Chemistry Update

Newsletter 350, 19 December 2022

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Calendar of Events

RSC-SCIG Sustainable Coatings Conference
Speakers: Various
Date: Tuesday 10 January
Time: 9am—4.30pm
Location: C/F106, GCCE

Teledyne table-top exhibition
Date: Thursday 12 January
Time: 9am—2pm
Location: Chemistry A Block foyer

UCAS Visit Days
Dates: 17, 19, 26 & 31 January
Time: 12pm—4pm

Green Chemistry Seminar
Speaker: Dr Vipul Patel, Grünenthal GmbH
Date: Tuesday 17 January
Time: 1pm—2pm
Location: C/F106, GCCE

Merck table-top exhibition
Date: Wednesday 18 January
Time: 9am—2pm
Location: Chemistry A Block foyer

McCamley Lecture
Date: Wednesday 18 January
Time: 1pm—3pm

Radleys exhibition
Date: Thursday 19 January
Time: 10am—2pm
Location: Chemistry A Block foyer

Green Chemistry Seminar
Speaker: Darren Stead, AstraZeneca
Date: Friday 20 January
Time: 1pm—2pm
Location: C/F106, GCCE

Date of Next Issue:
27 January 2023

MChem student solves adsorption problem

Olivia Dalby (MChem, 2021) has had her MChem project work, providing new insights into adsorption on solid surfaces, published in the journal Langmuir as the lead author.

The adsorption of chemical species on surfaces is important across a range of disciplines, such as understanding the effect of humidity on the moisture content of food or the water content of cement paste. Adsorption isotherms are routinely measured when characterising battery and porous materials. However, explaining and modelling such isotherms based on the underlying molecular interactions is a very challenging task, especially when the surface is heterogeneous, meaning that adsorption can take place in a stepwise manner.

Olivia carried out a theoretical study, supervised by Dr Seishi Shimizu focusing on these challenging adsorption isotherms. Her task was made even more difficult by the pre-existence of more than 80 different isotherm models, each having different scopes and premises.

Olivia focused on particularly challenging stepwise and multiple-stepwise isotherms. These are usually observed in heterogeneous surfaces that contain pores of both microscopic and mesoscopic sizes. Unlike previous approaches that start from an assumed adsorption mechanism, Olivia helped to establish a novel, unified approach, that can model all types of isotherms, based directly on the fundamental principles of statistical thermodynamics.

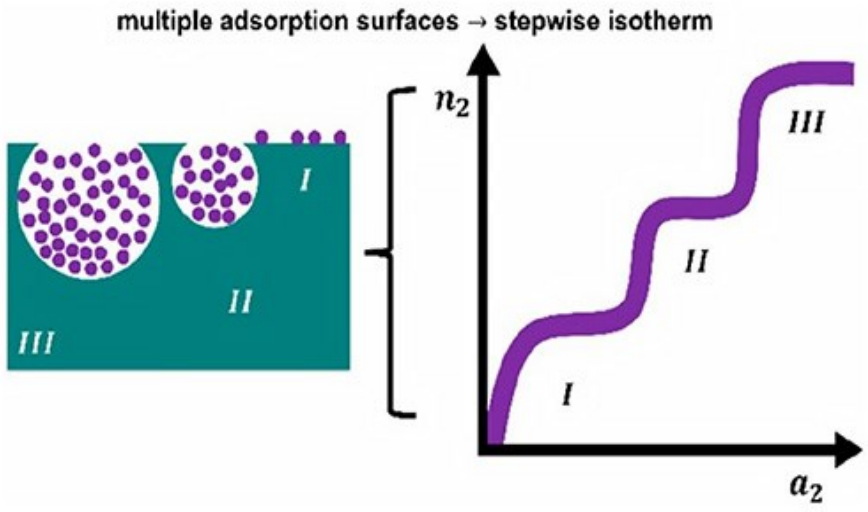


Figure: Stepwise adsorption on a heterogeneous solid surface.

The paper comes with an interactive web-based app written by Professor Steven Abbott working at TCNF Ltd, Ipswich. In this way, measured isotherm data can be directly analyzed by the new theory.

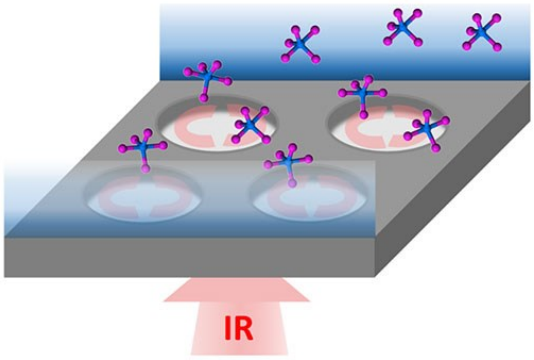
This work is the culmination of a long-time collaboration between Dr Shimizu and Professor Nobuyuki Matubayasi from Osaka University in Japan. The authors hope that the new unified theory will allow the simple modelling of all adsorption isotherms, rather than researchers having to select the appropriate model from many different possibilities.

Olivia said, “I am excited to see my MChem work published in Langmuir. I really enjoyed working on this with my supervisor, Dr Seishi Shimizu, and the coauthors, even with the challenges of online meetings in lockdown! I am proud of the work we achieved, and look forward to see how this paper may help future adsorption isotherm studies.”

Olivia’s work is published in *Langmuir*.

Enhancing the infrared detection of molecular fingerprints

A new approach, developed in York, significantly enhances molecular detection in dilute solutions and opens exciting new possibilities in terms of disease diagnosis.



The ability to determine the molecular composition of liquid mixtures is needed across a wide range of science, from monitoring chemical reactions to the analysis of biomedical samples. However, the complexity of such systems, and the low levels of some analytes of interest, can make this analysis particularly challenging.

Infrared (IR) spectroscopy is a powerful analytical tool because the signals act as highly distinctive 'fingerprints', based on the precise details of the molecular structure. Unfortunately, applications of IR spectroscopy are limited by its relatively low sensitivity.

In order to address this issue, a team based in York led by Professor Neil Hunt in the Department of Chemistry and Professor Thomas Krauss of the School of Physics, Engineering and Technology have taken a surface modification approach.

The team produced a series of silicon surfaces patterned on the micro-scale (smaller than the thickness of human hair). When samples are placed on these surfaces, the IR signals are enhanced by 10-100 times, thus allowing molecules to be detected at much lower concentrations than was previously possible.

Importantly, the enhanced electric field associated with these unique patterned surfaces, that creates the enhancement in signal intensity, extends deeper into the material being analysed than currently used metal surfaces. This means that the IR signals of dilute liquids can be enhanced and properly analysed for the first time.

Dr Soheila Kharratian, a postdoctoral research associate in the Hunt lab, and first author on the paper explains: "Being able to analyse the composition of dilute liquids with IR is a very significant breakthrough. In the future, this might find application in the analysis of blood samples.

"For example, it may be possible to precisely monitor the levels of pharmaceuticals and their metabolites in the bloodstream. Alternatively, specific molecules present within the blood may even act as detectable fingerprints of certain diseases."

This research has been published in *Chemical Science*.

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.

Introducing Jenny Glynn, New Student Wellbeing Officer

Scan QR Code to book a meeting

Hello everyone!

I thought I would introduce myself, my name is Jenny Glynn and I am the Student Wellbeing Officer for Chemistry, Biology, Biochemistry, Biomedical and Natural Sciences.

I will be mainly based in Chemistry Block A, Room 117 on Mondays and Wednesdays to Fridays where I can offer face-to-face, Zoom, walks or phone call appointments. On Tuesdays, I will be available for only Zoom or phone calls.

To make an appointment, please book a slot in my calendar.

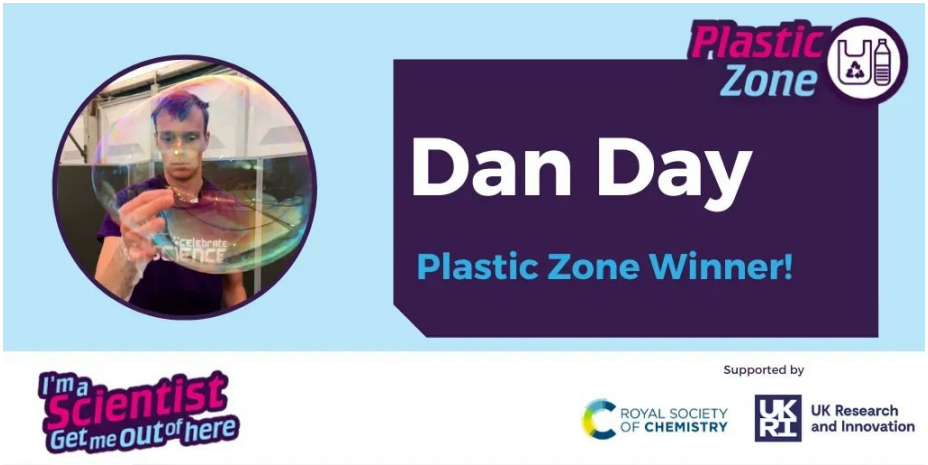
You can also contact be via email: jennifer.glynn@york.ac.uk

If you are a member of staff:

If you wish to refer a student, please fill in this Google Referral Form.

You can also contact me via email.

I'm a Scientist – Plastic Zone Outreach Winner



Green Chemistry Centre of Excellence (GCCE) PDRA Dan Day recently took part in the RSC- and UKRI-funded, 'I'm a Scientist Plastic Zone' outreach event. *I'm a Scientist* connects school students with scientists through live online chats to give them the opportunity to find out what it is like to pursue a career in science. The plastic zone drew lots of questions on environmental issues with plastics, which allowed Dan to communicate some of the recent results from the University of York coordinated CHAMPION research project into bio-based polymers. Over the course of the month, Dan was voted the favourite scientist by the students, for which he was awarded £500 to spend on more outreach activities in the future. *I'm a Scientist* runs many different themes and is a great way to communicate your research with many students without geographical restrictions so have a look into it if you are interested in doing more outreach.

Roxana's return to the Green Chemistry Centre of Excellence

"I have a long history with the GCCE: I graduated with a Masters by Research and a PhD. In 2015, I enrolled on an MSc by Research in Green Chemistry, where I completed a thesis entitled 'Adsorption of small polarisable molecules using mesoporous carbonaceous materials', which was focused on the use of Starbon® materials in gas adsorption. In 2017, I started my PhD entitled 'Applications of the novel bio-derived solvent Cyrene in polymer chemistry' in collaboration with Circa Group. My PhD thesis was based on the replacement of toxic polar aprotic solvents with Cyrene in applications such as filtration membranes, wire coatings, graffiti removal, extraction of bioactive compounds from food waste and carbon nanotubes dispersions.

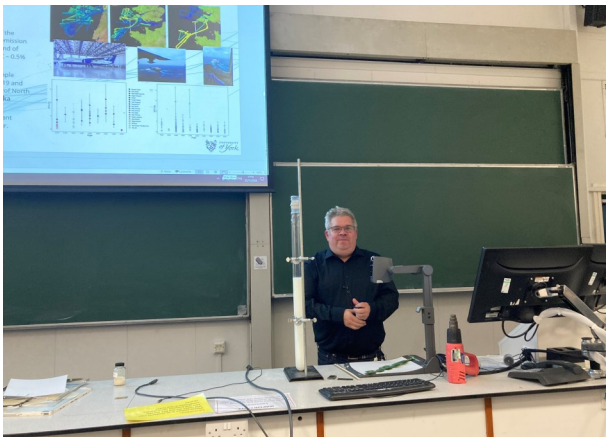
"Since l finished my PhD, I've been working in industry and had two jobs at AgrifoodX and Chip[s] Board. As a proud green chemist, I replaced various chemicals and solvents with greener alternatives for more sustainable processes. During my time in industry, l worked with Natural Deep Eutectic Solvents and green conventional solvents (lactic acid). I used deep eutectic solvents to extract bioactive compounds from food waste and developed new solvents from this class; at least one patent will be released based on the new class of solvents. Next, as the lead of the downstream department, l developed the process of the extraction and purification of lactic acid from potato waste at plant scale. Also, l designed the pilot plant of the downstream process and led various projects with the BDC and the University of Loughborough.

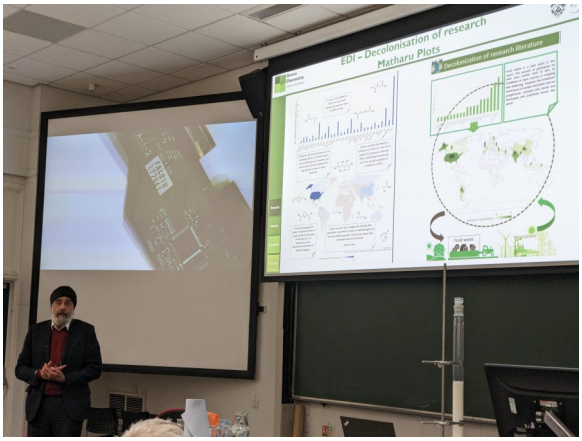
"I came back to work for the new Circa Renewable Chemistry Institute (CRCI) to continue my collaboration with Professor James Clark and Circa Group because it was great to work with the people involved in my PhD. I left University with many ideas that l could not materialise during my PhD. I also feel that l grew more during my time in industry and l strongly believe that l can bring back more knowledge which will help me materialise the research ideas l possess. I am happy to be back in York, which l consider home, and the GCCE, where l made great friends."

- Dr Roxana Milescu, CRCI Technical Manager

Inaugural Lectures held on 23 November

Thank you Professor James Lee and Professor Avtar Matharu!





Nicky Waller wins Special Recognition Award for Outstanding Contribution to STEM Education in the North East

Nicky Waller, who has worked for the Centre for Industry Education Collaboration (CIEC) in the Department for nearly 20 years, has recently added another accolade to her collection. On Friday 11 November at the 2022 North East STEM Awards, she was presented with the "Special Recognition Award for Outstanding Contribution to STEM Education in the North East". This is not the first honour that Nicky has received; last year she received the Excellence in Primary Education award from the Royal Society of Chemistry for sustained contributions to the professional development of primary teachers in the teaching of science. Previously, in 2017, she was awarded with Primary Science Teacher of the Year from the Institute of Physics.

After receiving the latest recognition, Nicky told us:

> "*I was absolutely over the moon to receive the outstanding contribution to STEM education award. There are many people doing exceptional things to promote the STEM agenda across the northeast, and to be recognised amongst these people and their organisations is a real honour*."

Needless to say, her colleagues at CIEC are not surprised; they have seen how she inspires primary school children and their teachers in her work for CIEC, and helps to raise the aspirations of the young people she works with. Moreover, she is a positive influence for the whole CIEC team as she embodies the CIEC ethos of looking for, and building on, the best in people thus helping them to be the best that they can be. CIEC director, Joy Parvin, told us:

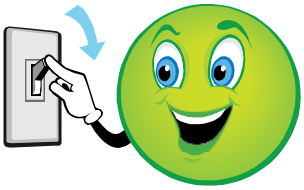
> "*I am so proud to see Nicky receiving the recognition that she deserves. I have seen how she uses her skills to raise the life chances of children while dispelling stereotypes of science careers and industries.*"

Nicky won't be letting the grass grow under her feet. Early in the new year, Joy and Nicky are due to deliver a keynote address at the Association for Science Education annual conference. After that she will continue her work on a variety of projects for CIEC, including Best Evidence in Science Teaching, leading primary courses at the National STEM Learning Centre, Thinking Doing Talking Science, Teacher Assessment in Primary Science and Children Challenging Industry.

Green Impact

Please switch-off over Christmas

Over the Christmas break, please can you ensure the following is turned off (preferably turn off at the wall):



- Computers
- Printers
- Monitors
- Lights
- Photocopiers
- Any equipment that does not need to be kept running over this period

Please turn down the heating to the minimum settings where possible (radiators, thermostat controls and thermostatic radiator controls). Please also turn off any air conditioning as well.

Think carefully about whether you need to leave your desktop switched on for the whole of the break and the environmental impact of this. You should only leave your PC on if you think you definitely will need to access your PC remotely via the Virtual Desktop Service (VDS) i.e. to access specific software on your PC. Remember you can still have remote access to the Virtual Private Network (VPN) which includes filestore access and web based apps without your PC being left switched on. Further information on remote access can be found on the IT Services - Work off campus pages.

Save your Christmas stamps!

Used stamps are collected and given to the Royal National Institute of Blind People (RNIB). The charity sells the stamps to generate revenue for their work.

Any and all stamps welcome!

Find a collection envelope located at **Chemistry reception**.

Green tips for Christmas

◊ **Heating** - try not to turn the heating up too much - wrap up in a jumper/blanket instead and wear layers.

◊ **Recycling** - recycle as much as you can - you might even be able to recycle wrapping paper (check on your Council's website - may need to remove sellotape) or use up old Christmas cards for scrap paper.

◊ **Food waste** - try not to cook more than you need or try to use up left over food the next day or store in the fridge or freezer.

◊ **Water** - use a dishwasher for full loads - otherwise try to wash up (and turn the tap off between each use). Only boil as much water as you need in the kettle.

◊ **Oven** - don't open the oven door if possible as this wastes energy. Cook more things at the same time by using smaller oven trays, for instance.

◊ **Fridge** - don't open the fridge too often (leave the door open for a longer period of time while you take out the items you need is more efficient than opening and closing the door several times).

◊ **Driving** – try to reduce the number of trips you have to make, for example try to combine outings, go shopping fewer times. Also, in the cold weather, try not to keep your car running when you start it up in the morning (it is more efficient to go straight away – de-ice your car before you turn the engine on).

Sparrowhawk pays a visit to the Department of Chemistry

The University of York's security team had a busy morning recently, successfully rescuing this handsome sparrowhawk that had become trapped in the Department of Chemistry:

MChem student Megan Goss designs Christmas jumper

Green Chemistry MChem student Megan Goss's talents aren't just limited to chemistry… she designed this Christmas jumper herself!