



Calendar of Events

Research Seminar

Speaker: Andrew Feilden, BiCycle
Therapeutics
Date: Wednesday 8 November
Time: 1pm-2pm
Location: C/B/101

Academic Promotions Seminar

Date: Friday 10 November
Time: 12.30pm-1.30pm
Location: C/A/122

Research Seminar

Speaker: Jeff Peischl, CIRES/NOAA
Date: Monday 13 November
Time: 11am-12pm
Location: C/G/111

Diwali Celebration

Date: Monday 13 November
Time: 12.30pm-1.30pm
Location: C/B/101

UCAS Visit Day

Date: Wednesday 15 November
Time: 12pm-5pm

McCamley Lecture

Speaker: Andrew Jupp, University of
Birmingham
Date: Wednesday 15 November
Time: 1pm-2pm
Location: SLB/118

Staff Wellbeing Bake Sale

Date: Wednesday 15 November
Time: 2pm-4pm
Location: D-Block Tea Room

Research Forum on Publishing High Impact Work

Date: Thursday 16 November
Time: 12pm-2pm
Location: C/A/102

Research Seminar

Speaker: Eloise Marais, University
College London
Date: Friday 17 November
Time: 12pm-1pm
Location: C/A/101

Research Seminar

Speaker: Prof Akhil Sahoo, University
of Hyderabad, India
Date: Monday 20 November
Time: 1pm-2pm
Location: C/A/122

UCAS Visit Day

Date: Wednesday 22 November
Time: 12pm-5pm

Research Seminar

Speaker: Dr Kate Harris, University of
Newcastle
Date: Wednesday 22 November
Time: 1pm-2pm
Location: C/B/101

This issue:

New virus identified and
named after York - p2

Dr Seishi Shimizu's success in
Langmuir - p3

Nobel Prize winner opens
Eleanor and Guy Dodson
Building at University of York
- p4

Professor Avtar Matharu
responds to new report on
British Muslim transitions to
PGT studies - p5

The Brian Sutcliffe
Memorial Symposium - p6

Introducing your 2023
PDRA Committee
Representatives! - p7-8

KMS Winners Seminar - p8

New virus identified and named after York

A new study by researchers from the York Structural Biology Laboratory (YSBL) and the Department of Chemistry and the Department of Chemistry has identified and characterised a new type of virus which infects freshwater bacteria.

The virus has been called 'Jorvik' from the Viking name for York, the city where it was first discovered. The study was recently published in the journal iScience.

Jorvik does not infect humans but it infects bacteria found in aquatic ecosystems. These are indispensable for humankind; from food production to the global carbon cycle, water plays a role in vital planetary systems which sustain human life.

Identifying the virus is the first step in understanding how it affects our environment. As it infects members of the Rhodobacteraceae family, which have been found in a wide range of aquatic environments including oceans, it has the potential to be very widespread.

The presence or absence of the virus in aquatic ecosystems could also help us monitor the state of these ecosystems and react accordingly. Dr Pavol Bardy, lead author of the paper, explained: "Something similar is now being done with the human gut virome when an increased occurrence of certain virus families is linked to bowel issues. However, much more environmental research is required to be conducted on Jorvik in this regard to determine how it functions."

Dr Bardy was able to identify Jorvik in something of a lucky circumstance. While working on the bacteria called *Rhodobacter capsulatus*, he noticed it was producing a virus. He was then able to get a microscopy sample of the virus itself.

Dr Bardy explained: "For me, the most interesting part of this study was the discovery that Jorvik is very unstable when employing established laboratory protocols that have been in use from the beginning of bacterial virology.

That explains why this group of viruses remained hidden from us for many decades. Our luck was the fact that Jorvik resided as a dormant, persistent infection in one of our strains, similar to the human herpes virus that will reappear, for example, during stress. This is why we could periodically retrieve it from this strain and work with it."

The study reveals Jorvik represents the first member of an entire family of viruses. By comparison, the equivalent taxonomic family for humans also includes orangutans, gorillas and chimpanzees. Therefore Jorvik's discovery is key to finding, and understanding, more viruses like it.

Dr Seishi Shimizu's success in Langmuir

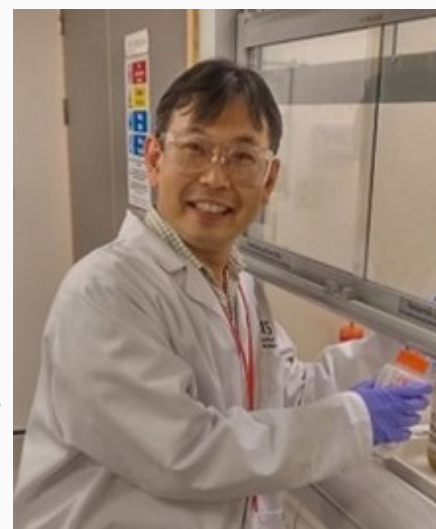
An academic in the Department of Chemistry has had outstanding success with achieving 4 out of 20 of the “Most Read” articles in Langmuir, a leading international journal dealing with surface and colloid chemistry.

Dr Seishi Shimizu is based at the York Structural Biology Laboratory (YSBL) and his recent research papers, which focus on sorption isotherms, have proved popular with the Langmuir readers. Sorption isotherms are important in a range of disciplines and applications, such as how food moisture content and cement paste change with humidity, measurement of the porosity of materials, and the characterisation of battery electrodes. However, there have been some fundamental flaws in the way sorption analysis is carried out conventionally.

In collaboration with Professor Nobuyuki Matubayasi of Osaka University, Japan, Dr Shimizu has answered this question. Instead of adding yet another model to an already well-populated catalogue that exist already, they started from the fundamental principles of statistical thermodynamics and established:

- the universal basic equations for sorption isotherms (valid for any surface shape and geometry, incorporating adsorption and absorption)
- a universal method to derive isotherms via differential equations
- capacity for modelling all six IUPAC isotherm types by the combination of only two statistical thermodynamic isotherms

The most popular isotherm models, Langmuir, BET, and GAB, are the special and restricted cases, based on idealized assumptions, of Dr Shimizu's isotherm.



Dr Shimizu extended his theory further to sorption from solution, where the simplistic adaptation of the gas adsorption model precluded clarity for decades. Many of his theories have been made interactive, and are therefore usable for practitioners with their own data.

Dr Shimizu said: “I thank Professor Matubayasi for an incredibly fruitful long-term collaboration, Professor Steven Abbott for making the theory usable via his apps, and the York Structural Biology Laboratory for its stimulating interdisciplinary research environment. I am happy that there are still important problems to be tackled by pen and paper.”

The four Shimizu-Matubayasi papers that made it in the 20 Most Read articles (30 days) in Langmuir are:

- Understanding Sorption Mechanisms Directly from Isotherms, Langmuir, 2023, 39, 6113.
- Surface Area Estimation: Replacing the Brunauer–Emmett–Teller Model with the Statistical Thermodynamic Fluctuation Theory, Langmuir, 2022, 38, 7989.
- Sorption from Solution: A Statistical Thermodynamic Fluctuation Theory, Langmuir, 2023, 39, 12987.
- Cooperativity in Sorption Isotherms, Langmuir, 2023, 39, 13820.

Nobel Prize winner opens Eleanor and Guy Dodson Building at University of York

Nobel Prize winner Dr Richard Henderson has officially opened the University of York's Eleanor and Guy Dodson Building.



From left to right: Professor Tony Wilkinson, Professor Duncan Bruce, Professor Caroline Dessent, Professor Eleanor Dodson, Professor Matthias Ruth, Dr Richard Henderson and Dr Jamie Blaza. Image credit: University of York.

The state-of-the-art building enables world-leading research to take place into the molecular structure of biomolecules by providing optimal conditions for electron cryo-microscopy.

Electron microscopes allow scientists to visualise the proteins and other biological molecules that sustain life. Understanding the structure of these molecules aids the design of new medicines, for example antibiotics or vaccines.

The building's name pays tribute to the pivotal role played by Eleanor and the late Guy Dodson in establishing the world-renowned York Structural Biology Laboratory (YSBL) within the Department of Chemistry.

Dr Henderson was awarded the Nobel Prize in Chemistry 2017 for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution.

Dr Henderson said: "The understanding of biological structures has grown in importance and impact over many decades since the 1950s.

"It now forms the foundation of much of biology and medicine, so the inauguration of the Eleanor and Guy Dodson building at the University of York is a key part of the future access to the methodology by present and future scientists."

The building was designed around the specific requirements of structural biology hardware and provides low-vibration, low-humidity, constant-temperature conditions for the electron cryo-microscopy suite.

Its construction was funded by a generous grant from the Wolfson Foundation and the University of York, while the equipment was funded by the Wellcome Trust, Biotechnology and Biological Sciences Research Council, and Dr Anthony H Wild, an early York Chemistry graduate and generous benefactor to the University of York.

Dr Jamie Blaza, the academic lead on the cryoEM facility, added: "Our key pieces of equipment, the electron microscope, NMR magnet, x-ray source, and crystallisation space, all have demanding environmental requirements for optimal performance.

"Even harder than that, they all have different requirements to each other. By providing us with a building designed from scratch around these activities, the Eleanor and Guy Dodson Building will offer YSBL a perfect home to our structural biology equipment for decades to come."

Watch the full recording of the public lecture [here](#)

Professor Avtar Matharu responds to new report on British Muslim transitions to PGT studies

The Aziz Foundation has launched a major report on British Muslim transitions to PGT studies entitled "Transitions: British Muslims between undergraduate and PGT studies". Professor Avtar Matharu was invited to give a formal response at the launch event which took place on Thursday 26th October at University College London.

The report explored representation, experiences of discrimination, financial pressures and, post-Masters expectations.

The report made four recommendations:

1. HEI's to consider adoption of the working definition of 'Islamophobia'.
2. Parity of esteem and financial resources between pre-entry WP and postgraduate WP, with the latter taken as seriously as if the regulatory obligation had already been extended.
3. Ring-fencing of scholarships as a form of positive action
4. HEI's to be proactive in incorporating 'British Muslims' as a disadvantaged group in Access and Participation Plans, with targets set relating to participation, retention and attainment.



The Brian Sutcliffe Memorial Symposium – 11 October

Whether colleague, teacher, PhD supervisor or fellow Union activist, everyone who met Brian Sutcliffe knew that he was someone special. Last month, we learnt so much of why – his awesomely wide and deep knowledge, his ability to inspire, to teach, to entertain, his dedication to supporting colleagues in difficulty, or his determination to use theory to understand the very fundamental questions of chemistry. Those with long memories – Brian retired in 1998 after 33 years in the Department – were genuinely privileged to know him. Talking of long memories, David Waddington took us back much further – to Brian's recruitment 58 years ago at the very start of our Department of Chemistry. We hosted Brian's family, several of our original academic staff and one of the earliest research students at the event.

To celebrate Brian's legacy, we had invited two former students, Hazel Cox and Fred Manby, and one research collaborator, Jonathan Tennyson, to speak. Hazel had come to York to do a mathematics PhD but ended up as a chemist and is now a professor of chemistry. Fred came to York as an "innumerate" (his word) undergraduate and was inspired by Brian's lectures to become a theorist rather than an organic chemist as he anticipated. His path has taken him, via a professorship of theoretical chemistry in Bristol, to California as Chief Technology Officer of a software company (Entos) that uses machine intelligence to design new drugs. Jonathan met Brian when he was a postdoc in Nijmegen and Brian was a visiting professor. Their long-standing collaboration enabled them to calculate the vibrational spectra of very hot, very small molecules with fabulous precision. Their prediction of the spectrum of H_3^+ led to their first triumph – the recognition that H_3^+ was present in the aurora of Jupiter and that their theory could act as a thermometer. That turned Jonathan from a chemist to an astronomer. Thirty years later, the same theoretical methods allow imaging of gas turbine measurements and measurement of the temperature of wildfires from space. Nowadays Jonathan is a professor of physics in UCL, runs citizen science projects with schoolchildren and has a software company (Quantemol) to exploit the Tennyson-Sutcliffe methods. Don't let anyone tell you that theoretical chemistry isn't useful!

The symposium was really a double bill. The second half celebrated Peter Karadakov's promotion to a professorship and his new look at aromaticity as well as the work of two early career researchers, Cate Anstoter (now in Edinburgh) who studies excited states of gas-phase anions and Conor Rankine who uses machine intelligence to analyse X-ray spectra in condensed phases.



Introducing your 2023 PDRA Committee Representatives!

Our Chemistry Postdoctoral Representatives are the conduit to voice praise, concerns, suggestions and feedback of the early career research and teaching communities to the Department and serve to help shape the policies that directly impact on your training, research, professional development and cultural experience at York. Thank you in advance for engaging with them productively so that they can serve effectively on our behalf. Huge thanks you to this year's Postdoctoral Representatives for taking up the mantle!



Dr Naomi Farren, Carslaw Group, WACL
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Research theme: Atmospheric Chemistry
Committee: Departmental Research Committee (DRC)

Hi, I'm Naomi, an atmospheric scientist based at the Wolfson Atmospheric Chemistry Labs. I am really pleased to be continuing my role as PDRA rep for the Departmental Research Committee this year. My role is to provide input from the early career perspective on aspects of departmental research activity and strategy, such as fellowship and research grant applications, allocation of resources, and department research themes. If you have any concerns, feedback or suggestions relating to this, please feel free to email me or come and find me in WACL (C/G/119). Thanks!



Dr Matthew Gill, McGonigal Group
matthew.gill@york.ac.uk

Research Theme: Molecular Materials
Committee: Safety Management Group (SMG)

Greetings all, I am the Postdoc representative for the Safety Management Group. So for at least the next year I will be your voice in the department for all things safety related! If you have any safety matters or suggestions that you would like raising at the meetings please let me know, especially around the department's policies or how things are done here in York. Feel free to email me, or pop upstairs and say hello, I work in the E202 office or E214 lab.



Dr Beth Nelson, Carpenter and Lee Groups, WACL
beth.nelson@york.ac.uk

Research theme: Atmospheric Chemistry, Digital Chemistry
Committee: Equality, Diversity & Inclusion Committee (ChemEDI)

As the PDRA representative for Chemistry Equality, Diversity and Inclusion (ChemEDI), I am committed to providing a route for which PDRA specific EDI suggestions, ideas, and complaints are acknowledged and actioned. Please email me if there is absolutely anything you wish to be raised on behalf of yourself or the PDRA community (anonymously or otherwise), so we can work toward creating a more inclusive Department.



Dr Rabia Ayub, McGonigal Group
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Research theme: Molecular Materials
Committee: Board of Studies (BoS)

I am computational organic chemist working on the design singlet-fission chromophores for applications in the solar cells as Marie-Sklodowska Curie Postdoc Fellow (MSCA). As the PDRA Rep on the Board of the Studies, I'm excited to learn a lot and contribute to our aims to ensure the performance and quality assurance of Chemistry teaching at York. You can find me in E214 and E202. Feel free to approach me in case of any questions or feedback (I'm also on the Chemistry Postdoctoral Society Committee so get in touch to get involved!)



Dr Aisha Bismillah, McGonigal Group
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Research theme: Molecular Materials
Committee: NMR Committee

Hi everyone :) I'm Aisha, a PDRA in the McGonigal group. I'm a physical organic chemist in the field of Supramolecular Chemistry and my research focuses on 'shapeshifting' systems. I'm a heavy NMR user (specifically variable-temperature) hence why I was interested in becoming a member of the NMR committee. As a member of the NMR committee, I'm looking to listen to the voice of the postgraduate community in terms of NMR and determine whether changes can be implemented, so feel free to contact me with any comments.

KMS Winners Seminar 2023

The Winners of this year's KMS prize each delivered a fantastic talk about their research at a seminar on 18 October. Having been shortlisted from 14 nominations, our three winners had been interviewed and selected by an academic panel back in the summer and each won a prize from the Kathleen Mary Stott Memorial fund.

The seminar was followed by a drinks reception to celebrate our winners.

Ana Silva Terra (MEH)

Towards analytical applications using SABRE-hyperpolarised ^{19}F benchtop NMR

Samuel Cliff (JDL/SJM/MS)

Understanding evolving urban air pollution sources with emissions measurement applications

Helena Lancaster (ASW/SBD/RNP)

Shining Light on the Hydrosilylation Reaction : a Kinetic and Mechanistic Study



Congratulations to all nominees as well as our winners, and thank you to the KMS Panel, Jamie Blaza (Chair), Meghan Halse and Chris Spicer.