Chemistry Update

Newsletter 294, 23 February 2018

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Calendar of Events

Chemistry @ York
Date: Friday 23 February
Time: 10am—4pm
Location: C/B/101 & C/B102

Research Seminar
Speaker: Prof Warren Warren, Duke University
Date: Friday 23 February
Time: 1pm—2pm
Location: C/A122

JISC EdTech in Higher Education Interactive Award Lecture
Speakers: Dr Glenn Hurst, University of York & Verity Nalley, DigiLab
Date: Wednesday 28 February
Time: 2pm—3.30pm
Location: C/B102

Research Seminar
Speaker: Prof Mike Ashfold, University of Bristol
Date: Wednesday 7 March
Time: 1pm—2pm
Location: C/B102

Equality and Diversity Lunchtime Forum
Impostor syndrome: Am I the only person that feels like a fraud?
Date: Thursday 8 March
Time: 12pm—1pm
Location: C/B101

Chemical *Inter*Actions International Picnic
Date: Thursday 15 March
Time: 12.30pm—2pm
Location: C/A122

6th UK Solar Fuels Symposium
Date: 19-20 March 2018
Location: Department of Chemistry

Inorganic Seminar
Speaker: Prof Lee Brammer, University of Sheffield
Date: Wednesday 21 March
Time: 1pm—2pm
Location: C/A122

Salters' Festival of Chemistry
Date: Thursday 22 March
Time: 10am—3.30pm
Location: Department of Chemistry

RSC Analytical Biosciences Early Career Researcher Meeting
Date: 22-23 March
Location: Department of Chemistry

Durham ECR Mini-Symposium
Speakers: Dr Alyssa Avestro, Dr Matthew Kitching & Dr James Walton, University of Durham
Date: Wednesday 28 March
Time: 12.30pm—2pm
Location: C/B/101

Date of Next Issue:
23 March 2018

Atmospheric Chemists and Defra Talk Air Quality

Scientists at York discuss the role of research in support of the Government's UK Clean Air Strategy.

Leading UK air quality scientists joined officials from the Department for Environment Food and Rural Affairs (Defra) to discuss research in support of the Government's UK Clean Air Strategy. At the second National Centre for Atmospheric Science (NCAS) Air Quality Forum, experts and policy makers were brought together in Westminster to think about the priorities for air pollution research. The United Nations Environment Programme declared air pollution as the World's worst environmental health risk, with the Royal College of Physicians estimating that it is linked to 40,000 deaths per year in the UK. The Secretary of State for the Environment, Michael Gove, has stated that the Clean Air Strategy, due to be published in 2018, will address all forms of air pollution, not just transport, delivering cleaner air for the whole country.

Defra Chief Scientific Adviser, Professor Ian Boyd, kicked off the policy forum with a challenge to the research community to consider their role in moving towards a more multidisciplinary, whole system approach to environmental issues. This set the tone for a day of discussions featuring priorities for research, dealing with uncertainty, effective science communication, and the interplay of engineering, social and physical sciences to drive innovation.

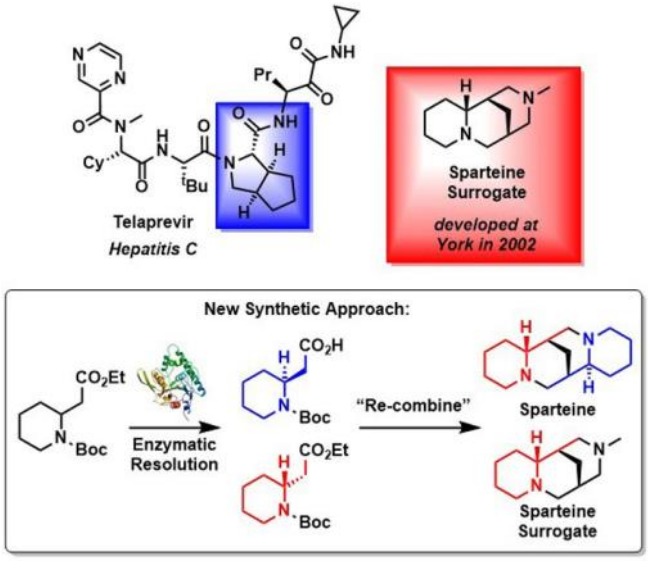
The forum, organised by Dr Sarah Moller from the Wolfson Atmospheric Chemistry Laboratories (WACL) at the University of York, was rather different to many scientific meetings in that presentations were short, only ten minutes, and intended to stimulate discussion and challenge thinking. The aim was to initiate conversations between policy officials and experts that could lead to future collaboration and knowledge exchange.

Harriet Wallace, Defra Deputy Director for Air Quality and Industrial Emissions, introduced the attendees to the Clean Air Strategy that the Government intends to publish later this year. The presentation was followed by a lively discussion session, chaired by Professor Ally Lewis from WACL. Contributions were many and varied, with experts offering advice, challenge and evidence to support and strengthen the themes being considered for inclusion in the strategy.

Attendees included experts from UK universities, research institutes, the Joint Nature Conservation Committee, the Environment Agency, Natural England and the Met Office, as well as Defra officials and research council representatives. Dr Moller said, "I was delighted with how open everyone was to sharing views and discussing their work. This was a great opportunity to bring together communities who don't interact as a group very often. The event seems to have been a real success". Dr Moller added "but that is just the beginning. I now need to make sure that the interactions and ideas sparked by the day's discussions are followed up and that the potential for research impact and knowledge exchange is maximised".

York Chemists Solve Long-Term Supply Issues of Sparteine Chiral Ligands

Scientists from the Department of Chemistry have developed a new synthetic route that delivers significant quantities of two very important sparteine-based chiral ligands that could help in future development of drug molecules.



Sparteine and the sparteine surrogate, developed in York in 2002, are chiral ligands with the potential to synthesise mirror-image 'enantiomeric' compounds that have been widely used in metal-mediated reactions to tackle complex synthetic problems and generate drug molecules. For example, researchers at Vertex who developed the Hepatitis C drug Telapravir, showed that the sparteine surrogate could be used to synthesise the part of the drug molecule highlighted in blue.

However, there are issues with the long-term supply of both sparteine, which is extracted from scotch broom, and the sparteine surrogate, which derives from cytisine and is extracted from the seeds of the Laburnum tree. Sparteine itself became unavailable in 2010 and has been scarce ever since. Chemists at Vertex recently rejected a multi-kg scale route using the sparteine surrogate since "inquiries about long-term, high-volume supply of cytisine had been met with concerns about production variability, due mainly to reliance on cytisine isolation from natural sources".

These problems with long-term supply motivated the development of a new approach by Professor Peter O'Brien's group in the Department of Chemistry at the University of York. Their route uses common feedstock chemicals to make these chiral ligands on an unprecedented scale, moving away from the precarious use of naturally occurring compounds, and hence allowing supply issues to be addressed. Their innovative approach utilises the enzymatic resolution and separation of the mirror-image forms of a simple intermediate. For sparteine, these were then recombined to generate the complexity required in the target ligand.

Dr James Firth, lead chemist on the project, said: "Our approach to the family of sparteine chiral ligands allows synthesis of either mirror-image form on a gram-scale for the first time. Hopefully this will help ease supply issues, helping both fundamental research and drug production".

The work has attracted attention and recently featured in the popular pharma blog "In the Pipeline" by Derek Lowe.

The research is published in *Angewandte Chemie International Edition* and was funded by EPSRC, Astra Zeneca and F. Hoffman-La Roche.

Four Hot Papers in Three Different RSC Journals

Four papers published in 2017 from the Shimizu group have been chosen as Hot Papers in three different Royal Society of Chemistry journals (*Physical Chemistry Chemical Physics*, *Green Chemistry* and *Food & Function*).

The review on food-flavour interactions published in *Food & Function* was also featured as the front cover for the second time in a row, and the tutorial review on greener solution chemistry in *Green Chemistry* is the Shimizu Group's first-ever publication in the journal.

The journal *Physical Chemistry Chemical Physics* chose two papers, a perspective paper on the theory of hydrotropes pioneered by the Shimizu Group, as well as simulation work led by a team in Stuttgart which confirmed the theoretical calculations of Joshua Reid (PhD, 2018), originally made back in 2015 (*PCCP* 17, 14710, 2015).

The published work was performed in collaboration with Professor Nobuyuki Matubayasi of Osaka University, Professor Steven Abbott of TCNF Ltd, Ipswich, and Professors Fyta and Smiatek of Stuttgart University. Dr Seishi Shimizu is a member of York Structural Biology Laboratory (YSBL).

- Read the review paper "*Quantifying non-specific interactions between flavour and food biomolecules*"
- Read the perspective paper "*Unifying hydrotropy under Gibbs phase rule*"
- Read the tutorial review paper "*Practical molecular thermodynamics for greener solution chemistry*"
- Read the paper "*The properties of residual water molecules in ionic liquids: a comparison between direct and inverse Kirkwood–Buff approaches*"

Professor James Clark Awarded Senior Fudan Fellow Title

Professor James Clark has been awarded the title "Senior Fudan Fellow" for 2018-19. Fudan Fellows are meant to promote academic collaboration between Fudan faculty and leading research centres outside of China.

Fudan University is widely considered to be the top university in China outside of Beijing and is ranked number 40 in the QS World rankings and no. 3 for BRICS (Association of five major emerging national economies: Brazil, Russia, India, China and South Africa). It is over 100 years old and has almost 30,000 students half of whom are postgraduates. James and colleagues in the Green Chemistry Centre of Excellence (GCCE) will work with Fudan scientists on getting chemical value from waste including the use of York microwave technology. Drs Alice Fan and James "Jimbo" Sherwood will join James in Fudan later this year.

Unlocking Wood Biomass

Researchers in the Department of Chemistry have discovered a set of enzymes capable of breaking down one of the main components of wood. The enzymes could potentially contribute to the conversion of wood biomass into valuable chemical commodities.

The use of wood is taking on a new importance, as it is one of the most promising sources of advanced biofuels and plant-derived products. Notwithstanding its potential, however, cost-effective conversion of wood feedstocks is limited by a single key factor: its resistance to degradation by enzyme cocktails. As a result, current wood biorefineries utilize energy-demanding pre-treatment processes.

In new research, Professors Paul Walton and Gideon Davies from the University of York worked with French researchers from CNRS Marseille to discover enzymes that greatly increase the potential use of wood as a feedstock. In work published in Nature Chemical Biology, the research team reports a new family of enzymes called lytic polysaccharide monooxygenases (LPMOs). Importantly, LPMOs have been shown by the team to be capable of breaking down xylans, a form of recalcitrant polysaccharide commonly found in wood biomass. The new enzymes are isolated from fungi, which themselves play a vital role in the terrestrial carbon cycle and dominate wood decomposition in forests.

The research builds on the key discovery that LPMOs are copper-containing enzymes, as reported by the team in York back in 2010. Specifically, the new discovery of the ability of lytic xylan oxidase to break down challenging wood biomass advances knowledge of the way in which woody biomass degrades in nature. Furthermore, these enzymes may underpin the development of improved enzyme cocktails for biorefinery applications using wood – unlocking its conversion into a wide range of valuable commodities.

This research, published in *Nature Chemical Biology* was funded by the European Commission, the UK Biotechnology and Biological Sciences Research Council (BBSRC) the Centre National de la Recherche Scientifique (CNRS), and the French Infrastructure for Integrated Structural Biology (FRISBI).

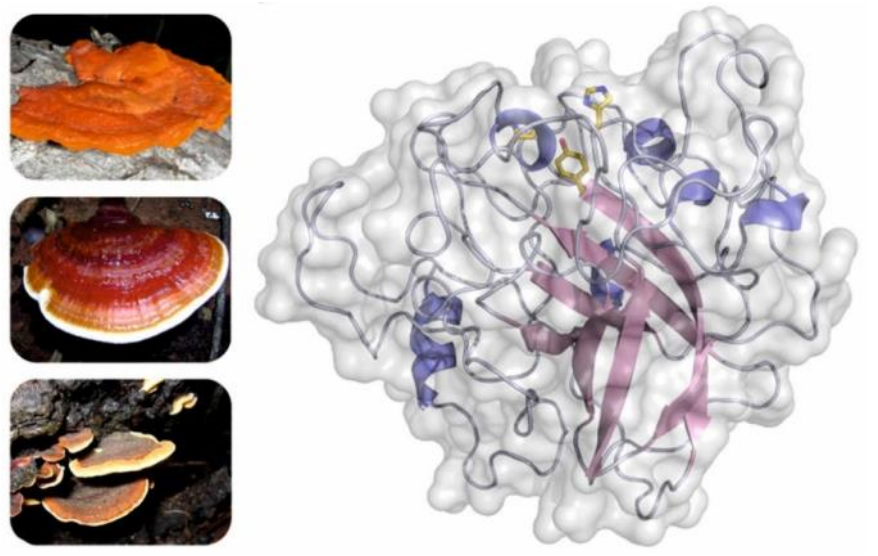


Image of fungi which possess the newly disovered lytic xylan oxygenase enzymes, and an overall three dimensional structure of one of this class of enzymes.

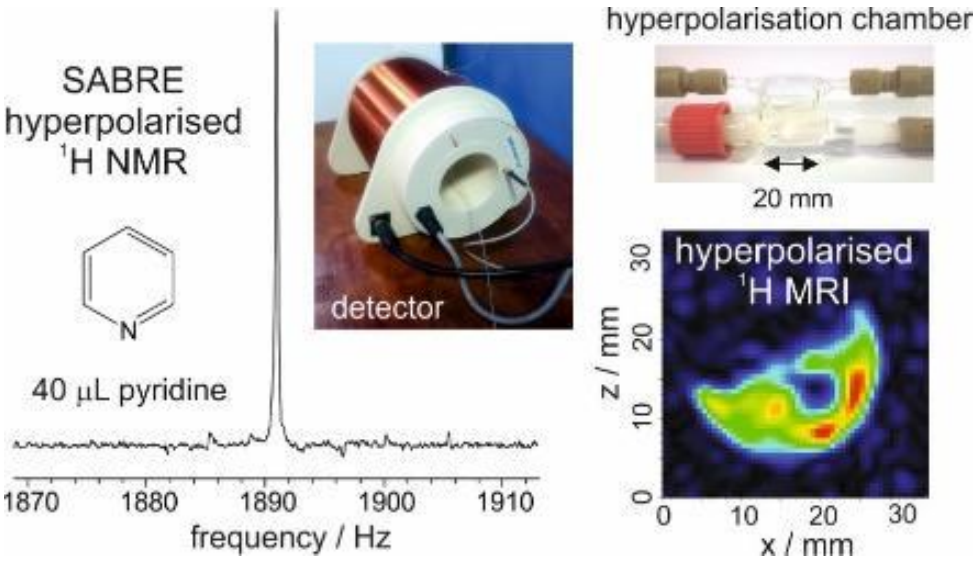
EPSRC New Investigator Award for Dr Meghan Halse

Dr Meghan Halse has been awarded £210,439 from the Engineering and Physical Sciences Research Council (EPSRC) to support research on "Lighting up Magnetic Resonance: SABRE optimisation powered by in situ detection".

MRI and NMR are powerful tools in applications ranging from synthetic chemistry to medical diagnosis. However, such instruments are very expensive because they rely on large magnets to provide strong signals. Hyperpolarisation methods, such as the signal amplification by reversible exchange (SABRE) method invented here in York, dramatically improve the intensity of the NMR/ MRI signals of target molecules by up to 100,000 times. These signal gains can be exploited either to reduce the cost of the technique by working in a weak magnetic field or to open up new applications: for example, hyperpolarisation methods provide new routes to probe disease in clinical MRI.

The SABRE technique holds particular promise for low-cost NMR and MRI applications because the enhanced signals are generated using magnetic fields that are 10,000 times weaker than a normal NMR spectrometer. In this work, a low-magnetic-field NMR apparatus will be used as a platform to directly study the SABRE process in the precise conditions where the amplified signals are generated. This will provide previously inaccessible information about how the technique works and will allow us to explore new methods for improving the efficiency of SABRE. The ultimate goal is to provide a route to the rapid optimisation of SABRE for a broad range of chemical systems and thus enable widespread applications of the method in areas like medicine and industrial manufacturing.

This research will be carried out by Dr Meghan Halse within the Centre for Hyperpolarisation in Magnetic Resonance (CHyM) at the University of York. EPSRC is the UK's main agency for funding research in engineering and the physical sciences. EPSRC invests around £800 million a year in research and training, to help the nation handle the next generation of technological change.



SABRE hyperpolarisation enables NMR and MRI in magnetic fields as low as the Earth's magnetic field (50 µT), which is 200,000 times weaker than a standard NMR spectrometer (e.g. 9.4 T)

The Things We Do for Impact

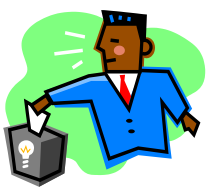
In January, Professor Michael North and Dr Alison Parkin published a joint paper on CO_2 electrochemistry using sea water as electrolyte and waste metals within the anode in *ChemSusChem*. This work has already been attracting a lot of interest, helped by a University of York press release. Already the paper has been highlighted in 'Chem' and an interview with Michael North and Alison Parkin about the paper has been published in 'Materials World'.

Earlier this month, the Department of Chemistry hosted Reuters who came to make a 5 minute news story on the technology for global syndication to both online and broadcast news organisations. Filming started in Whitby with the collection of sea water. If the filming had been in August this could have been a good excuse for a day out at the seaside, as it was, we had to collect the sea water in sub zero temperatures and in the middle of a snow storm. Fortunately Dr Katie Lamb and current PhD student Mark Dowsett were not going to let adverse weather get in the way of their film careers. We returned to York in a hurry (not even stopping for fish and chips) when the snow storm turned into a blizzard. The afternoon was then spent filming indoors in laboratories and the GCCE Industrial Engagement Facility.

The finished film can be viewed at: https://uk.reuters.com/video/2018/02/13/using-seawater-and-crisp-packets-to-cut?videoId=400858757&videoChannel=4000&channelName=Technology

Katie and Mark collecting sea water whilst being filmed.

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.

O'Brien Group News

Hanna Klein from the O'Brien group recently attended a Training Network (FragNet) meeting on fragment-based drug discovery in Barcelona, Spain. FragNet is part of an EU funded Marie Skłodowska-Curie Innovative Training Network (ITN) set up to train a new generation of researchers in all aspects of Fragment-Based Ligand Design (FBLD). Professor Rod Hubbard is the York PI for this project. The workshop, which took place 22-26 January, is the third in a series of meetings aimed at exchanging project results and providing training in scientific topics and transferable skills. A variety of projects based on fragment library design, biophysical screening techniques, computational methods and applications were presented. Hanna gave two separate presentations on her work on the design, synthesis and screening of a 3-D fragment library. The latter half of the workshop focused on training in computational and transferable skills.

Hanna commented "The conference was a great chance to learn about computational modelling techniques and gain insight into the latest challenges of FBLD. It was also good to catch up with the other 14 early stage researchers involved in the program, find out about their progress and discuss future opportunities for collaboration."

New Starters

Adrian Chu, PDRA in YSBL
Room: Biology L1; Extension: 8818; Email: adrian.chu@york.ac.uk

Buthaina Albanyan, PDRA
Room: D115/D126 ; Extension: 2599/4184; Email: buthaina.albanyan@york.ac.uk

Dr Ana Campo Rodrigo, PDRA
Room: D115/D126 ; Extension: 2599/4184; Email: ana.camporodrigo@york.ac.uk

Dr James Bennett, Associate Lecturer
Room: C/A049 ; Extension: 4539; Email: james.bennett@york.ac.uk

CIEC at 2018 NEPIC Annual Industry Awards Dinner

The region's brightest youngsters, best companies and tireless contributors were celebrated at the 2018 NEPIC (North East of England Process Industry Cluster) Annual Industry Awards Dinner at Hardwick Hall, Sedgefield on Friday 19 January.

Sixteen awards were presented in front of 420 industry guests, with a total of twenty four thousand pounds in prize funds donated over the course of the evening. The Centre for Industry Education Collaboration (CIEC)'s advisory teacher, Nicky Waller, was there to support The Village Primary School, Thornaby - the winning school in the Primary School Environmental Award category, sponsored by BOC.

Many of the winning organisations each received £2000 to donate to a local school or educational project of their choice. Wilton based company, Micropore, was the winner of this year's Innovation Award and chose to donate their £2000 to CIEC's very own Children Challenging Industry Programme.

The Outstanding Contribution Award this year was won by recently retired CEO of NEPIC, Dr Stan Higgins OBE. Stan has been a long standing supporter of CIEC and our work with primary schools and also chose to donate his £2000 prize money to the Children Challenging Industry programme.

The award ceremony was followed by an exciting evening of celebrations and networking. We would like to thank Micropore and Dr Stan Higgins for their overwhelming contributions of support.

Representatives of Micropore and Stan Higgins presenting their donations to CIEC to Nicky Waller

Nicky and a representative from the village school receiving a cheque on behalf of the school

Workshop Series:
Sustainable Manufacturing for the Chemical Industry

Increasing demand for chemicals worldwide, depleting resources, stricter legislation and the rising cost of waste disposal are placing increasing pressure on the chemical and related industries. For any organisation to survive in the current climate, the issue of sustainability must be fundamental to the way it operates. A sustainable manufacturing approach will enable economic growth to be combined with environmental and social sustainability, and will be realised via collaboration between a multidisciplinary community including chemists, biologists, engineers, environmental scientists, economists and policy makers. Hence employees with new skills, knowledge and experience are needed.

Benefits

After close consultation with industry, this course of five interactive workshops has been designed to provide an insight into the issues surrounding sustainable manufacturing including change management, commercialisation, environmental impact, circular economy, legislation and bio-resources including the conversion of waste into valuable products. The multidisciplinary course content will incorporate industrial case studies, providing access to real business issues, and will be delivered by experts from departments across campus as well as from industry.

The interactive nature of the workshops will also provide opportunities for open discussion and debate, as well as the chance to network with like-minded individuals on-campus. Some of the workshops will be followed by additional networking sessions where refreshments will also be provided.

Who is it for?

These workshops are open to all on campus with an interest in the future of sustainable manufacturing. Graduates, PhDs and postdocs are particularly encouraged to attend.

How do I sign up?

Follow the links on the next page to register your attendance at each of these workshops via Eventbrite. Attendance at all five workshops is not compulsory but is encouraged. Places are limited and will be allocated on a first come, first served basis.

Content

One of the workshops 'Safer Chemicals for Healthy Buildings?' has already passed but there are still spaces at the following workshops (the fifth workshop is TBC):

28 February 2018	**Where there's muck there's brass?**	Dr Liz Rylott, Centre for Novel Agricultural Products (CNAP), Dept. of Biology
7 March 2018	**Business Case for Green**	Professor Peter Ball, Management School
14 March 2018	**Green Chemistry Marketing to the Global Research Community**	Dr Jane Murray, Merck

To find out more detail on the individual workshops please visit the links above or alternatively contact Dr Rob McElroy (rob.mcelroy@york.ac.uk) or Louise Summerton (louise.summerton@york.ac.uk).

Talking Chemistry

Annie Hodgson is working with Lynda Dunlop from the Department of Education on an exciting project to introduce philosophical enquiry in chemistry into schools. This project is supported by the Royal Society of Chemistry (RSC), who were so intrigued by the novelty of the concept that they sent a representative to observe a recent workshop.

Students taking part in a "Hot Seat" exercise while debating key issues about chemistry

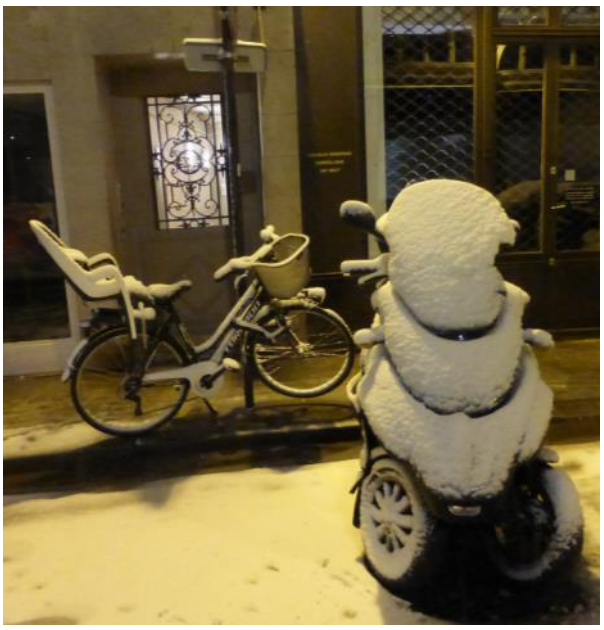
The aim of the project is to explore the potential for philosophical dialogue to support chemistry teaching and learning in schools. The idea is to send pairs, or small groups, of university students into secondary schools to run workshops with the young people. The students are in year 2 of their studies and are drawn from the Departments of Chemistry, Education, and Philosophy. So far the students have attended two half-day workshops to train them in how to plan and run sessions in schools. The next step is to place the students in their host schools.

Watch this space…

"Odile Eisenstein Investiture" by Professor Robin Perutz

"I was lucky enough to be invited to the investiture of Odile Eisenstein, our Honorary Visiting Professor, as an Officer of the Légion d'Honneur. This event was quite different from Britain's way of awarding honours. We met at the 17th century Institute de France, the very grand home of the French academies by the banks of the Seine. There are about 30 members of the French Academy who are chemists, including two women, of whom Odile is one. The Vice-President of the Academy of Science gave a fine tribute to Odile's research, especially her most recent contributions, in front of about 30 guests in a small tapestry lined room before presenting the honour. Odile replied with an account of how she had been brought up in a single-parent family by a mother who had total faith in the value of education for her daughter. Her mother was still traumatised by her experience of Paris as a Jewish immigrant during the war, losing her first husband to arrest and Auschwitz, while she herself had to move from one safe house to the next. After the champagne, we went out to very quiet and white streets and the realisation that Paris is no better at dealing with snow than London."

Institut de France



Paris in the snow

Green Impact

Sustainable Shopping

Consider buying products that reduce impact on the environment. The following websites give information on buying more sustainable /ethically sourced products:

- www.ethicalconsumer.org - Click on 'Full A to Z list' to find out about products (out of 20, the higher the rating the better). The surface level detail is free, for more detail you will have to pay a subscription.
- www.thegoodshoppingguide.com is similar to the above. There is also an app.

Buy FSC certified wood products and Rainforest Alliance certified products (www.rainforest-alliance.org/shopthefrog). Consider buying environmental cleaning products, such as Ecover.

Information on what and where to buy Fairtrade products:

www.fairtrade.org.uk/en/buying-fairtrade

BigBarn—find local food - www.bigbarn.co.uk

Why buy new books? Simply buy second hand books online:

www.worldofbooks.com (free delivery)

www.abebooks.co.uk

Buy from charity shops – reuse items rather than buying new (and save money!). There are quite a few charity shops in York (see Goodramgate). Search for 'charity shops' in York on www.yell.com.

Support your local shop! www.visityork.org/shopping is a good websites for information about which shops to go to in York.

Eat Seasonably

eatseasonably.co.uk/what-to-eat-now/calendar

You can click on the different types of vegetables and tips are also displayed on how you can use them.

Best to eat in **February** – Savoy cabbage and leeks

Best to eat in **March** – Spring green cabbage

Consider also growing your own vegetables – you don't need much space. See above Eat Seasonably website on what to grow, when.

Chemical *Inter*Actions

Social Group Open to All in the Department of Chemistry

International Picnic

Thursday 15 March 2018

12.30 – 2pm in C/A122

Bring food from your region or home country for others to try

All welcome

Bring your friends

Celebrate the diversity of staff and students in the Department

We will provide soft drinks, plates, napkins and plastic cutlery

To help us plan for the event, please sign up via the link below or the QR code: https://tinyurl.com/y7hyfmfa

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Email: chemical-interactions-group@york.ac.uk

www.facebook.com/ChemInteractions

Athena SWAN Gold Award

DEPARTMENT OF CHEMISTRY
york.ac.uk/Chemistry

UNIVERSITY of York

Equality and Diversity Lunchtime Forum

Impostor syndrome:

Am I the only person that feels like a fraud?

All staff and students welcome

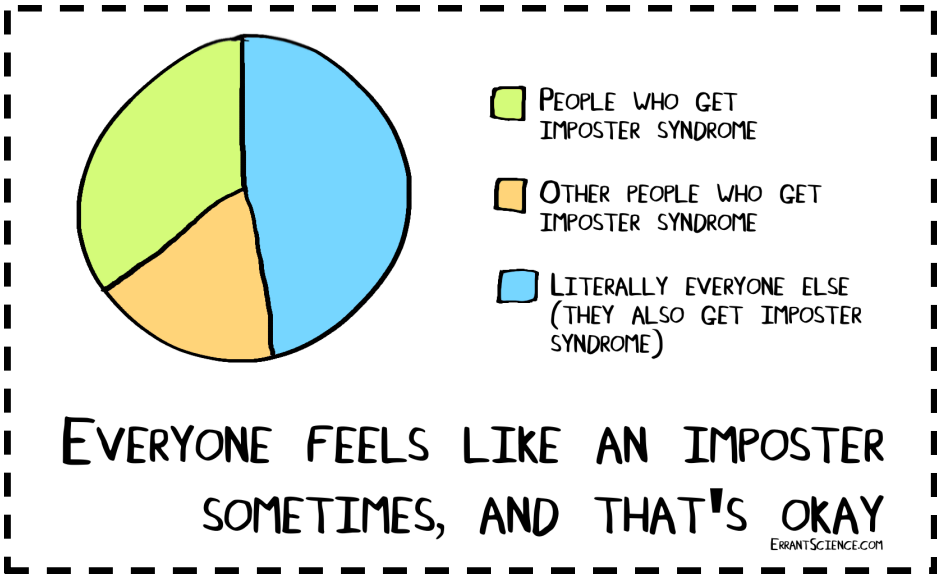
Imposter syndrome is the feeling that you are not as good as people think you are and one day you will be found out. It is very common in academia.

Come along to chat and learn a bit more about this issue.

Meet others in the department who are interested in equality and diversity and share your experiences.

Thursday 8th March

12-1 pm, C/B101



Bring your lunch and a mug - tea and coffee provided

Please contact caroline.dessent@york.ac.uk or leonie.jones@york.ac.uk for more information