

Chemistry Update

Newsletter 320, 30 April 2020

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Calendar of Events

Virtual coffee break for chemistry postdocs and staff

Date: Friday 1 May

Time: 2pm

Homeworking can be very isolating. The Graduate School Board Postdoctoral representative, Kelly Pereira, is holding an informal virtual 'hangout' for all postdocs and staff who wish to join. This hangout is designed to allow everyone to chat, using Zoom 'breakout rooms', moving individuals between different virtual rooms of ~ 3 people every 5 to 10 minutes (depending on numbers). Anyone who would like to join and doesn't have the link can email Kelly directly at kelly.pereira@york.ac.uk.

Virtual Seminar: "The Development of Expertise in Structure Elucidation using NMR Spectroscopy"

Speaker: Prof Ginger Schultz, University of Michigan

Date: Wednesday 13 May

Time: 2pm—3pm

Physical Chemistry Virtual Seminar

Speaker: Dr Melanie Britton, University of Birmingham

Date: Wednesday 20 May

Time: 1pm—3pm (tbc)

Virtual Seminar: "Singlet-assisted diffusion NMR methods"

Speaker: Dr Giuseppe Pileio, University of Southampton

Date: Wednesday 27 May

Time: 2pm—3pm

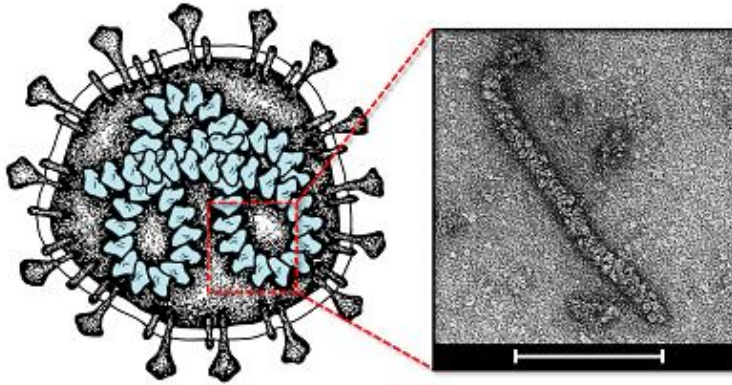
Date of Next Issue:

29 May 2020

New insights into COVID-19

Research from the Department of Chemistry in York is providing vital insights into the novel Coronavirus SARS-CoV-2, and may help underpin antibody tests and future therapies.

Ongoing work in York during the global COVID-19 pandemic, led by Professor Fred Antson, aims to determine a high resolution structure of an important protein in the SARS-CoV-2 virus. Achieving this would provide detailed information about how this virus assembles and replicates.



Left, illustration of SARS-CoV-2 virion in cross-section, with nucleocapsid protein coloured blue. Right, negatively stained transmission electron micrograph showing a nucleocapsid assembly, produced by researchers in YSBL (scale bar 100nm). Image credit: Jake Smith, Oliver Bayfield.

Much work globally has focused on the 'spike' proteins on the exterior of the virus, but the protein of interest to the team in York is the nucleocapsid protein (highlighted in blue in the image). This protein binds to the viral RNA forming a long helix-like assembly that is condensed inside the virus particle, safeguarding the RNA from degradation.

The researchers had the relevant gene synthesised in early March, and started working on protein expression and characterisation just as the UK was going into lockdown.

A high resolution structure of the nucleocapsid protein assembly could help in the development of antiviral drugs that disrupt the protein-protein or protein-nucleic acid interactions that are critical for virus assembly

This may allow the development of drugs to treat not only COVID-19, but also SARS-CoV and MERS-CoV, as well as other related coronaviruses that may emerge in the future.

The team, consisting of Postdoctoral Researcher Dr Oliver Bayfield and PhD students Dorothy Hawkins and De-Sheng Ker have been working in shifts around the clock so that they can follow social distancing guidelines whilst maximising the progress of their research.

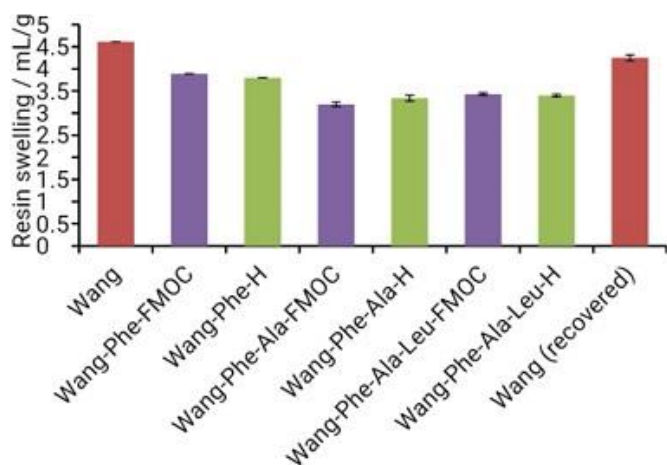
The researchers are collaborating with Dr Becky Thompson, the cryo-electron microscopy facility manager and senior support scientist at Leeds. With Becky, they are collecting the vital high-resolution microscopy data on the protein and protein-RNA complexes produced in York.

The team have also been sending purified protein and the gene that encodes several protein constructs produced at York, to labs in Sheffield, Oxford, and London. These materials are playing an important role in helping develop antibody tests for COVID-19 that will ultimately determine who has been infected with the disease.

Since starting work on SARS-CoV-2, the team have received messages and offers of support from colleagues across the University, and have been receiving enquires about collaboration almost daily. The work shows how scientists can very rapidly contribute to enhancing understanding in the face of a global pandemic, and is something very positive for science that is emerging from this troubling time.

York Chemistry undergraduates publish world-leading research paper

Work carried out by eight University of York Chemistry undergraduates results in a major publication in an international open access chemistry journal.



The students, led by Professor Michael North and Dr Anne Routledge, investigated how physical and chemical characteristics associated with polymeric resins affect their ability to interact with 15 sustainable solvents. The work has been published in open access chemistry journal, [ChemistryOpen \(2020, 9, 431–441\)](#).

Understanding how polymers interact with solvents - especially with new, environmentally friendly and sustainable solvents - is a major challenge, with applications to areas as diverse as pharmaceutical synthesis, polymer synthesis, graffiti removal and plastic recycling.

The complex 3D structure of polymers makes this a challenging area to study. The results of the students' work indicated that the chemical properties of the polymer had a larger influence on the solvent interaction than the physical properties. This is particularly important for the solid phase multi-step synthesis of pharmaceuticals (eg antiviral drugs) because the chemical properties of the polymer change as the synthesis proceeds. In particular, the results show that the optimal solvent may be different for each step of the synthesis. However, by understanding how the solvents and polymer interact, it becomes possible to choose a single solvent (or solvent mixture) which performs well for every step of the synthesis.

The students involved were Chidi Amadi-Kamalu, Holly Clarke, Matthew McRobie, James Mortimer, Dani Sibbald, Matthew Tickias, Kai Tse, Helen Willway and Yanrui Ran; they carried out the work for various projects, such as the BSc group project, the Year 4 MChem project and summer student projects.



Yanrui Ran was the only postgraduate student (MSc) who worked on the paper. In addition to contributing to the research, the students gained experience in working as a team and statistically analysing their experimental results for reproducibility.

Professor Michael North said: "This work is an example of how the University of York chemistry degrees encourage the embedding of cutting edge research into the undergraduate curriculum. It is by no means unique, but is unusual in having involved such a large number of undergraduates and only one postgraduate student."

Decorated gel bead 'doughnuts' with activity against drug-resistant bacteria

Core shell gel beads can be decorated with silver nanoparticles and show antimicrobial activity against drug-resistant bacteria.



Antibiotic-resistant bacteria are a major problem in modern healthcare, and can cause significant complications in hospitals for bone and wound healing. With problems such as these in mind, the development of antibacterial gels that can be used to help wound healing and bone regrowth is a vital.

Professor David Smith and his research group have expertise in developing soft biocompatible gels that self-assemble from simple molecular-scale building blocks. In recent studies they used one of their self-assembled gels as the 'filling' in a natural alginate polymer gel shell to create innovative core-shell gel beads that could be compared to jam-filled doughnuts.

They reasoned that these gel beads, which can be easily made, handled and manipulated could potentially be useful for preventing infections in orthopaedic and wound-healing applications, where gel bead systems are already in clinical use.

Decorated

In the same way that doughnuts can be decorated with other ingredients, Dr Carmen Piras, working in Professor Smith's team, reasoned that her gel beads could also be 'decorated' with other components to give them the required antibacterial properties. As the additional ingredient, she selected silver nanoparticles, which are known to be active against multiple drug-resistant bacterial strains and can promote bone growth. The use of silver nanoparticles on orthopaedic implants to avoid infections has recently gained some interest as an alternative to the administration of antibiotics.

In order to decorate the gel beads, Dr Piras made use of the unique properties of the self-assembled gel bead filling, which is able to reduce precious metals such as silver, to form metal nanoparticles. In this way, the gel beads could be effectively loaded up with the active ingredient.

Demonstration

Working with Dr Clare Mahon, Dr Piras demonstrated that the decorated gel bead doughnuts had antimicrobial activity against drug-resistant bacteria, in particular, vancomycin-resistant enterococci and pseudomonas aeruginosa, both of which are highly problematic hospital-acquired infections.

Dr Piras explained: "These gel beads are very easy to make and manipulate. They would be straightforward for surgeons to apply into wounds during orthopaedic surgery, and their antibacterial properties could potentially make them valuable for patients during the healing process."

The research was funded by [EPSRC](#) and the [European Commission](#) and is published in [Chemistry—A European Journal](#).

New study reveals York's air quality improves by 30 per cent during lockdown

York's air quality has improved significantly during the coronavirus lockdown, according to research by a University of York academic



Dr David Carslaw, from the Department of Chemistry, who is an expert in urban air pollution has analysed data from local traffic monitoring sites as part of an ongoing project. The data was compared against an estimated “business as usual” level.

The analysis shows improvements in air quality (nitrogen dioxide concentrations) of 30 per cent on average across the city.

Significant drop

The most significant drop across the city was a 43 per cent reduction in nitrogen dioxide concentrations in Fishergate. There was a 28 per cent reduction in Fulford Road and a 29 per cent reduction in both Gillygate and Lawrence Street. The lowest drop was recorded in Bootham of 16 per cent.

According to Defra's clean air strategy 2019 there are a number of deaths a year nationally, and children are suffering life-long health problems, as a result of poor air quality.

Air pollution

Dr David Carslaw said: “There has been widespread coverage of how air pollution has changed due to the COVID-19 pandemic. The satellite measurements sourced have been especially compelling, showing the before and after situation for many of the world's cities. We do of course have hundreds of ground-based continuous air pollution monitors across the UK that can also be investigated to better understand the changes in air pollution at a local level.

“This analysis is a first look at some potential changes in air pollution due to COVID-19. As more data becomes available, the robustness of these estimated changes should increase. However, it is already clear that there has been a dramatic and mostly consistent decrease in poor air quality (NO_x) across a wide range of sites, including York.”

Invested

Cllr Paula Widdowson, the City of York's executive member for the environment and climate change, said: “The impact of the Coronavirus lockdown has had a significant impact on air quality in the city. The council has invested in a number of measures in recent years to help improve air quality in York, and we will continue to do so for the benefit of our communities.”

Prof Alastair Lewis leads UK government effort to understand impact of air pollution changes during Covid-19 crisis

Professor Alastair Lewis of the University of York's Department of Chemistry is leading a national scientific advisory group calling for scientists and researchers to share their data on air pollution during the Coronavirus pandemic.



The pandemic has seen unprecedented changes in living and working patterns and is likely to have had a significant, but as yet unquantified, effect on air pollution in the UK.

Professor Alastair Lewis is the Chair of the UK Government independent science advisory group on air pollution - the Defra Air Quality Expert Group (AQEG) - who will use the data to inform future air quality management.

Air pollution

The AQEG is calling for evidence to address a series of urgent short-term issues related to recent and ongoing changes in UK air quality. These include:

- areas of socioeconomic activity that will or have shown a decrease in air pollution emissions
- changes in indoor and outdoor air quality
- how public exposure to air pollution has changed as a consequence of recent restrictions on movement
- how altered emissions of air pollutants over the next three months might affect UK summertime air quality
- the impact of air quality on viral infection

Professor Lewis, from the University's Department of Chemistry, said: "Evidence and insight into possible changes to the factors that control air pollution will help us to refine and improve how we deliver the best possible air quality for the UK."

"Air pollution has a significant adverse effect on public health affecting a broad spectrum of the population. It is a particularly significant environmental risk factor for vulnerable groups including those with underlying respiratory and cardiovascular diseases."

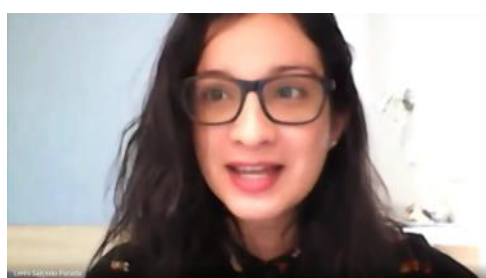
Emissions

Current restrictions on travel will have changed road transport emissions, and altered the locations where people are currently exposed to pollution. The relative mixtures of different pollutants being emitted in the UK may also have changed.

But in order to provide more accurate assessment of the potential impacts of air pollution in the coming months, better estimates of UK emissions, concentrations and exposure during COVID-19 are needed, said the advisory group.

Evidence and analysis are being sought from any relevant experts working in the field of air pollution science, technology or management. These might be based on existing measurements (such as local authority and research data, earth observation, activity information, or emissions reporting), atmospheric modelling or theoretical analysis, as well as scenario modelling and sensitivity analysis.

MSc Green Chemistry World Earth Day Meeting



MSc Green Chemistry Meeting for World Earth Day 2020

67 views



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Wednesday 22 April was World Earth Day, and students and staff from our MSc Green Chemistry course met virtually to discuss what the day means to them both personally and as practitioners of sustainable chemistry. A wide variety of home countries were represented, including Greece, China, UK, Pakistan, Columbia, Mexico and Nigeria and students were given the opportunity to share their thoughts in their native languages. Themes of hope, listening and working through issues collectively came up as well as the importance of small changes to our daily lives. The meeting was led by Dr Avtar Matharu, and you can see the [full recording on our YouTube channel](#).

STEM Village Symposium 2020 • Friday 28 August

Message from Derek Wann: The STEM Village were planning to hold a Symposium in June in Edinburgh at which researchers from the LGBTQ+ community - from PhD students to Professors - could present their research in any area of STEM. Since it's looking like social distancing will be necessary for the foreseeable future, it's unlikely that a physical conference will be possible. So, they're putting together a virtual conference! If anyone is interested in participating please complete [this registration form](#) (even if you registered before). If anyone has already submitted an abstract, please contact the organisers who can transfer it to your new registration: thestemvillage@gmail.com.

Online Department suggestion box



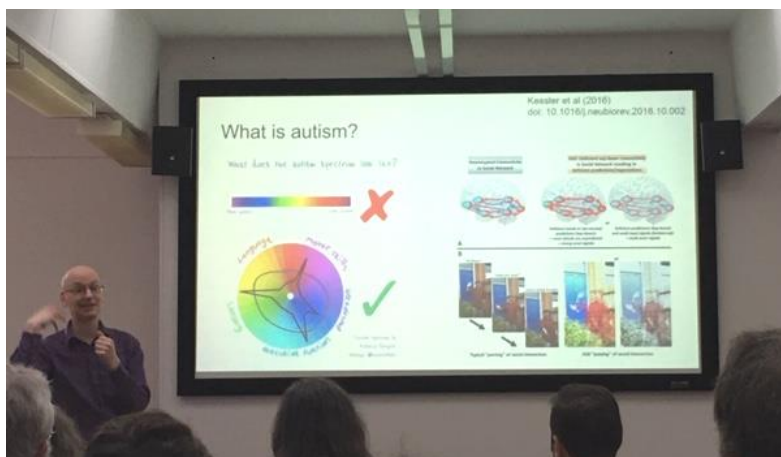
The online Equality and Diversity suggestion box has been extended to be a suggestion box for the whole Department. You can submit your thoughts/suggestions/ideas for general Departmental matters as well as matters relating to Equality and Diversity. You can find the Google form on the intranet homepage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

Chemical Interactions Equality and Diversity Seminar: Professor Kevin Cowtan



At the end of February, back in the days before social distancing when we could sit next to one another in lecture rooms, Professor Kevin Cowtan gave a Chemical Interactions talk under the theme of equality and diversity. The talk, entitled “Doing science from the intersection of colour blindness, autism and gender ambiguity”, provided a fascinating insight into Kevin's research career, the challenges he faces on a daily basis, and the strategies that he employs to try and overcome these.

It was a wonderfully honest talk that provided a lot of food for thought in terms of how we interact with one another, and how we can all be a little more mindful and understanding of the challenges that some people may be dealing with. This talk was very well attended with a full room of 50-60 people, both staff and students.



New starters

Freya Squires, PDRA - Data Analysis

Room: C/G116 (WACL); Ext: 4759; Email: freya.squires@york.ac.uk

Nico Seling, PDRA in Organic and Biomaterials Chemistry

Room: C/E202 & E214; Ext: 2593; Email: nico.seling@york.ac.uk

Will Drysdale, PDRA in Air Pollution Flux Measurements

Room: C/G116 (WACL); Ext: 4758; Email: will.drysdale@york.ac.uk

