetic reactions

In a landmark study, researchers from the Department of Chemistry have gained new mechanistic insights into C-H activation, a vital chemical reaction process.

The activation of a C-H bond at a metal centre, and its subsequent functionalization, is undeniably one of the most important breakthroughs in organic and synthetic chemistry in the last 15 years. It provides access to important chemical building blocks for the agrochemical, materials and pharmaceutical sectors. Even though scientists have figured out how to carry out many complex C-H activation processes, there remain mysteries around the mechanistic steps that take place.

In research published in *Journal of the American Chemical Society*, Professor Ian Fairlamb and Dr Jason Lynam, working with scientists from Syngenta and the STFC Central Laser Facility used fast laser methods to understand the deprotonation step, which allows C−H bond activation at a manganese(I) centre. The activation of a C-H bond by formal deprotonation is extremely difficult to observe because of how rapidly the process takes place.



Front to back: Ian Fairlamb, Jason Lynam, Jonathan Eastwood and Anders Hammarback working on the Time-Resolved Infrared Spectrometer at the STFC

Computational modelling was used to map out intermediate steps and likely transition state structures. However, this approach requires experimental validation to give a true and clear picture of the complete reaction pathway. Therefore, the team devised a direct strategy to observe the microscopic reverse of the deprotonation (activation) step – the protonation of a photochemically-activated complex, namely [Mn(ppy)$(CO)_4$] (ppy = 2-phenylpyridyl).

The observation and quantification of the microscopic reverse of the deprotonation processes enabled direct translation to the forward process involved in C-H bond activation. Time-resolved infrared spectroscopy (TRIR) was used to take snapshots of the catalytic reaction over picosecond to millisecond time scale, allowing experimental observation of the computationally-predicted pathway.

The team was therefore able to provide direct and compelling evidence for the key intermediates and processes predicted within the reaction mechanism for the first time. This gave rise to unprecedented levels of detail that would have been missed using alternative approaches.

The research is published in *Journal of the American Chemical Society* **2021**, 143, 1356-1364.

One year on feature

The University has published a feature One year on: Supporting students through a year of Covid-19 which amongst lots of activities across the University specifically mentioned work by Green Chemistry technicians in supporting the MSc in Green Chemistry and Sustainable Industrial Technology.

Social Research and Air Quality: STFC, Social Sciences and SAQN

The STFC Air Quality Network (SAQN) held an event on 26 January 2021 to ask how social sciences undertake and interact with air quality research. The meeting explored the capabilities that the Science and Technology Facilities Council (STFC) have to support social science research and whether collaborations could be built between different disciplines to address air quality challenges.

The meeting, held online, heard from social scientists researching air quality, and from STFC departments with the potential to support these types of research. Participants discussed ways for STFC to work with social science, and more broadly the possibilities of interdisciplinary work to tackle air quality challenges. Recordings of the presentations and discussion panel are available on the SAQN website, along with a set of next steps to be taken based on participants' input.

The SAQN also held a training session for members on using the Centre for Environmental Data Analysis (CEDA) and the JASMIN supercomputer facility. The recording of this event and accompanying slides are also available on the SAQN website, and would be useful for any researchers interested in making use of these facilities.

International Day of Women and Girls in Science

Jon Agire reports back on the profiles that were recently created in YSBL to showcase the work of female scientists.

To mark the International Day of Women and Girls in Science on 11 February, the YSBL community on Discord (our cakeless coffee haven in COVID times) decided it was about time we publicly showcased our female scientists' contributions to the lab, science and society. We quickly devised a fairly standard set of questions, and we put together a shared document containing a list of names and email addresses that, in true YSBL fashion, got so long we shall be publishing profiles for years to come. Having turned the questions into a form, we reached out to past and present YSBL women and hoped for the best.

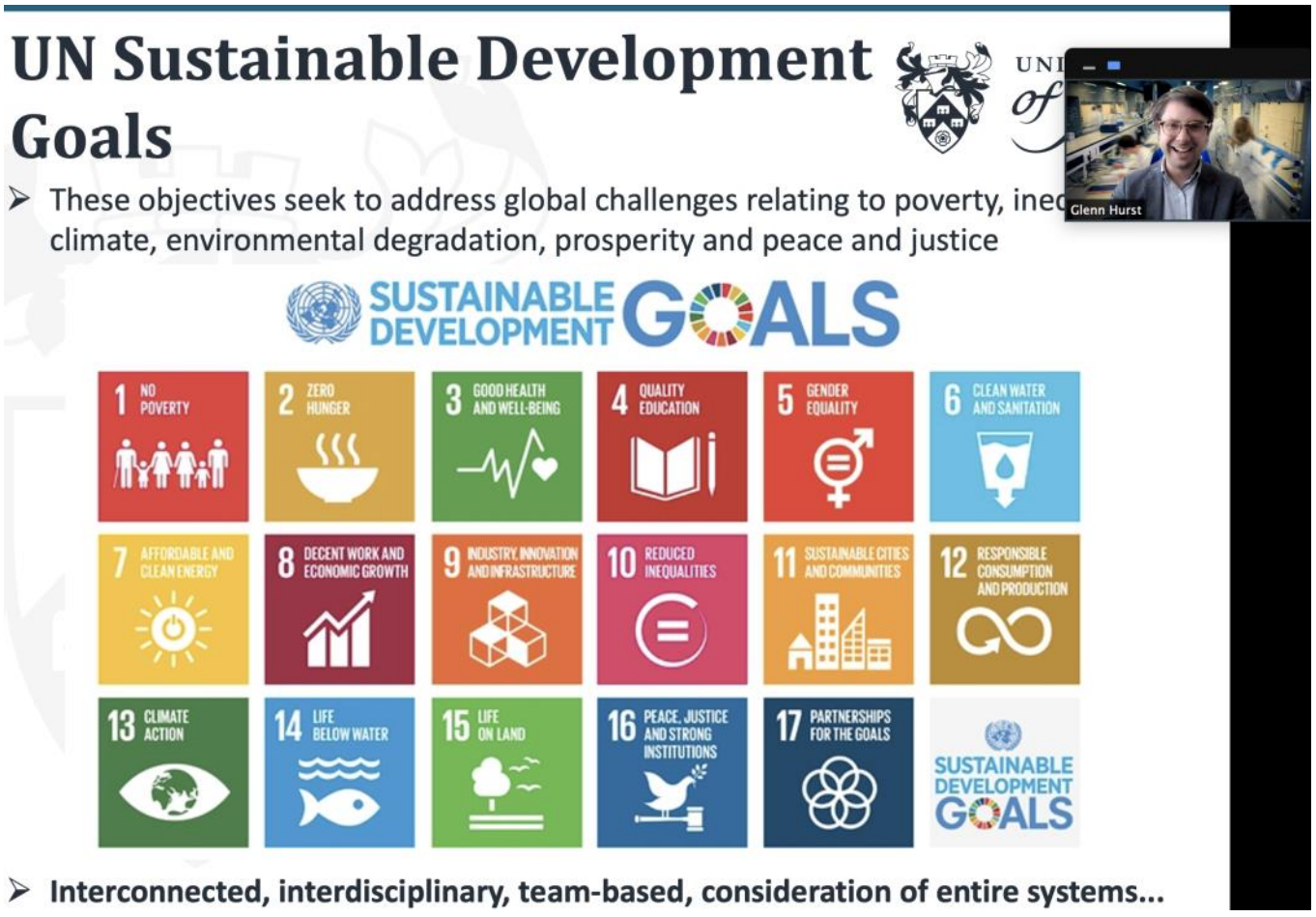
And *the best* did answer.

We published 19 profiles across many different career stages, from current PhD students to established academics and industry professionals. From their experiences, we can see that much of the motivation that led them to a career in STEM came from school teachers. *Motivated* school teachers, with wildly differing attitudes towards girls and women. Some did spot their potential, but others completely missed it or, even worse, tried to discourage them – interestingly, this had the opposite effect in some of our interviewees, who showed admirable tenacity. The most repeated message *to their younger selves* – a set question we asked – flagged up that they should have taken themselves more seriously. This is something I will certainly be remarking to my now teenage daughter.

The experience has been positive, and we will surely repeat it next year, and for as long as it takes until the battle for equality is won.

Dr Glenn Hurst advises the United Nations and commences new $250k green chemistry education project

In March, Dr Glenn Hurst was invited by the Chemicals and Health Branch of the United Nations Environment Programme (UNEP) to provide expertise and to prepare a specialised manual for global green and sustainable chemistry education at all levels from primary school through to university and beyond as part of development training for industrial professionals. Additionally, the manual will not only be implemented in formal education settings but informal environments too such as community and spiritual centres. The construction of this manual is in response to resolution 4/8 at the 4th meeting of the United Nations Environment Assembly (UNEA-4) where the UNEP developed a framework manual on green and sustainable chemistry over the past year, highlighting the requirement to design a globally transferrable educational template and set of recommendations for teaching green and sustainable chemistry. A portfolio of case studies developed by Glenn and colleagues at the Green Chemistry Centre of Excellence has been included as exemplars in the manual.



Glenn is also part of the leadership team for the recently funded Green Chemistry Teaching and Learning Community (GCTLC) project ($250,000 from the Argosy Foundation). In conjunction with the American Chemical Society Green Chemistry Institute and Beyond Benign, this project will develop an online hub needed to support the adoption of green chemistry and hasten the transformation of chemistry

education. The hub will house educational resources and provide an interactive global networking and collaboration platform. Through this, community members will be able to locate vetted resources for teaching core chemistry concepts with a green chemistry lens, discuss approaches with like-minded colleagues and share a diversity of ideas needed to advance chemistry education to a place where students are prepared to take sustainable action, aligned with the United Nations Sustainable Development Goals. Effectively, the aim of this project is to shift the global community from one of practice to transformation. As part of this work, Glenn is specifically focusing on enhancing collaboration, engagement and training provisions while nurturing the development of new leaders in green chemistry education with the hope that there will be evidence of the emergence of new global leadership and representation from diverse voices.

Closer to the chalkface (or in reality, 'via Zoom'), Glenn was invited to deliver a virtual lecture on 'Empowering the next generation to propel us towards a greener and more sustainable society' to Harrow School Scientific Society on Thursday 11 March. The diverse and interdisciplinary lecture, which brought in elements of philosophy, science history and research-led examples of working with students as partners on projects aligned with the United Nations Sustainable Development Goals through embracing a systems thinking theoretical framework of learning, was very well received by the society at Harrow. Glenn has since been invited to deliver a lecture to Bede School in Sussex as part of 'The 42 Club' where 'inspiring online lectures are delivered by speakers at the top of their fields covering a range of topics from STEM and philosophy to business and law.'

Cyrene™ production to increase

The Green Chemistry Centre of Excellence (GCCE)'s industrial collaborator Circa Group have successfully raised over €50 million through a private placement enabling them to fund the construction of a one thousand tonne a year plant for the manufacture of Cyrene™, the solvent invented in collaboration with the GCCE. The plant will be located in France, and larger manufacturing plants are already being planned to meet the increasing interest in Cyrene. Shares in the company are expected to be listed on Euronext Growth Oslo.

Cyrene is a novel biobased solvent that can replace existing, toxic and fossil-based solvents like NMP and DMF in some applications. The total market potential for Cyrene is estimated to be more than one million tonnes, and there are currently almost no viable and safe alternatives available at large scale. Global chemicals distribution giant, Merck KGaA, has already provided a Letter of Intent covering the entire Cyrene production capacity of the French plant.

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 on the intranet homepage or at this link.

YSBL student takes part in *I'm a Scientist, Get Me Out Of Here*

"Throughout February I took part in "I'm a Scientist, Get Me Out Of Here", an online engagement activity designed to give school pupils of all ages an opportunity to ask real scientists about their work. 867 students took part throughout the month, asking myself and 23 other scientists questions about everything from our day to day lab work to our career path into our current roles. The event involved the students voting for their favourite scientist, with the prize being £500 to go towards science outreach; and after my participation, I was fortunate enough to be voted the winner.

"I plan to use the money to develop outreach activities based around my work with protein engineering for use at future in-person outreach events with my research group. I really enjoyed taking part in the live chats, particularly talking to the students who asked really insightful questions and I hope it has encouraged the students to consider career paths that they wouldn't otherwise be exposed to. I would definitely suggest that anyone who is interested in public outreach should apply."

- Amelia Gilio, PhD student in YSBL

New starters

Dr Naeem Iqbal, PDRA in Free Radical Chemistry and Radical Detection
Room: C/E014; Ext: 4587; Email: naeem.iqbal@york.ac.uk

Hester De Groot, HR Administrator
Room: C/A121; Ext: 2716; Email: hester.degroot@york.ac.uk

Neil Scott, Postdoctoral Research Associate
Room: C/E202; Ext: 2556; Email: neil.scott@york.ac.uk