CatalysisHub NEWSLETTER

UKCC 2023 Poster prize winners

Highlights of 2022

Dissemination and networking are a vital part of the scientific process, and the Hub has actively sought virtual mechanisms for interaction throughout 2022 including a diverse webinar program, training seminars, workshops, discussion meetings and conferences. The access to virtual events has been a positive outcome of lockdown and the Hub as seen much wider global attendance of events and webinars that is possible for in person conferences. It has also been possible to host training events aimed at PHDs, PDRAS and ECRS.

Research has continued across the Hub and there have been several scientific highlights. These include a new commissioning of a multi capillary reactor for XAFS and other analysis allowing higher throughput. The data project has continued developing workflows for catalysis especially in collaboration with the facilities on the Harwell campus to allow more efficient processing of the large amounts of data in facilities experiments. Modelling work has been undertaken to understand mechanisms for the Pincer Catalysis and utilise this to look at heterogeneous alternatives. Neutron techniques have been utilised for greater understanding of MTH reactions. In the Water and energy theme interesting insights have been gained into using Ionic liquid gels as immobilisation for biocatalytic chemical synthesis. An ATR – Photoelectrochemical cell is being developed to treat high ionic strength wastewater. In the circular economy theme catalytic cascades are being investigated for biomass valorisation. Grafted solid acid catalysts have been shown to have high TON and techniques such as XPS are being used to understand the increased activity.

The BAG access to B18 at diamond has continued and for the first time since March 2020 we have been able to perform *in situ* measurements. This was enabled by the expert team at Harwell who were allowed access and able to run experiments for members from other institutions. Beamtimes at ISIS and CLF have also restarted with reduced capacity. The Hub also continues to develop analytic techniques with the Synchrotron, Neutron and Laser facilities. This relationship with the Facilities at Harwell has enabled some experiment in this 2m world and researchers have helped test remote capabilities on B18 at Diamond as well as socially distanced experiments at ISIS and CLF.

Events 2022

Consultation with the UK Catalysis Hub for National Data needs workshop 1 March 2022

The Hub held a hybrid workshop to consult on data needs and wants of the catalysis community that should be delivered by a national data infrastructure. The UK Catalysis Hub has recognised, particularly in its 2nd phase, the need for the development of a data infrastructure to capitalise on its results. There is now the opportunity for the Hub to benefit from a UKRI investment in a national data infrastructure for the physical sciences, a crucial investment towards making catalysis research in the UK fully digitally enabled. This cross-technique infrastructure would integrate data across existing initiatives such as the STFC Facilities, Academic institutions etc., to: Support multiscale modelling and multimodal research; Leverage simulation data to drive experimental science and vice versa; Surface data from many sources; Provide reference-quality data; Standardise, normalise and aggregate data and metadata; Enable data to be exploited by AI methods; Support workflows that automate data processing; Seamlessly access performance compute for scaling up; Be a place for curation of legacy beyond individual projects. A pilot phase of the Physical Science Data Infrastructure (PSDI) has been funded following the submission of a Statement of Need. The pilot aims to plan the next phases of the PSDI via a number of activities, including workshops with major initiatives such as the UK Catalysis Hub. The workshop featured talks by Richard Catlow, UCL/Cardiff, Barbara Montanari, STFC, Abraham Nieva de la Hidalga – UK Catalysis Hub and Mark Pera-Titus, Cardiff. They were followed by a panel discussion chaired by: Ian Silverwood, ISIS, Matthew Quesne, Cardiff, Anthony Green, Manchester and break out sessions. The workshop's report will be written to feed into a proposal for an investment as part of the UKRI Digital Research Infrastructure.

UK Catalysis Hub May Town Hall Meeting 4 May 2022

The UK Catalysis Hub Town meeting took place on 4th May to discuss a potential evolution and future of the UK catalysis Hub.

The main aim of the meeting was to provide the data and community input to inform the critical opportunities as the Hub evolves to continue to meet the current challenges in catalysis, and the UK.

The agenda for the meeting included: Current state of the catalysis research for sustainable manufacturing, an international perspective, an industrial perspective, discussion and feedback and next steps.

UK Catalysis Hub Summer Conference 2022 20 & 21 June 2022

On the 20th and 21st of June 2022 the UK Catalysis Hub held its annual summer conference and networking meeting. The Conference took place at the Rutherford Appleton Laboratory, Harwell Campus, Oxfordshire. The event was a hybrid event with the option to attend virtually for those who could not attend in person.

The conference began at lunchtime on the 20th with lectures, a poster session and exhibition on the evening of the 20th June and dinner by invitation.

Exhibitions on the evening of the 20th June featured work developing catalytic processes for Net zero including more effective use of water and energy, waste minimisation, and material reuse and reduction by scientists from institutions across the UK connected with the UK Catalysis Hub. Exhibitions included; A step towards net zero carbon emissions, Catalysis in Schools Outreach, How Catalysis can Enable a Sustainable Future Beyond Oil: The Royal Society Summer Science Exhibition 2022, Replacing mercury with gold catalysts for a cleaner route to production of polyvinyl chloride (PVC), Prof. Charlotte Williams' Group and poster prize sponsors Enabled Future.

Exhibitions included;

A step towards net zero carbon emissions
The replacement of conventional fossil fuels (coal, crude oil and natural gas) and their derivatives such as gasoline, olefins and aromatics with carbon neutral renewable resources (e.g., atmospheric CO2 and biomass/bio-waste) holds the key to achieve the UK's ambitious target of net zero carbon emissions by 2050. This exhibit illustrated the potential of carbon neutral renewable methanol to hydrocarbons (MTH), a process that can achieve net zero carbon emissions from vehicles and polymer/chemical industries with the existing infrastructure. Dr. Santhosh Matam, Dr. A. Logsdail, Prof. A. Beale, Dr. E. Campbell, Dr. N.

Dummer, Dr. M. Wilding, Prof. M. Bowker, Prof. D. Willock and Prof. Sir C. Richard A. Catlow, FRS

Catalysis in Schools Outreach
Inspiring the next generation of catalytic chemists is an important activity for all researchers. This exhibit featured some recent activities that have been developed to give school pupils some hands-on insights into chemistry in general and catalysis in particular. They also illustrated how low-cost digital technology can be used to enhance experiments aimed at secondary school pupils. Dr. David Willock, Cardiff University

How Catalysis can Enable a Sustainable Future Beyond Oil: The Royal Society Summer Science Exhibition 2022
The UK's ambition to achieve net zero carbon emissions by 2050 will not be possible without new and innovative catalysis. The exhibit previewed their offering for the The Royal Society Summer Science Exhibition with activities and displays that highlight to the public; (1) How integrated petroleum products are currently to our daily lives, beyond "just fuel". (2) The fundamental concepts of catalysis and how it will enable us to move beyond oil. (3) The extent of the scientific challenges in enacting this change through catalysis and how it requires a collaborative effort between different scientific, engineering communities, and national facilities. They had a selection of the displays intended for the exhibition in the summer. Dr. Simon Kondrat, Prof. Sandie Dann & Anna Leather Loughborough University.

Replacing mercury with gold catalysts for a cleaner route to production of polyvinyl chloride (PVC)
Polyvinyl chloride (PVC) is the world's third most produced polymer after polyethylene and polypropylene. Until recently the formation of vinyl chloride monomer (VCM), the precursor to PVC, has relied on the use of a highly toxic mercuric chloride catalyst for acetylene hydrochlorination. This exhibit summarised the successful development of a gold catalyst for this reaction, and highlights the importance of close links between industry and academia. Dr Samuel Pattisson, Prof. Graham Hutchings' research group, Cardiff University

Prof. Charlotte Williams' Group
At the University of Oxford, Professor Williams and her team investigate how to make sustainable plastics. To do this, they take molecules derived from waste products, such as carbon dioxide and citrus peel, and transform them into long chains, known as polymers. These polymers can be used as the key ingredient for materials with a range of applications, from shoes to mattress foam, to sealants and adhesives. Compared with plastics derived from fossil fuels, these new materials have a decreased environmental impact and will help us in our effort to reach Net Zero. In the exhibit, scientists from the Williams group showcased some of their CO_2-derived materials. Attendees were also able to play games to help them understand the science of plastics and watch videos demonstrating how the team at Oxford conducts research. Professor Charlotte Williams, Dr Ryan Kerr, Dr Arron Deacy, Dr Thom McGuire, Dr Greg Sulley and Kam Poon

A poster session ran alongside the exhibition showcasing work from the Hub postdocs. Our poster prize winners this year were Edward Jones, Catherine Spencer, Shaojun Xu and Anastasia Zaleska. The poster prize was kindly sponsored by Enabled Future.

Prof. Andrew Harrison, OBE, FRSE, FRS, CEO, Diamond Light Source gave a public lecture at the UK Catalysis Hub summer conference. He spoke about his work at Diamond on Covid and the scientific opportunities with Diamond II for scientific research.

Speakers at the UK Catalysis Hub summer conference included researchers from the Catalysis Hub, internationally renowned speakers and industrialists covering a range of topics in catalysis.

Recordings available to watch at https://youtube.com/playlist?list=PL3naBfxaSBmUvOK4zZTeoXCfXAxAkGP8-

UK Catalysis Hub and Harwell XPS workshop on photoelectron spectroscopy for catalysis
22 September 2022

The Harwell XPS & UK Catalysis Hub Workshop took place on Thursday September 22 at the Research Complex at Harwell. Attendees gathered for a day long hybrid event to learn about XPS and how it can be used to aid research in Catalysis! With speakers from HarwellXPS and beyond taking a detailed look at the technique of XPS including; XPS theory, experimental design, theory and understanding and describing your data.

Recording available to watch at https://ukcatalysishub.co.uk/uk-catalysis-hub-and-xps-harwell-workshop-on-photoelectron-spectroscopy-for-catalysis/

VI - UKEM Emissions Control Workshop
20 October 2022

The interactive workshop offered an open forum for technical discussion about the current challenges facing the automotive industry and provide experts from industry and academia the opportunity to share knowledge and ground-breaking technologies with colleagues from around the UK. The workshop discussions were around significant research and the challenges of future regulation in a multi-pronged approach, investigating advanced combustion regimes, alternative fuels, and next-generation emissions control technology.

Speakers included: Dr Matthew Keenan (Ricardo), Dr Andrea Eva Pascui (Johnson Matthey), Dr Kelly Kousi (University of Surrey), Prof Robert Steinberger Wilckens (University of Birmingham), Dr Fergal Coleman (IonicRE), Claire Leishman (University of Edinburgh), Colette Larkin (University of Edinburgh), Dr Agnes Thornton (Sustainable Flight Solutions) and Dr Haresh Manyar (Queen's University Belfast).

UKEM serves as a powerful motivator for the continued growth of the automotive mobility industry and its contributors.

UK Catalysis Hub Winter Conference
29 - 30 November 2022

On the 29th & 30th of November 2022 the UK Catalysis Hub held its annual winter conference and networking meeting. The Conference took place at the Rutherford Appleton Laboratory, Harwell Campus, Oxfordshire. The conference began at lunchtime on the 29th with lectures, the JMT medal presentation, a poster session in the evening of the 29th November and dinner.

The Conference also included memorial sessions for Sir John Meurig Thomas, a distinguished professor in the field of catalysis who sadly passed away in 2020. He was a remarkable man and one of the most eminent figures in catalytic science in the past 100 years, who was a pioneer in many of the techniques and concepts that have now become standard in the field. He was generous with his time and support for the UK Catalysis Hub and its events and the Hub is proud to have established 2016 an annual award in honour of his achievements and this session also included the presentation of the JMT medal for Catalysis to Prof. Stuart Taylor (Cardiff).

Speakers at the UK Catalysis Hub winter conference included; Prof. Fraser Armstrong (Oxford), Dr. Benjamin Bhawal (Edinburgh), Daniil Boiko (Carnegie Mellon University), Prof. Paul Cox (Portsmouth), Prof. Sankar Gopinathan (UCL), Prof. Thomas Maschmeyer (Sydney), Gerhard Mestl (Clariant), Prof. Eranda Nikolla (University of Michigan), Dr. Firdaus Parveen (Liverpool), Prof. Robert Schlögl (Fritz-Haber-Institut der Max-Planck-Gesellschaft), Prof. Martin Schröder (Manchester), Prof. Magda Titirici (Imperial) and Prof. Paul Wright (St. Andrews).

Watch recordings of presentations from the conference at https://ukcatalysishub.co.uk/uk-catalysis-hub-winter-conference-2022/.

UKCC 2023
4 - 6 January 2023

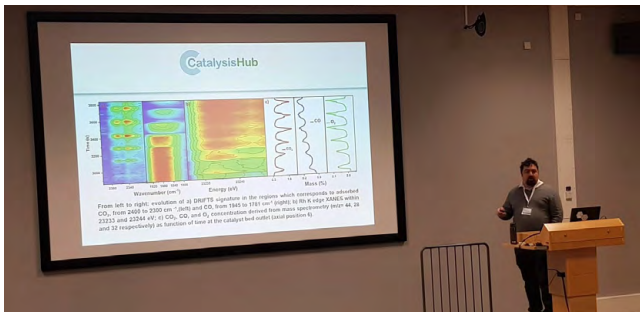
The ninth UKCC conference took place from the 4th - 6th January 2023. The conference was attended by over 100 delegates including academics, industrial researchers, experimentalists, theoreticians, and students.

Plenary speakers included: Prof. Javier Pérez-Ramírez (ETH Zürich), Prof. Unni Olsbye (University of Oslo), Prof. Emiel J.M. Hensen (Eindhoven University of Technology), Prof. Martin Schröder (The University of Manchester) and Dr. Sofia Diaz-Moreno (Diamond Light Source).

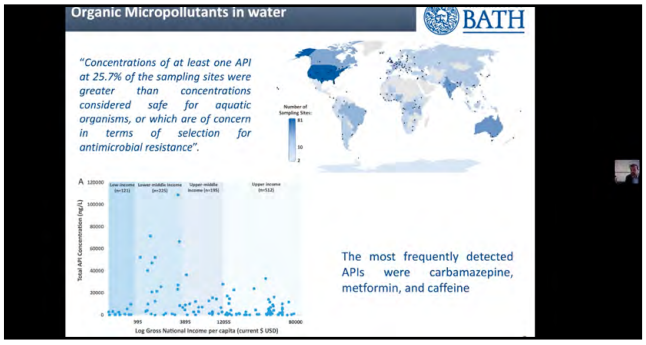
Keynote speakers included: Prof. Pieter Bruijnincx (Utrecht University, Netherlands), Dr. Antoine Buchard (University of Bath, UK), Dr. Marina Carravetta (University of Southampton, UK), Prof. Mark R. Crimmin (Imperial College London, UK), Dr. Melis Duyar (University of Surrey, UK), Dr. Peter Johnston (Johnson Matthey, UK), Prof. Wen-Feng Lin (Loughborough University, UK), Dr. Mark Muldoon (Queen's University Belfast, UK), Prof.

Glenn Sunley (BP, UK), Prof. Gosia Swadzba-Kwasny (Queen's University Belfast, UK) and Dr. Dan Zhou, (DENS Solutions, Netherlands).

The conference was supported by the UK Catalysis Hub with a session on catalysis featuring Hub PhD students and researchers. The scientific programme was organised around many aspects of catalysis, including organo/biocatalysis, heterogeneous catalysis, homogeneous catalysis and engineering.



Webinars: Photocatalytic Foams for Organic Micropollutant Degradation with Prof. Davide Mattia, 29 March 2022



The presence of micropollutants – pharmaceuticals, pesticides, phthalates and hormones in water is a major global health and environmental challenge. Conventional wastewater processes are not capable of effectively removing these compounds, often found at very low concentrations, µg L-1 or even ng L-1, leading to their discharge in surface and ground water. Photocatalytic processes, while effective at removing micropollutants, have not yet been deployed at industrial scale due to cost and safety concerns associated with the potential leaching of nanoparticle slurries on one hand, and the low activity of immobilized photocatalyst configurations on the other.

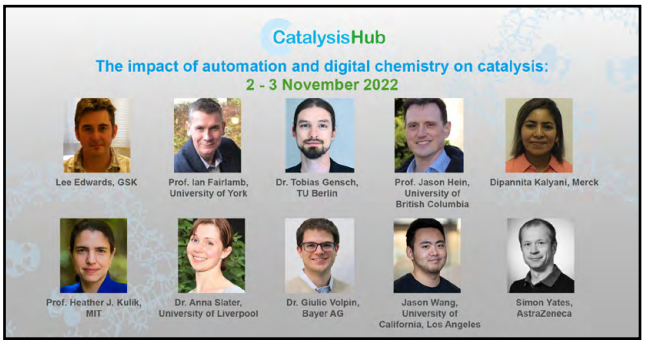
In this presentation Prof. Davide Mattia discussed his work to address these twin challenges by developing novel photocatalytic foams, whose activity is given by the material itself rather than grafted nanomaterials, as previously done. His initial work focused on sintering ZnO microparticles to obtain porous self-supporting foams. He has tested these foams in batch, recirculating batch and single pass reactor configurations, obtaining performances comparable to slurries. Since then, he has developed 'molecular foams', continuously interconnected porous structures, starting from metal oxide compounds, and he is now exploring 3D printing for photocatalytic foams.

Webinar with UK Catalysis Hub Director Prof. Matthew Davidson 4 October 2022

Director of the UK Catalysis Hub Matthew Davidson gave a webinar – Towards Sustainable Plastics: New Catalytic Approaches for Bio-based Polymers.

Recordings available to watch at https://ukcatalysishub.co.uk/webinar-with-uk-catalysis-hub-director-prof-matthew-davidson/

The impact of automation and digital chemistry on catalysis 2 – 3 November 2022



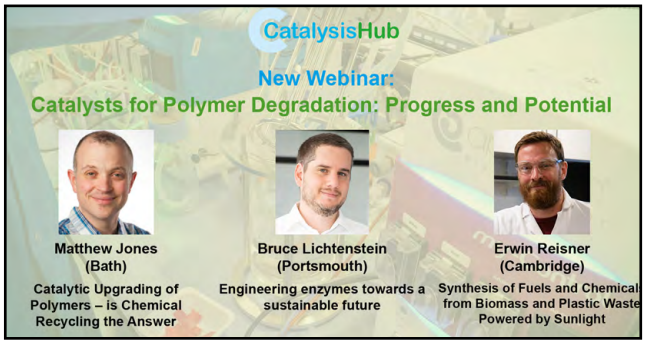
The UK Catalysis Hub and Centre for Rapid Online Analysis of Reactions (ROAR) hosted a virtual meeting to discuss the impact of automation and digital chemistry on catalysis. The discovery, design and optimisation of catalysed reactions are undergoing profound and transformative changes, driven by the growing use of automation/robotics, flow chemistry, and the integration of data and machine learning into workflows. This meeting was designed to allow pioneers and practitioners to share their experiences, followed by time for questions and panel discussions in each of the four focus areas (automation, digital chemistry, chemistry in flow and industry 4.0). The meeting included contributions from speakers based in both industry and academia, from the UK and abroad, as well as highlighting some of the UK's facilities open to external users in the UK.

Speakers included: Lee Edwards, GSK, Prof. Ian Fairlamb, University of York, Dr. Tobias Gensch, TU Berlin, Prof. Jason Hein, University of British Columbia, Dipannita Kalyani, Merck, Prof. Heather J. Kulik, MIT, Prof. Marc Pera Titus, Cardiff, Dr. Anna Slater, University of Liverpool,

Dr. Giulio Volpin, Bayer AG, Jason Wang, University of California, Los Angeles and Simon Yates, AstraZeneca.

Recordings available to watch at https://ukcatalysishub.co.uk/the-impact-of-automation-and-digital-chemistry-on-catalysis/

Catalysts for Polymer Degradation: Progress and Potential 14 November 2022



The UK Catalysis Hub hosted a virtual seminar "Catalysts for Polymer Degradation: Progress and Potential" for early career researchers on to discuss different catalytic solutions to plastic. The meeting had a series of talks in four topics on solutions from biocatalysts, homogeneous catalysis and heterogeneous catalysis with time for discussions afterwards.

Presentations included:
Matthew Jones (Bath) on Catalytic Upgrading of Polymers – is Chemical Recycling the Answer

The talk looked at the pros and cons of chemical recycling and different strategies. It then went into details of recent examples utilising Zn(II) and Mg(II) for polyester upgrading.

Bruce Lichtenstein (Portsmouth) on Engineering enzymes towards a sustainable future

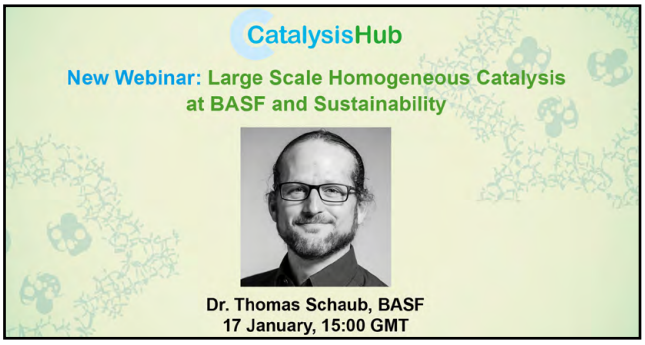
Plastics have revolutionised the way we live, yet the robust material properties that we depend upon have made them recalcitrant environmental pollutants. With most plastics deriving from petroleum feed stocks, and a developing appreciation of their potent negative effects in the environment and to human health, these polymers sit as targets of a global move towards sustainability. To address the needs for circularity in plastic use, they are taking a unified approach towards biological solutions to plastic pollution, with an emphasis on bioinformatics driven discovery of novel enzymes for plastic degradation, their engineering and laboratory evolution, and in the modelling and considerations for next generation plastic-depolymerase pairs. In this presentation, Bruce discussed recent results in the engineering of non-natural polymer degrading enzymes, highlighting new discoveries driven by enzyme engineering, and with a focus on identifying the properties of enzymes and plastics needed to close the gap between the relatively inexpensive petroleum feedstocks and the polymer breakdown products from enzymes.

Erwin Reisner (Cambridge) on Synthesis of Fuels and Chemicals from Biomass and Plastic Waste Powered by Sunlight

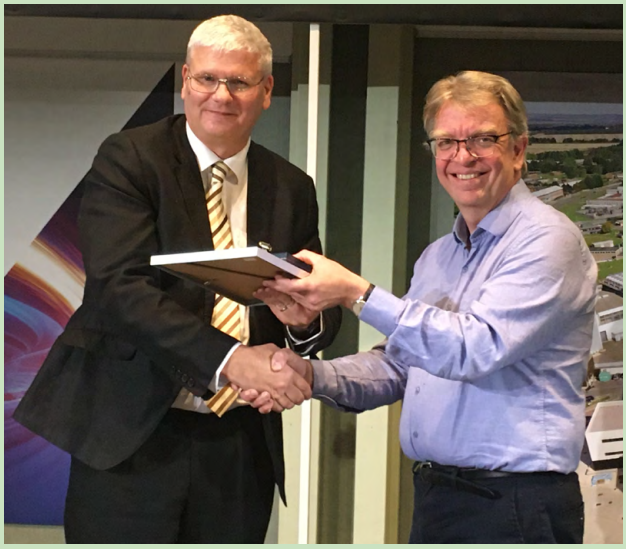
This presentation gave an overview on their recent progress in developing semiconductor nanoparticle systems and photoelectrochemical devices to convert biomass and plastic waste into sustainable hydrogen and valuable platform chemicals in a process generally known as photoreforming. The principles and design considerations for this solar-driven photo-reforming process were compared to traditional artificial photosynthetic systems as well as more conventional waste treatment processes and benefits and disadvantages discussed.

Recordings available to watch at https://ukcatalysishub.co.uk/catalysts-for-polymer-degradation-progress-and-potential/

Large Scale Homogeneous Catalysis at BASF and Sustainability 17 January 2023



BASF is applying homogenous catalysis for the production of organic products on a multi-million ton scale each year. In this webinar an overview on these large-scale process at BASF was provided by Dr. Thomas Schaub. He also explained how such an efficient process was developed. Addressing the challenges in terms of more sustainable processes in this field was also covered.



JMT Award Winner Announced

The UK Catalysis Hub have named Professor Stuart Taylor from Cardiff University as winner of the Sir John Meurig Thomas Catalysis Medal at the UK Catalysis Hub Winter Conference on the 29th of November 2022. Professor Stuart Taylor was selected from the nominations for top mid-career scientists working in the United Kingdom to win the medal for 2022. Judges of this year's Sir John Meurig Thomas Medal said, "We had a number of excellent applications but what really stood out was the impact of Stuart's work in its application to address the target problem, as well as clear future impact" and "were struck by the clear, demonstrable impact of his work in terms of environmental protection (the REF case study 2021), but also how this was combined with numerous impressive outputs across many other areas of catalysis. Achieved through sustaining a very high level of contributions for many years."

Professors Hutchings and Catlow agreed that it was most fitting that Stuart receives this recognition. "He has made many seminal contributions to heterogeneous catalysis translating fundamental catalysis into everyday use applications. He has pioneered innovative approaches to the synthesis of heterogeneous catalysts, developing fundamental understanding of catalytic processes. His catalyst discoveries are used in many commercial applications today benefiting society."

The medal honours the achievements of Sir John Meurig Thomas, a distinguished professor in the field of catalysis who sadly passed away in 2020. He was a remarkable man and one of the most eminent figures in catalytic science in the past 100 years, who was a pioneer in many of the techniques and concepts that have now become standard in the field. He was generous with his time and support for the UK Catalysis Hub and its events and the Hub is proud to have established 2016 an annual award in honour of his achievements. He will be missed by scientists in the Hub community and worldwide. The Sir John Meurig Thomas medal was presented at the end of a symposium on the first day of the conference in honour of Sir John Meurig Thomas's scientific achievements.

Professor Stuart Taylor delivered a lecture on catalysis to the UK Catalysis Hub Winter conference attended by over 100 people. He said on winning, "It is a privilege and a great honour to be awarded the 2022 JMT medal. I met Sir John many times, especially in his role as visiting Professor at Cardiff. He was always encouraging and enthusiastic and very gracious with his time and guidance, and his pioneering work influenced my own research. The award of the JMT medal reflects achievements over many years, and I am truly grateful to all of my students, colleagues and collaborators that have contributed and supported me."

Professor Stuart Taylor's work has focused on developing synthesis approaches to heterogeneous catalysts, delivering fundamental understanding of catalytic processes. Establishing relationships between catalyst structure and activity across a range of metal-nanoparticle and metal-oxide catalysts has driven the rational design of new catalysts, delivering impact across the important areas of energy, sustainability, green chemistry, and environmental protection. In particular, research has shaped environmental catalysis for life support and atmospheric emission control, including the discovery of highly-active copper manganese, nanocrystalline cobalt and cerium-based oxide catalysts. Catalyst preparation has also been exploited for upgrading inexpensive abundant feedstocks to more useful chemicals in sustainable approaches. Recent projects have pioneered bi-metallic supported nanoparticle catalysts for direct conversion of carbon dioxide to synthetic fuels, an important process for meeting net zero carbon targets.

The JMT medal was generously sponsored by BP, JM, Dr. Reddy's, Givaudan and Royal Society of Chemistry Applied Catalysis Group.

For more information and to watch a recording of Prof. Stuart Taylor's JMT lecture visit https://ukcatalysishub.co.uk/2022-jmt-medal-winner-announced/

Upcoming Events

Save the Date!

UK Catalysis Hub Summer Conference

17 - 18 July 2023

Harwell Campus, Oxfordshire

The UK Catalysis Hub Summer Conference 2022 will be held on **17th & 18th of July 2023** at Harwell Campus, Oxfordshire.

Talks will be starting at lunchtime on the 17th July with a poster session on the evening of the 17th July followed by a dinner at a local venue. The lectures continue on the 18th July until lunchtime.

Visit https://ukcatalysishub.co.uk/catalysis-hub-conferences/ for more information.

UK Catalysis Hub Webinars

ECR Seminar - Lignins

22 March 2023, 15:00 GMT

The UK Catalysis Hub are hosting a series of seminars for Early Career Researchers on the use of catalysts (bio, hetero- and homo-geneous) towards sustainable solutions in the carbon economy.

The next virtual seminar for Early Career Researchers will be on lignin related catalysis topics; particularly as a sustainable source of carbon feedstocks. Three talks followed with time for discussion.

Chair:
Bruce Lichtenstein, Portsmouth

Speakers:
Jeremy Luterbacher, École Polytechnique Fédérale de Lausanne (EPFL)

Lindsay Eltis, University of British Columbia

Shannon S. Stahl, University of Wisconsin – Madison

Register for free at https://ukcatalysishub.co.uk/early-career-researcher-symposium-lignins/

To find out about all our forthcoming webinars and register for them visit - https://ukcatalysishub.co.uk/webinars/

UK Catalysis Hub Phase II - Meet the team

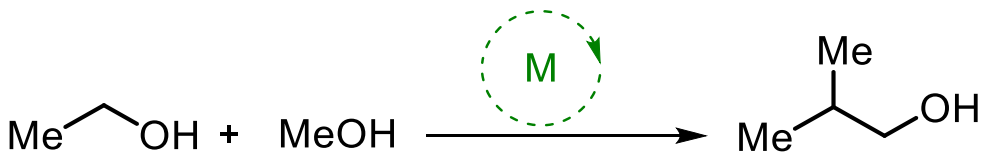
Join us in welcoming these new members of staff to the UK Catalysis Hub. We introduce them with a short profile of their background and what they will be working on with the UK Catalysis Hub.

Dr. Balakumar Emayavaramban - Catalyst development for bio alcohol synthesis and carbon dioxide valorisation reactions

I did my Master's in Chemistry at the National Institute of Technology Tiruchirappalli, India. I was first introduced to the field of catalysis during my Master's project, where I developed palladium catalysts for classical C-N coupling reactions. After my masters, I worked as a project assistant at the Indian Institute of Technology Guwahati for a period of six months. During this period, I synthesized chiral salen complexes for asymmetric cycloaddition reactions. These experiences early in my career motivated me to pursue further research in the field of catalysis.

I joined the Indian Institute of Technology Kanpur in 2014 for my Ph.D under the guidance of Dr. Basker Sundararaju. The main focus of my research was in base metal catalyzed (de)hydrogenative functionalization. I developed various iron and cobalt based homogeneous catalytic systems for C-C and C-N bond forming reactions. I employed two main approaches to construct C-C and C-N bonds; i) Hydrogen auto transfer reactions, and ii) reductive functionalization. This enabled the use of widely available and cheap alcohols as starting materials making this approach more attractive.

From October 2021 I joined the group of Prof. Duncan as a PDRA at Cardiff University. My role is to synthesize and characterize new and known organometallic complexes and their homogeneous catalytic screening for bio alcohol and carbon dioxide valorization reactions. A major focus of our project is to develop potential metal catalysts for the synthesis of the advanced biofuel isobutanol via the Guerbet reaction. The Guerbet reaction is a potential green process for bio alcohol synthesis by utilizing renewable feedstock chemicals and producing water as the sole side product. This current project is funded by EPSRC and the UK Catalysis Hub.



Author:

Dr. Balakumar Emayavaramban, Cardiff University

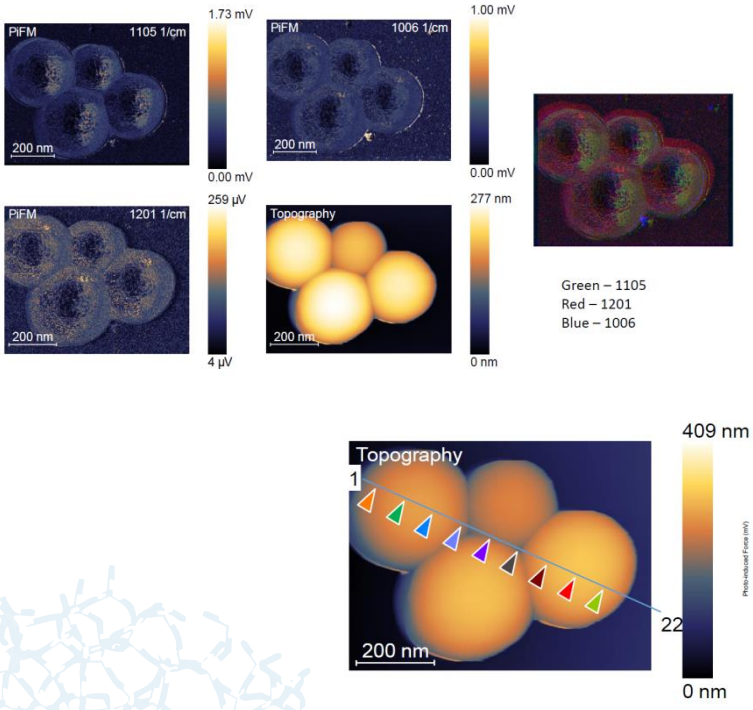
Dr Arthur Graf

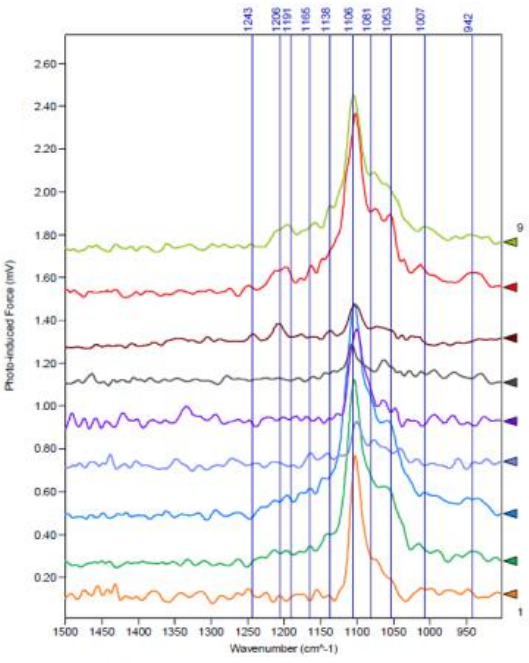
I got my PhD in chemical-physics/spectroscopy from the University of Sheffield last year under the supervision of Dr Adrien Chauvet. My research field is X-Ray Photoelectron Spectroscopy (XPS)/ surface science, which led me to join Prof. Phillip Davies at Cardiff University (CU)/HarwellXPS. I have also been privileged as an undergraduate to do research – including using the LNLS (Synchrotron light source in Brazil) – under the supervision of prof Maria Luiza Rocco and prof Cassia Turci (UFRJ). In Sheffield, I have investigated ultrafast relaxation and electron transfer in porphyrin systems, metal oxides and Ruthenium complexes. At HarwellXPS, I have been studying complex inorganic systems – quantum dots, explosive compounds and thermochromics using temperature-controlled XPS (heating and cooling/cryo).

My current project in the UK Catalysis Hub aims to use the newly acquired Photo-Induced Force Microscopy (PiFM) machine at CU as a tool to characterise Janus particles. PiFM not only allows investigation of materials morphology but also localised chemical characterisation; hence it maps the chemical properties of the material and how they are distributed over the structure. In the figure, Silica spheres are mapped using PiFM: the bright yellow colour is the IR signal corresponding to Silica vibrations. The technique obtained not only the sphere-shaped topography of the silica but also acquired IR spectra at different points within the material – confirming it is silica.

A Janus-like particle should have at least two chemically distinct sides or polarities; in the research, I'm doing a hydrophobic and hydrophilic side. In collaboration with prof. Marc Titus (CU), these Janus materials would be ideal for Pickering emulsions, where catalysis happens on the interface of non-mixable liquids. Therefore the PiFM will be able to identify with precision the different chemical sides of the particles, as well as how these differences are arranged within the material.

As an early-career researcher, I have won two competitive grants within the University of Sheffield to pursue my original ideas as side projects, and so far, joining the team at HarwellXPS has been an incredible experience – with the supervision of Dr David Morgan (CU/HarwellXPS), we are now organising the next international XPS Workshop to happen in 2024, in Cardiff. It is exciting to be able to contribute to such a big-scale event and be in close contact with the biggest names in my research interest field.





Author:

Dr Arthur Graf, Cardiff University

Dr Arran Plant – Development of heterogeneous catalysts for the reduction of CO_2 using NADH cofactors

My education background is fairly multidisciplinary, graduating with a Dual Hons in Chemistry and Physics at Keele University. I swiftly followed on to complete an MSc in Chemical Engineering at The University of Birmingham. My desire for learning continued and I developed a keen interest in reaction engineering and catalysis which directed me to pursue a PhD. I started my doctoral studies in 2017 at Lancaster University supervised by Dr Vesna Najdanovic and Professor Malcolm Joyce with funding from the EPSRC. This research focussed on developing radiation-catalysed chemical reactions utilizing ionising radiation from a 250 kW TRIGA (Training, Research, Isotopes, General Atomics) nuclear reactor, working in collaboration with members of the Reactor Physics Department at the Jožef Stefan Institute (JSI), Slovenia. I submitted my doctoral dissertation in 2022 titled “Radiation-directed production of chemical reagents and petroleum additives from waste organic feedstocks” which proposed a novel nuclear cogeneration process to produce renewable chemicals. During my doctoral studies, I also gained experience with electrochemistry in developing a bespoke high-pressure electrochemical reactor to reduce CO_2. One of the highlights of my career so far has been the opportunity to work at the TRIGA reactor facility and to experience a fission reactor in operation – seeing the characteristic blue glow of the Cherenkov radiation in person is quite remarkable!

I have recently joined the UK Catalysis Hub in late 2022, starting work as a PDRA in heterogeneous catalysis at Lancaster University led by Dr Xiaodong Wang in collaboration with Shelley Minteer (Utah), Russell Howe (Aberdeen), Alan McCue (Aberdeen), and Xinbin Ma (Tianjin). This project aims to develop a heterogeneous catalytic system to reduce CO_2 into simple molecules such as formic acid using cofactor NADH (reduced nicotinamide adenine dinucleotide) as a hydride donor (as per Figure 1). The effectiveness of low-cost metals and support materials for this reduction process is a focus of this work, ideally to discover a process that could be industrially competitive. This project continues the previous Catalysis Hub and EPSRC projects that have developed heterogeneous materials for NAD^+ (oxidised nicotinamide adenine dinucleotide) regeneration. I am excited about the opportunities to develop my analytical skills, network, and delve into this exciting new research topic!

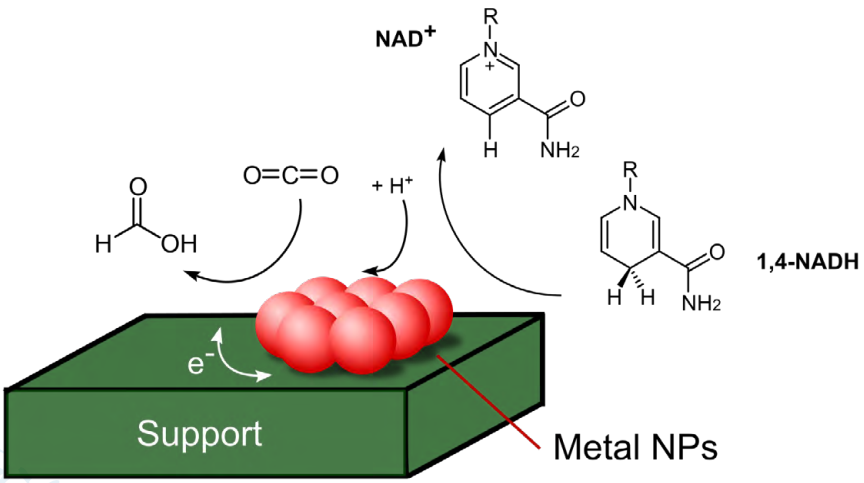


Figure 1: Reduction of CO_2 using supported-metal heterogeneous catalysis and the 1,4-NADH cofactor

Author:

Dr Arran Plant, Lancaster University

Dr Alexandros Symillidis - Engineering efficient and stable electrocatalysts for water splitting to green H_2 and O_2

My background is chemical engineering, with focus on electrochemistry, catalysis, hydrogen utilisation and fuel cells, catalytic hydrogenation and CO_2 recycling hydrogen production and electrolysis.

I did my undergraduate studies at the University of Patras, Greece, where I first came in contact with the core of a hydrogen-based energy system, the fuel cell, when I worked on my diploma thesis with the title "*Study of the triode operation of polymer electrolyte membrane fuel cells (PEMFC)*". My personal love for hydrogen and my awareness for the need for a clean energy system in order to achieve a better future for our planet urged me to work in this area. Continuing on the same path during my postgraduate studies in the same university, I completed my MSc research thesis titled "*Study of the metal – support interaction during the hydrogenation of CO_2 towards hydrocarbons using supported Ru and Co catalysts*", where hydrogen was utilised as means of recycling of carbonaceous emissions. Afterwards, during my PhD research in Loughborough University, UK, I had the chance to work again with fuel cells, but an alternative type, the DEFC, in my PhD thesis with the title "*Ethanol electro-oxidation at M/Pd/GC, Pd/PANI/GC and Pd/PANI fibrous electrodes in alkaline medium for direct ethanol fuel cells*", aiming for the development of Pd-based polymeric electrodes in a polyaniline(shell)/polyacrylonitrile-ionic liquid(core) configuration.

Currently (since October 2022), I am a research associate at the Department of Chemical Engineering of Loughborough University working on a UKCH-funded project for the development of transmission metal carbides (TMC)-supported Pt-electrodeposited electrocatalysts for hydrogen evolution (HER) in alkaline conditions. TMCs are earth-abundant, low-cost catalysts, stable in acidic and alkaline conditions and with electron configuration and catalytic properties similar to that of noble metals. Molybdenum and tungsten carbides have been found to demonstrate promising behaviour for H_2 production in both acidic and alkaline conditions. The primary focus-materials of this study are WC, β-Mo_2C and α-MoC_{1-x}. Especially the latter is known for its strong interactions with Pt, enhancing its catalytic properties and inducing its atomic dispersion. These electrocatalysts are being tested for HER in a half-cell configuration, but there are plans for scaling-up to a full-cell-test procedure. The purpose of this project is to contribute to the development of efficient, low-cost M/TMC electrocatalysts for alkaline HER with low noble metal content and, consequently, low cost.

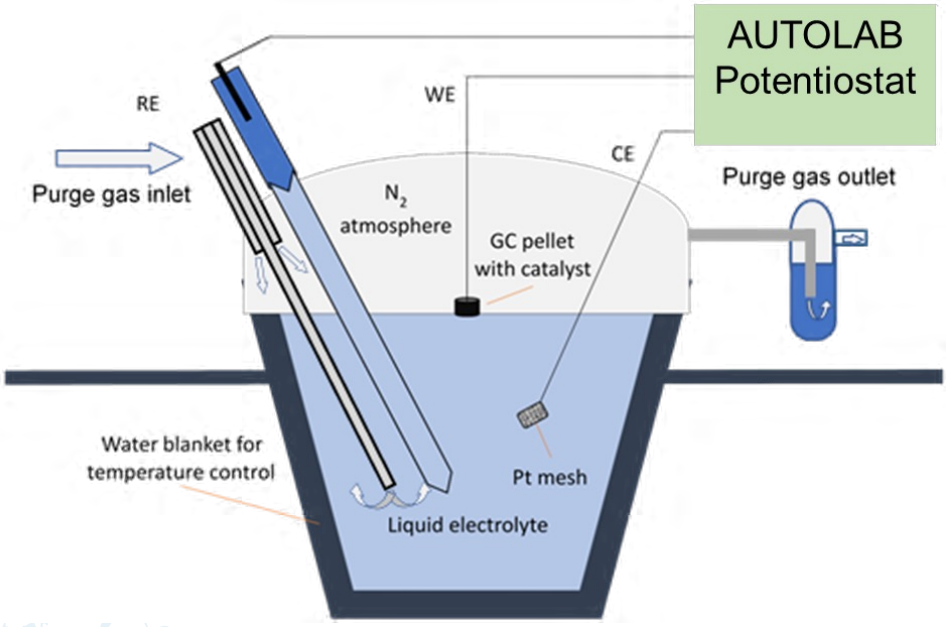


Figure 1: Schematic representation of a half-cell, where HER experiments are conducted. Electrocatalysts are deposited on the glassy carbon (GC) working electrode (WE).

Author:

Dr. Alexandros Symillidis, Loughborough University

UK Catalysis Hub Phase II - Departing team members

Join us in saying Goodbye to these members of staff who are leaving the UK Catalysis Hub. We would like to thank them for their work with us and here they give an overview of their work and memories.

Dr. June Callison - Lab Manager

I am writing this almost nine years to the day that I joined the UK Catalysis Hub as a Research Technician.

It was the beginning of the first phase of the Hub and I had heard of the job through previous colleagues, Emma Gibson and Ian Silverwood - both of whom I met whilst during my PhD at Professor David Lennon's lab in Glasgow and had both since moved onto PDRA positions at Harwell. My job at the time was to maintain the instruments in the Hub labs, along with helping on research projects.

I first worked alongside one of the Hub PDRAs, Khaled Mohammed, on the design of SnAlPO catalysts.[1] A project based on hydrogen production from the glycerol reforming reaction followed, under the supervision of Nikos Dimitratos and Peter Wells[2,3] showing that the synthesis temperature of Pt/Al_2O_3 catalysts influenced the metal particle size and therefore the catalytic activity. This project was continued by one of the Hubs first PhD students turned PDRA, Scott Rogers. I enjoyed working on these projects immensely and a particular highlight was a trip to Florence for the Europacat Conference to present the work on the Glycerol reforming project.

After the first five years under UCL, the Hub was awarded a new grant for phase two, now through Cardiff University where my job role changed to Lab Manager. Having watched the Harwell group grow at least four times the size, not even including the visiting researchers, this role was very much required!

Although for me it meant stepping back from 'hands on' science, I found the role challenging and very rewarding. I was able to implement new procedures into the labs that I hope, to this day improve the experience for all users and visitors working at the Hub. During this period, we have grown the scientific resources, installing new equipment such as a ChemBET, Ultrawave Digestor and a new FTIR/DRIFTS setup with high pressure capability.

One of the most rewarding things about being in this role is watching so many of the students and researchers that I have met through the years progress onto bigger and better things, from fellowships to beamline scientists.

Throughout my time at Harwell I've also become heavily involved in the Hub EXAFS BAG on B18 at Diamond. Working on this introduced me to a huge number of students and researchers in the UK Catalysis field, working on a variety of projects. For me, this has been one of the successes of the Hub and has led to numerous collaborations and publications, including an article in Nature Catalysis that I co-authored.[4]

Another strength that the Hub has had over the years is the development of relationships with the facilities at Harwell, mainly the Central Laser Facility (CLF), Diamond and ISIS, along with a close relationship with the core team at the Research Complex at Harwell. It is these relationships that has helped me to further my career as I move into the position of Deuteration Facility Operations Manager at ISIS. Even though I am moving on, I hope to be able to collaborate with the Hub going forward and continue to be a part of the team, after all I'll just be across the road!

I would also like to take this opportunity to thank every person that I have worked with whilst being at Harwell, which is a lot! Special thanks to Professor Sir Richard Catlow for giving me the opportunity to work in the Hub, Cath for dragging me to my first football session, the two Emma's for the support, Ines, the postdoc of the month, Monik for being the best lab Sheriff in town and to Josie for being a

great boss. There are many more that I am grateful to for the collaborations and friendship over the years, but I only have limited space here! I hope to stay in touch with everyone and wish all the Hub members a bright and successful future.

1. Mohammed, K. M. H. et al. Design and control of Lewis acid sites in Sn-substituted microporous architectures. *J Mater Chem A Mater* **4**, 5706–5712 (2016).

2. Subramanian, N. D., Callison, J., Catlow, C. R. A., Wells, P. P. & Dimitratos, N. Optimised hydrogen production by aqueous phase reforming of glycerol on Pt/Al2O3. *Int J Hydrogen Energy* **41**, 18441–18450 (2016).

3. Callison, J. et al. Directed aqueous-phase reforming of glycerol through tailored platinum nanoparticles. *Appl Catal B* **238**, 618–628 (2018).

4. Messinis, A. M. et al. The highly surprising behaviour of diphosphine ligands in iron-catalysed Negishi cross-coupling. *Nat Catal* **2**, 123–133 (2019).

Author:

Dr. June Callison, UK Catalysis Hub

UK Catalysis Hub Phase II - Visiting Researchers

Join us in welcoming these visiting researchers to the UK Catalysis Hub. We introduce them with a short profile of their background and what they have been working on with the UK Catalysis Hub.

Junhao Huang, PhD Student, Leibniz Institute for Catalysis, Germany – PhD visit opportunity LIKAT and UK Catalysis Hub

I am currently a PhD candidate from Leibniz institute for catalysis (LIKAT) in Germany under the supervision of Prof. Jennifer Strunk. My research interest is in the field of heterogeneous catalysis with a focus on the study of structure and reactivity relationship for Pd single-atom catalysts, using both experimental and theoretical methods. I have done the design, synthesis and characterization of materials and performed some calculations in LIKAT, but now I wanted to progress the understanding.

Funded by both the UK Catalysis Hub and LIKAT, I got this great opportunity to visit Dr. Andrew Logsdail's group at the Cardiff Catalysis Institute, Cardiff University to extend my knowledge of computational chemistry. I investigated these Pd catalysts using density functional theory (DFT) calculations, and I was able to discuss the results with the broader computational community. The new computational results in combination with the former experiments provide me with a completed picture of the electronic and coordination structure of this kind of single-atom catalyst, as a basis to understand the catalytic process.

During my visit, the first impression of the UK Catalysis Hub is its strong collaboration network. The Hub has close relationships with the universities, world leading facilities and industries, which aims to facilitate "multi–institutional, multi-disciplinary collaboration". My attention was most caught by the collaboration with Diamond Light Source. From an experimental point of view, the exploration of catalyst structure and understanding of the reaction mechanism are heavily dependent on advanced instruments as well as expert user knowledge.

Synchrotron science is one of the most powerful tools, which is available to scientific researchers, as it provides unparalleled resolution and insight. In the UK Catalysis Hub monthly group seminar, I was able to meet many experts on synchrotron radiation and communicated with them about my research, which inspired me a lot. In addition, the diversity of research directions supported by UK Catalysis Hub also deeply impressed me.

Taking the theoretical computing teams at Cardiff University as an example, their research involves homogeneous catalysis, heterogeneous catalysis, and biocatalysis, as well as the computational software development. The diversity of research approaches and interests give the possibility of idea exchange and creates new perspectives for recognizing and solving problems.

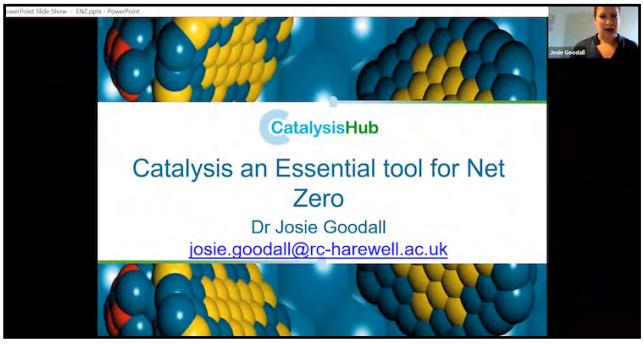
As I always believed, communication and collaboration could promote and produce better results, and talking and sharing would make things easier. I would like to thank the UK Catalysis Hub for the support throughout the visit, which has elevated our scientific understanding and provided a platform for delivering enhanced catalytic chemistry.

Author:

Junhao Huang, Leibniz Institute for Catalysis

Catalysis for net zero

Catalysis: the essential tool for achieving resilience in a net zero carbon society. Achieving a net zero carbon society is impossible without catalysis; catalysts are central to efficient chemical processes and manufacturing, controlling both the rates and energy demand of chemical reactions. For society, catalysis is essential to deliver the materials, energy vectors, fertilizers, medicines, electronics and products we need. It is also essential to implement and deliver the net zero agenda, from 'green' hydrogen, to large-scale energy storage, from a re-imagined fully sustainable chemical industry to green steel – advances in catalysis will deliver these future manufacturing industries. Find out more about the ways the UK Catalysis Hub is working to achieve a net zero carbon society below



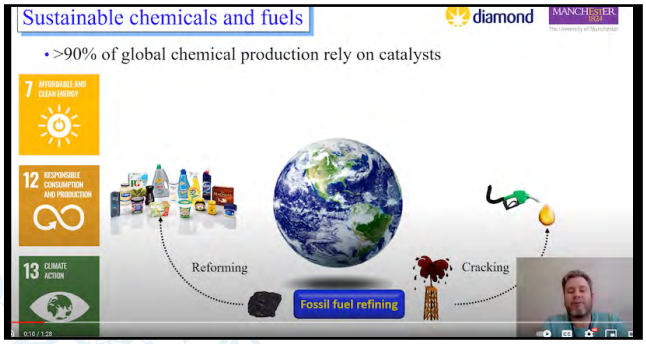
Catalysis an essential tool for net zero presentation by Dr Josie Goodall

Dr. Josie Goodall gave a video presentation in the virtual showcase at the Engineering and Physical Sciences Research Council (EPSRC) Engineering Net Zero week event in June 2022 with an overview of how catalysis is essential to achieve net zero goals.

Recording available to watch at https://ukcatalysishub.co.uk/catalysis-an-essential-tool-for-net-zero-presentation-by-dr-josie-goodall/

Other projects that were featured in the EPSRC presentation included:

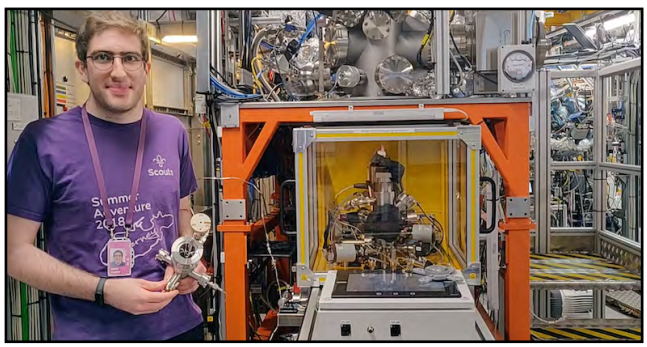
Sustainable fuels and chemicals from biomass by Christopher M. A. Parlett



Lignocellulosic biomass represents a sustainable feedstock for the production of carbon-based chemicals and fuels, which can function as drop-in replacements for conventional fossil fuel derived equivalents. Furthermore, using non-edible plant matter, such as agricultural and forestry residues or the cultivation of energy crops (on waste ground), circumvents the food v fuel debate and can add value to perceived waste. Developing this renewable feedstock is critical to meeting both the demands of a growing global population and UK targets for achieving net-zero. However, stark differences in the chemical composition of lignocellulose to conventional feedstocks dictate different processing conditions and catalytic material properties, such as lower temperatures, aqueous phase reaction media, and capacity to decrease oxygen content of the feedstock. To further complicate the situation, the complex nature of lignocellulose hampers its direct valorisation, with processing entailing an array of distinct different chemical reactions. The development of one-pot processes for biomass valorisation, therefore, requires multifunctional materials with the ability to facilitate more than one class of chemical transformations. At the Catalysis Hub, we are currently developing novel multifunctional catalysts, with nanoscale control, for multistep catalytic cascade conversion of sugars (cellulose and hemicellulose derived) into an array of products, including fuels, solvents, and biopolymer monomers..

Recording available to watch at https://ukcatalysishub.co.uk/sustainable-fuels-and-chemicals-from-biomass-by-dr-christopher-m-a-parlett/

Video on Net Zero research work by PhD student James Counter at the B07 beamline, Diamond Light Source



Heterogeneous catalysis research has as one of its main objectives the derivation of structure-activity links. These relationships relate catalytic performance, such as reactant conversion, product selectivity, and reaction mechanism, with physical sample composition, such as active metal distribution, pore network properties, and support shape and structure. By encouraging

knowledge-based design and operation of catalytic processes rather than trial-and-error experimental or synthetic approaches, understanding structure-activity links is a difficult but essential step in building more effective and stable catalysts.

The B07 team has been working on new sample environments for the catalysis community. In particularly, James project focuses on the design and development of electrochemical cells for in-situ NAP-XPS/NEXAFS investigations of water splitting reactions for green hydrogen production. The more accurate and realistic the characterization in spatial and time domains and in terms of reaction conditions with careful approach, the more information can be harvested regarding structure-activity relationships. Therefore, the new samples environment at B07 beamline provides opportunities for collaboration with national and international research communities to develop new materials and robust technology to address clean energy and environmental issues, contributing to the COP26 major goal of Net Zero target by 2050.

Recording available to watch at https://ukcatalysishub.co.uk/video-on-net-zero-research-work-by-phd-student-james-counter-at-the-b07-beamline-diamond-light-source/

Stable and economic catalysts for green hydrogen

Dr Yagya Regmi from Manchester Metropolitan University explains how his group is exploring platinum coated titanium dioxide as supports for iridium catalysts to help reduce the amount of iridium in water electrolysers and lower cost of hydrogen from electrolysis.

Reducing the amount of iridium in water electrolysers without compromising performance is essential to lower cost of hydrogen from electrolysis. One of the pathways used in catalysis is to utilise high surface area supports. In this project, we are exploring platinum coated titanium dioxide as supports for iridium catalysts. Platinum is necessary to improve conductivity of the support motifs. Our strategy is to rapidly test plethora of supported catalysts in a half-cell configuration using rotating disk electrodes. Only those catalysts that show promising activity and durability in half-cell are then integrated into the electrolyser. This approach is economic and efficient since integrating catalysts into membrane electrode assemblies and running electrolyser tests are resource and time intensive. However, there are challenges associated with replicating activity and durability from half-cell to device performance. Thus, we also explore methodologies and strategies to optimise our half-cell investigations to mimic full device conditions more closely. During this UK Catalysis Hub funded project, we have demonstrated that our strategy to engineer iridium catalysts has led to greater than 50% reduction in iridium content necessary in water electrolysers. And yet, our devices show performance and durability comparable to state-of-the-art technology.

Recording available to watch at https://ukcatalysishub.co.uk/exploring-platinum-coated-titanium-dioxide-as-supports-for-iridium-catalysts/

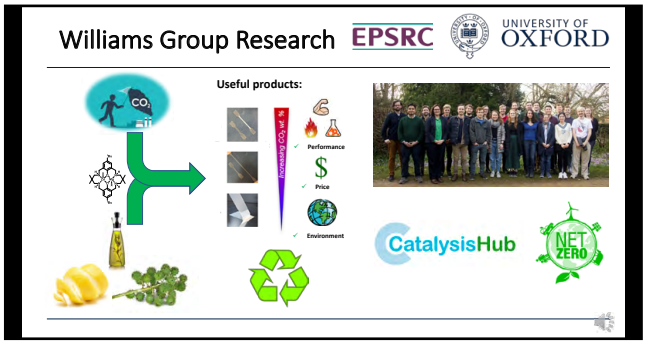
Dr Xue Han from the University of Manchester on her project and net zero research exploiting low grade thermal energy

Dr. Xue Han from School of Chemistry, University of Manchester talks about her project and the net zero research they are undertaking.

Currently, space heating using gas boilers and cooling using electric air-conditioner account for more than 20% of UK's carbon emission. The aim of my research is, instead of burning fossil fuels or totally relying on electricity, to exploit low grade thermal energy to realise heating and cooling. These energies are readily available as solar and geothermal energies or can be obtained from the waste heat of various industries, so they are sustainable and free. The technology is based on the phenomenon of adsorption-driven heat-transfer, which uses water as working fluid, and a porous sorbent material to cycle the adsorption and desorption of water. I am currently working on developing advanced porous materials such as metal-organic frameworks (MOFs) for this application. With the success in obtaining MOFs that are of high stability, high water uptake and can be regenerated at low temperatures, this research will make great contribution to decarbonization of heating and cooling.

Recording available to watch at https://ukcatalysishub.co.uk/dr-xue-han-from-the-university-of-manchester-on-her-project-and-net-zero-research-exploiting-low-grade-thermal-energy/

Selective Polymerisation



The research investigated using the Hub funding remains at an early stage as would be expected with EPSRC funded fundamental research. Nonetheless, the target area – making useful products from carbon dioxide, is one in which there is potential for both environmental and commercial impact. It is relevant to note that there is a UK based company, Econic technologies, formed on the basis of earlier catalytic science from C. K. Williams which has commercialized catalysts for carbon dioxide/epoxide copolymerization (https://econic-technologies.com/) The product polycarbonate polyols are attracting increasing industrial attention as components in polyurethanes, a large commodity sector of the polymer market. Thus, the discoveries of the EPSRC Catalysis Hub funding are relevant to an emerging sector in both the polymer and polymerization catalysis sectors.

There is also a demonstrated environmental benefit to using carbon dioxide to make polymers – in effect there is a 'triple win', as for every tonne of carbon dioxide used to make polymers, there is a three-tonne saving in CO_2 emissions. This arises because the carbon dioxide replaces epoxide in the conventional process and thus by avoiding petrochemical use there are emissions savings also.

The early-stage research in catalysis funded by the UK Catalysis Hub has allowed a broader range of polymers to be prepared from CO_2. This is important because in the future, equivalent cost and environmental benefits could be envisaged in sectors beyond polyurethanes. For instance, some of the polymers prepared using switchable catalysis show good elastomeric behaviour so may be suitable as replacements for commodity materials like SBS (styrene-butadiene-styrene). The catalysis has also been used to produce fully bio-based and degradable pressure sensitive adhesives, ductile plastics, and improve the material properties of the most widely used bioplastic, PLA. Lastly, funding from the UK Catalysis Hub led directly to the discovery of a chemical recycling method of polycarbonates; this is an important result in the context of future waste management and carbon-capture processes.

Another impact area that has been developed thanks to the Catalysis Hub funding is the outreach and demonstration of the concept to the general public. Between October 2021 and March 2022, an exhibit of the group's research was on display at the London design museum which was visited by over 20,000 people. People were inspired to find that everyday materials can be formed in a sustainable way from waste products (e.g. citrus peel). Excitingly, the exhibit will be on display in Hong Kong and Paris in the near future. The group is also heavily involved in the University of Oxford's outreach program. Researchers regularly run workshops with school children (10-18 years) and display our work at science stalls in local museums. For example, at the Oxford University Natural History Museum as part of their Super Science Saturday Online fair in 2020. The interactive and virtual exhibit used a polymer lifecycle to stimulate engagement, discussion and exploration through a series of tasks to our approach to improve sustainability across the life cycle. Charlotte Williams presented at COP26 highlighting the opportunity for innovation to create methods to add value to carbon dioxide wastes and to transform them into useful products, like polymers. Charlotte also regularly contributes to general interest science pieces regarding plastic waste (e.g. Nature News feature on carbon upcycling, New Scientist articles 'from pollution to solution', Chemistry World, the Periodic) and has previously presented our work to a general audience on.

Recording available to watch at https://ukcatalysishub.co.uk/selective-polymerisation-2022/

STFC UKRI Social Media Campaign on engineering Net Zero

UK Catalysis Hub projects were chosen to feature in the STFC UKRI social media campaign on engineering net zero which took place over two week in early July 2022. Details of the projects are below.

Methanol to hydrocarbons (MTH) for Net Zero

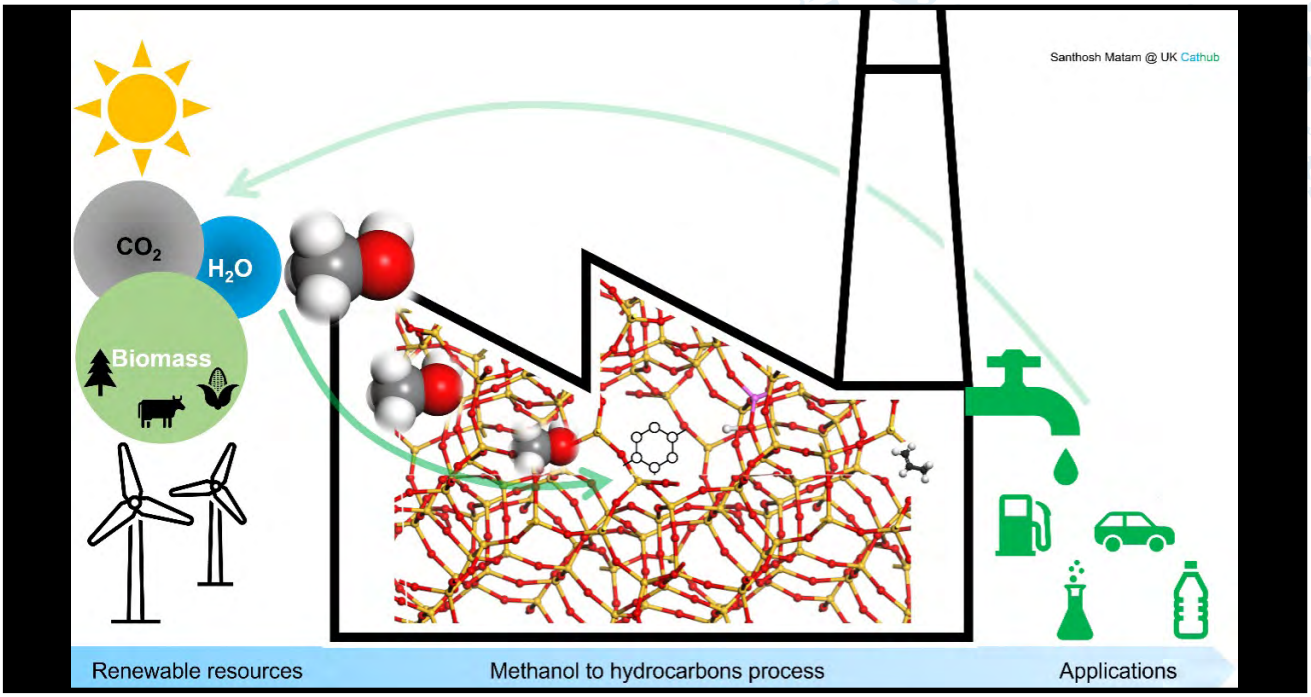


Figure 1. Schematic representation of renewable resources based MTH process

Methanol to hydrocarbons (MTH) is an important petrochemical process due to its ability to replace conventional fossil fuels (e.g., coal and crude oil) based gasoline, olefins and aromatics production with carbon neutral renewable methanol feedstock, which can be derived from CO_2 reduction with H_2O. The MTH process can reduce the net carbon emissions from vehicles and polymer (e.g., polypropylene) industries with the existing infrastructure, and hence it can potentially play a key role in the UK's ambitious target of achieving net zero carbon emissions by 2050 (Fig. 1).

Given the commercial and environmental significance of the process, a great deal of research has been dedicated by the scientific community and industry to better understand the fundamental reaction and deactivation mechanisms and to design and develop zeolite (catalyst that drives the MTH reaction) porous architecture. The Research Complex at Harwell is ideally located within the proximity of neutron and X-ray sources and is well equipped with lasers and other key facilities including computational expertise. This enables us to investigate comprehensively the MTH reaction on zeolites ZSM-5 and SAPO-34 with a wide range of time (ps-minutes), space (nm-μm) and depth (surface-bulk) resolutions. The complementary techniques reveal that:

i) Methanol forms methoxy species (a key intermediate) at the active acidic site of the zeolite

ii) Methoxy species breakaway under certain conditions as propylene and ethylene molecules (olefins), which are the first C-C bond containing molecules formed from C1 methanol molecules

iii) Part of olefins polymerise and cyclise to yield aromatics like alkylated benzenes

iv) Aromatics are the precursors for the zeolite deactivation

v) Computational tools aid to interpret the complex spectroscopic data and to validate results.

Direct Hydrogenation of Captured Carbon Dioxide using a Heterogeneous Catalyst

To achieve net zero, captured carbon dioxide must be efficiently utilised and recycled. A research team led by Dr Simon Kondrat (Loughborough University) and the UK Catalysis Hub are developing robust heterogeneous catalysts to directly produce methanol from amine captured carbon dioxide, which in the process regenerates the original amine. Using a theory led approach, facilitated by the expertise at the Research Complex at Harwell and Diamond Light Source, key properties of the catalyst are identified to assist in its design and characterisation. Successful catalysts could facilitate decentralised utilisation of CO_2 and maximise energy savings though limiting CO_2 storage and transportation.

Using a modelling led approach we are designing novel single-site heterogeneous catalysts for the single step hydrogenation of amine captured CO_2 to produce methanol and regenerate the amine. The project, as part of the UK Catalysis Hub, has identified key properties and transition states of current homogeneous catalysts and uses this knowledge to develop new heterogeneous catalysts.

The drive for net zero CO_2 requires new technologies that, (a) produce no CO_2 emissions and/or (b) effectively utilise CO_2 produced in processes. Ideally, we can recycle emitted CO_2 for use in chemical processes. Synthesis of methanol from the hydrogenation of captured CO_2 with H_2 produced from excess renewable energy is such a CO_2 utilisation stratergy. Yet, separation (a high-energy thermal step in commercial amine capture technologies), concentration and transportation of captured CO_2 limit application. An exciting prospect is direct catalytic methanol production from captured CO_2 that simultaneously regenerates the amine capture technology.

Homogeneous Ru pincer complex catalysts facilitate this reaction, but selectivity issues, deactivation and processing challenges call for the development of a robust heterogeneous equivalent. To date, no heterogeneous catalyst can turnover amine captured CO_2 to methanol. In addition, selectivity to methanol is highly dependent on the amine used.

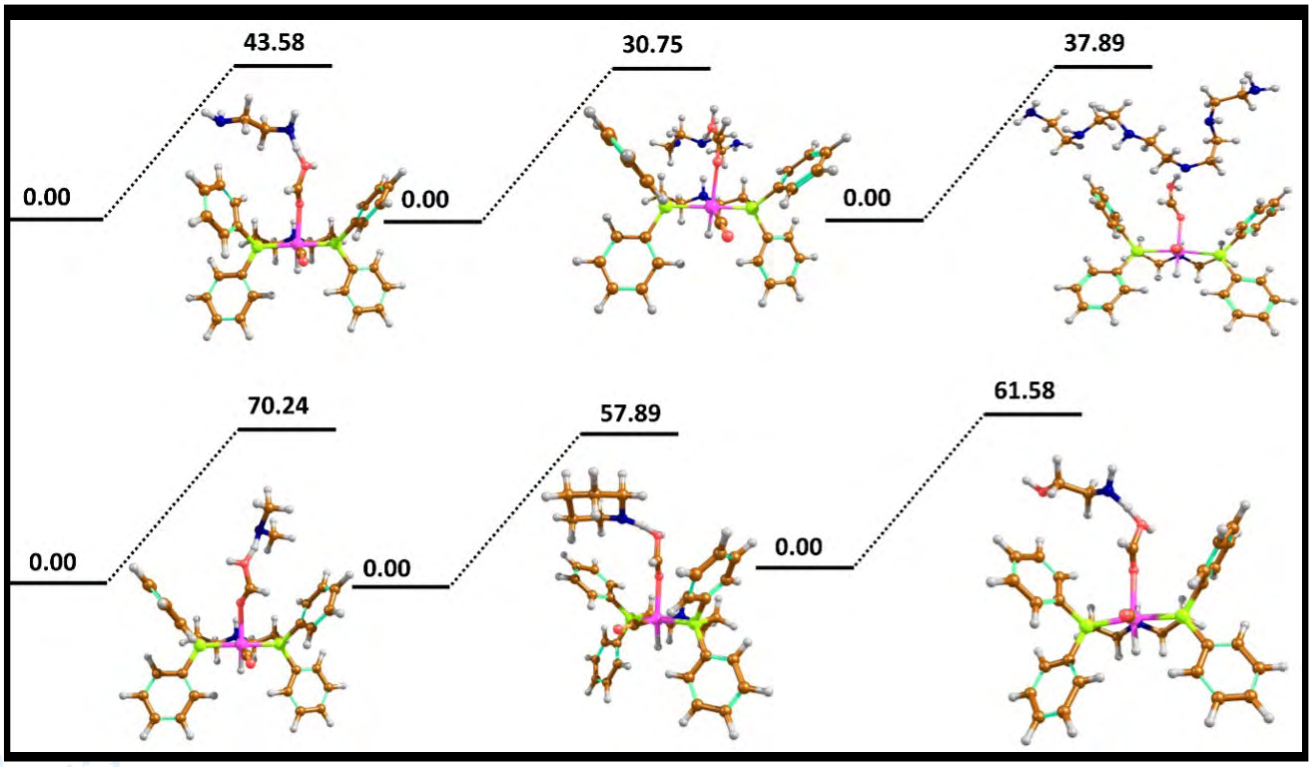
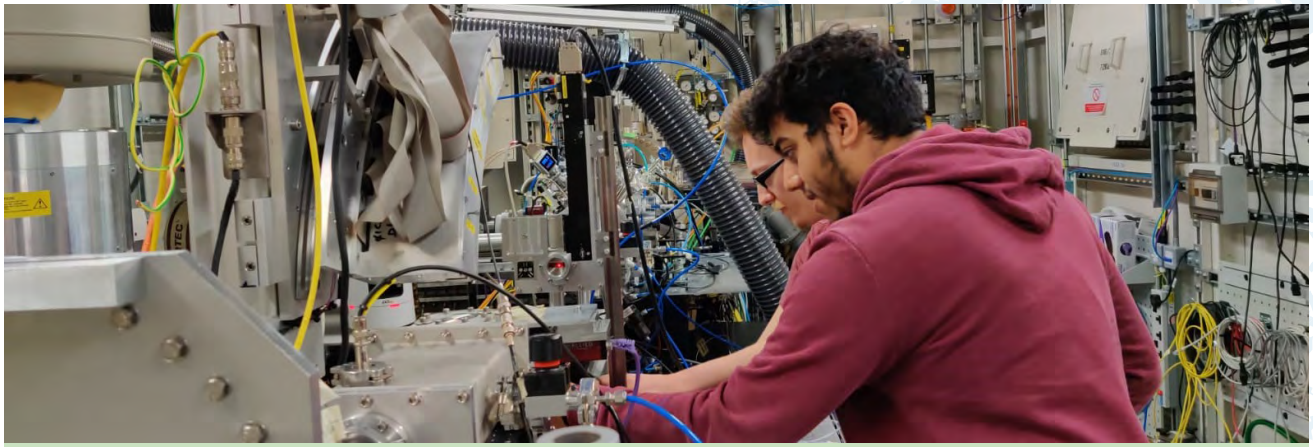


Figure 1. Reaction barriers for hydrogen transfer to Ru-Pincer bound formic acid, for the formation of formamide and H_2O. (top) reaction barriers for amines that promote methanol formation, (bottom) reaction barriers for the amines that promote either formamide or formate formation. All free energies were calculated at UB3LYP/TZVP level of theory and given in kcal/mol.



(PDF) Block Allocation Group (BAG) access at Diamond

The UK Catalysis Hub has two block allocation groups (BAG) of beamtime at the Diamond Light Source. The well-established X-ray absorption spectroscopy (XAS) BAG at B18 has two allocations of three days scheduled for each run cycle. The beamtime allocations for AP31 have been completed in April, September, and December 2022. Both *in situ* and *ex situ* experiments have been completed and it has been possible to invite users from several different groups to visit Diamond and participate in the experiments. Recent highlights of this beamtime included collection of *operando* data using a specially designed electrochemical cell operated in transmission geometry. Future beamtimes have been scheduled for March 2023 and we are again able to welcome users to participate in this experiment.

The UK Catalysis Hub has been awarded a block allocation group for X-ray Pair Distribution Function analysis (XPDF) at I15 and both *in situ* and *ex situ* measurements performed in cycle AP31. There are currently upgrades being undertaken at I15-1 and the next XPDF beamtime is tentatively scheduled for April 2023. This allocation with comprise both *ex situ* (powder) measurements and *in situ* experiments using several different sample environments, including the electrochemical cell used at B18. The XPDF technique is amenable to rapid data collection and therefore there is often a large amount of data produced which can be daunting and can mean that the technique is not fully utilised. Since one of the goals of the **XPDF BAG** is to introduce the technique to new users from within the catalysis community we have scheduled a **one-day workshop** ahead of the I15-1 allocation. This is scheduled for the **28th March 2023**. The workshop will introduce the PDF technique and will also provide a hands-on introduction to data analysis. We will provide three example data sets which will be of immediate interest to the catalysis community, and which were collected at I15-1 during 2022. These will include small- and large box modelling of core-shell nanoparticles, a study of Ru nanoparticles produced by in situ-reduction of RuCl3 that illustrates the complementary nature of XAS and XPDF studies and finally a large-box analysis of *in situ* data collected for single atom Pd supported on a metal-organic framework (MOF). Not only does this workshop aim to introduce XPDF to the catalysis community but it will also provide the opportunity for participants to discuss potential and develop experiments ahead of the scheduled beamtime and take part in the experiment. Register for the workshop at https://us7.list-manage.com/survey?u=d87bdd5885222dbe7040c85ff&id=5919c96184&e=|UNIQID|

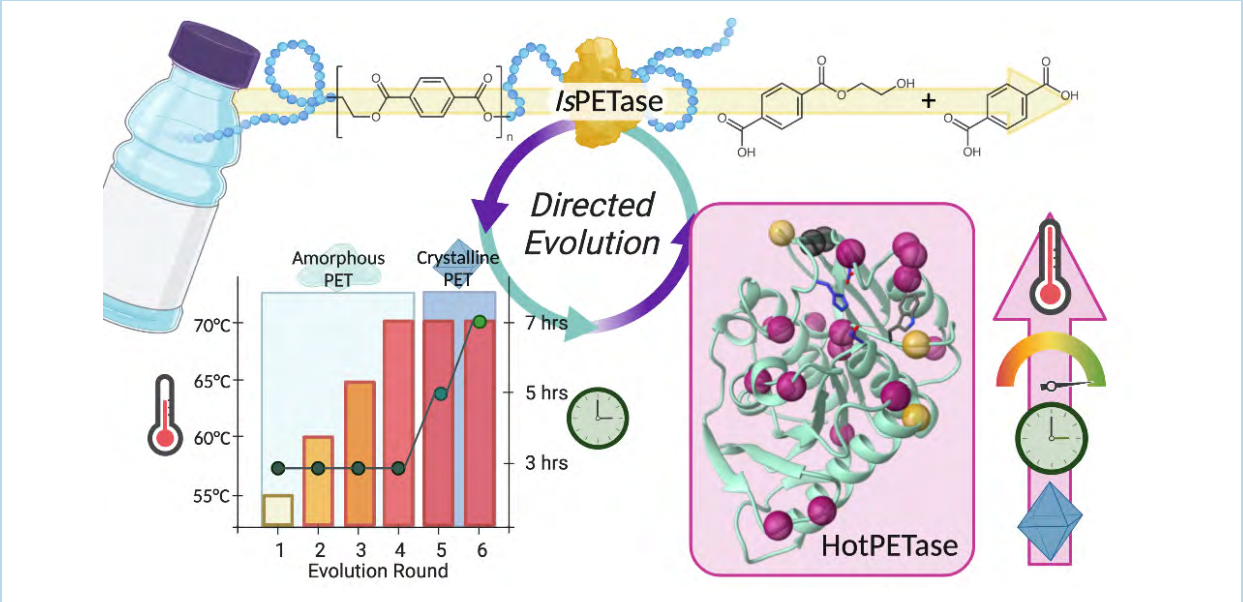
For more information on BAG access visit https://ukcatalysishub.co.uk/bag-at-diamond-light-source/. If you would like to discuss the PDF experiments or combined experiments please contact Dr Martin Wilding (WildingM2@cardiff.ac.uk).

To introduce the technique to the Catalysis Hub, Dr Phil Chater from I15-1 presented a webinar on the 7th February. The seminar introduced the PDF technique and described how it has been applied to local structure studies on catalysts. The webinar also explained how the plan PDF experiments and discussed the training and outreach components of the BAG and the development of streamlined processing and analysis for selected, commonly encountered systems. Recording available to watch at https://ukcatalysishub.co.uk/pair-distribution-function-pdf-block-allocation-group-bag-access-at-diamond/

Publications:

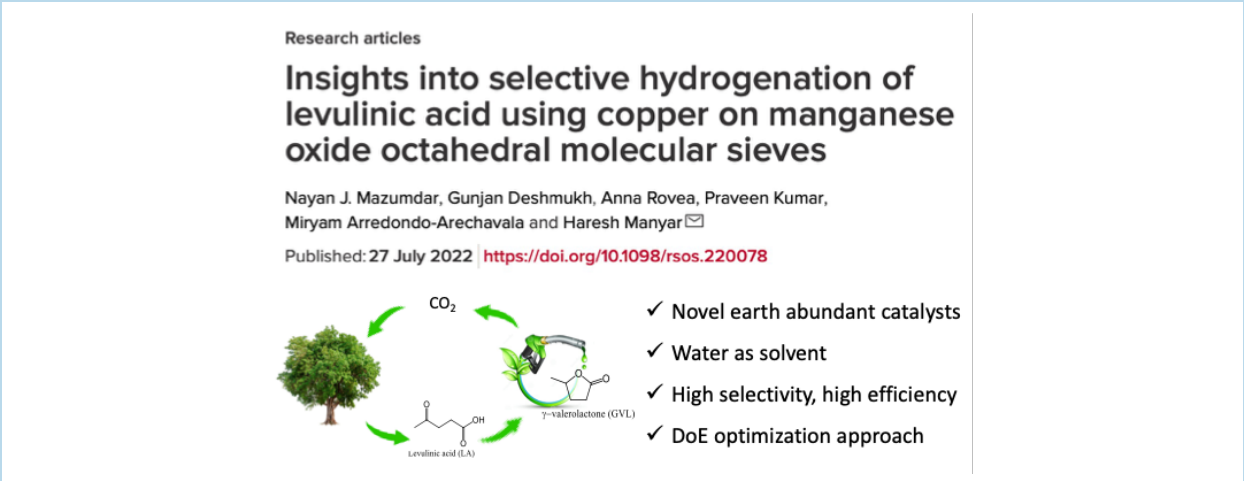
Directed evolution of an efficient and thermostable PET depolymerase

An article by researchers at the University of Manchester in collaboration with the UK Catalysis Hub has been published in Nature Catalysis describing the evolution of an efficient PET depolymerase that can deconstruct semi-crystalline PET plastic into its component monomers at elevated temperatures. The engineering of this enzyme was enabled by the development of a high-throughput, automated PET depolymerisation screening and analysis workflow, allowing thousands of enzyme variants to be assessed in a few days. The resulting engineered enzyme, HotPETase, can operate above the glass transition temperature of PET (60-70°C), is able to deconstruct crystalline PET more rapidly than other reported PETases, and can selectively depolymerise the PET portion of a real-world packaging composite film lid that is challenging to recycle using other methods. Read the article online at: https://doi.org/10.1038/s41929-022-00821-3.



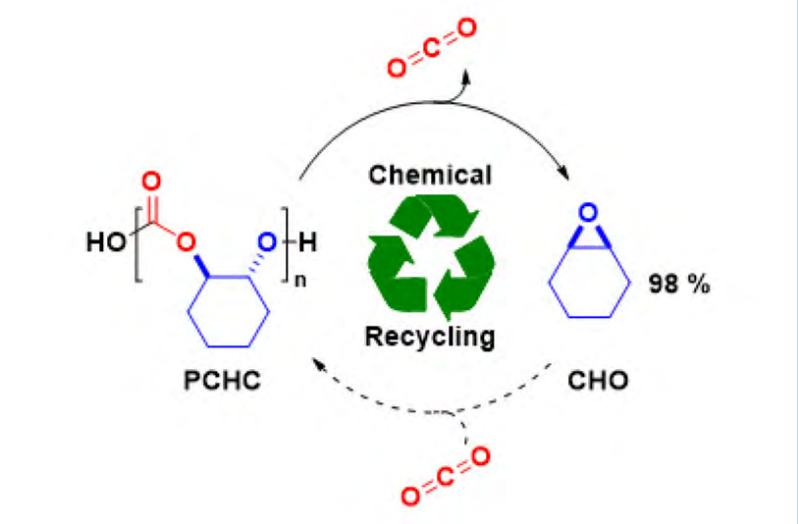
Insights into selective hydrogenation of levulinic acid using copper on manganese oxide octahedral molecular sieves

The researchers at Queen's University Belfast (QUB) UK in collaboration with the UK Catalysis Hub, have developed a new catalytic process for liquid phase hydrogenation of biomass derived levulinic acid to g-valerolactone (GVL) using Copper on manganese oxide catalysts in water as solvent. GVL is one of the key platform chemicals, for application as fuel additive and a precursor to produce sustainable jet fuels and renewable fuel range hydrocarbons. The GVL technology developed by QUB researchers is an important milestone on the road to net zero emissions. To read the full article visit https://doi.org/10.1098/rsos.220078.



Publications cont:

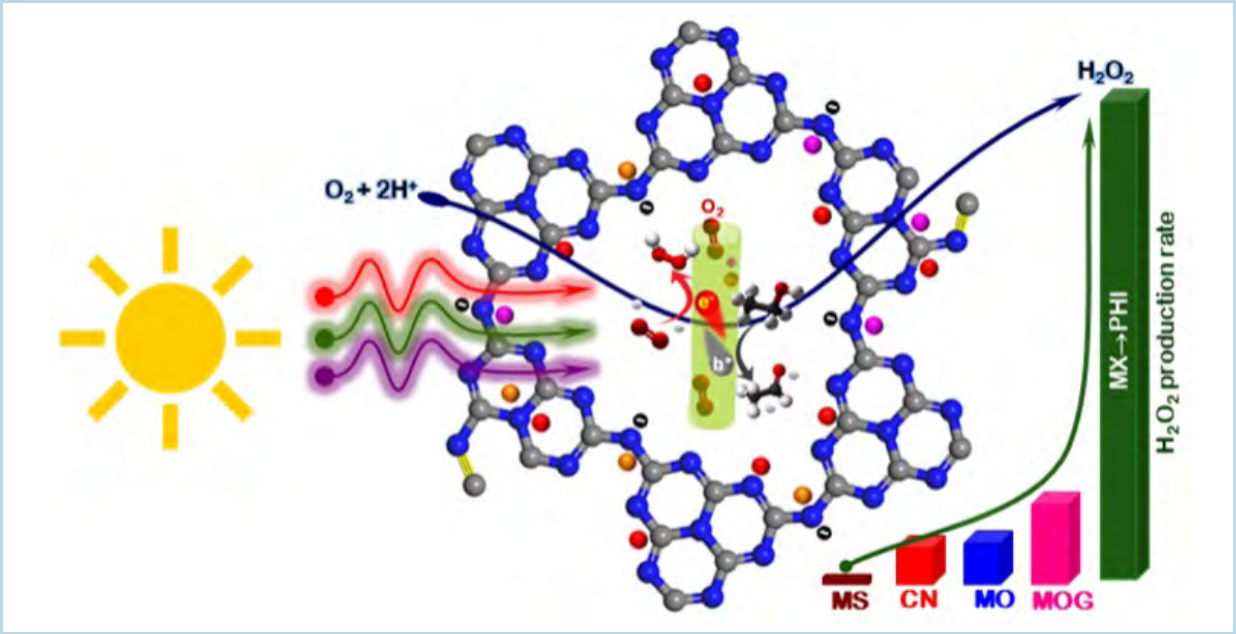
Chemical Recycling of Poly(Cyclohexene Carbonate) Using a Di-MgII Catalyst



Chemical recycling of polymers to true monomers is pivotal for a circular plastics economy. In this work, the team across Bath and Oxford in collaboration with the UK Catalysis Hub reported the first catalysed chemical recycling of the widely investigated carbon dioxide derived polymer, poly(cyclohexene carbonate), to cyclohexene oxide and CO2. The reaction requires dinuclear catalysis, with a di-MgII catalyst showing both high monomer selectivity (>98 %) and activity (TOF=150 h−1, 0.33 mol %, 120 °C). A joint experimental and computational (DFT) investigation revealed that the depolymerisation occurs via a chain-end catalysed depolymerization mechanism, and that the high selectivity arises from the Mg-alkoxide catalysed epoxide extrusion being kinetically favourable compared to cyclic carbonate formation. To read the full article visit https://doi.org/10.1002/anie.202201785

Enhanced H2O2 Production via Photocatalytic O2 Reduction over Structurally-Modified Poly(heptazine imide)

Dr Pankaj Sharma has a new paper in collaboration with the Cardiff Catalysis Institute and UCL Chemistry - Enhanced H2O2 Production via Photocatalytic O2 Reduction over Structurally-Modified Poly(heptazine imide). The paper describes the synthesis and potential use of an alkali metal-halide modulated C-N based poly(heptazine imide) (MX→PHI) molecular photocatalyst to produce green energy carrier (H2O2). Higher solar H2O2 production rate for MX→PHI has been reported. The work was done at Research Complex at Harwell and Diamond Light Source. Read more at https://pubs.acs.org/doi/10.1021/acs.chemmater.2c00528.



Future Publications

Acknowledgements

When publishing work from UK Catalysis Hub: please include the following acknowledgments:

From December 2018 – Phase II – Please acknowledge the UK Catalysis Hub using your project grant number

"UK Catalysis Hub is kindly thanked for resources and support provided via our membership of the UK Catalysis Hub Consortium and funded by EPSRC grant: EP/R026939/1, EP/R026815/1, EP/R026645/1, EP/R027129/1 or EP/M013219/1(biocatalysis))"

Between 2013 – 2018 – Phase I

"UK Catalysis Hub is kindly thanked for resources and support provided via our membership of the UK Catalysis Hub Consortium and funded by EPSRC grant: EP/K014706/2, EP/K014668/1, EP/K014854/1, EP/K014714/1 or EP/M013219/1"

When publishing work performed at the Research Complex please also include the following text (replacing X an Y with the relevant information):

"This research has been performed with the use of facilities at the Research Complex at Harwell including 'X' and 'Y' equipment. The authors would like to thank the Research Complex for access and support to these facilities and equipment."

Please also inform the Project Manager - Dr. Josie Goodall of all publications arising from Hub Projects.

Let us know about your publications:

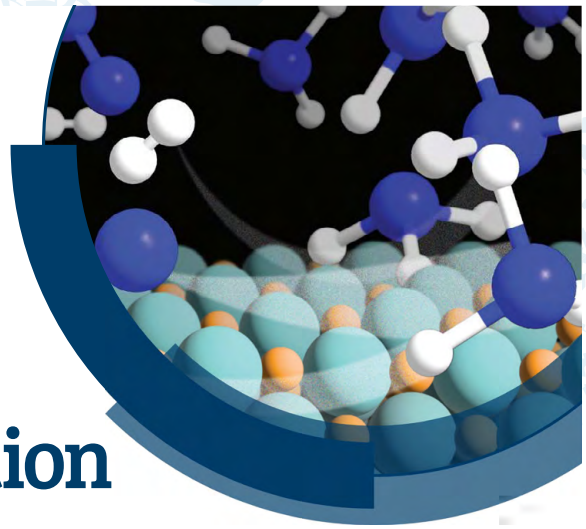
The UK catalysis Hub wants to hear your news. Please contact the Office Manager to contribute to the research highlights and publications in our newsletter.
Office Manager:
Corinne Anyika
corinne.anyika@rc-harwell.ac.uk

Visit https://ukcatalysishub.co.uk/news/

or follow us on Twitter for more news: Twitter:@UKCatalysisHub

Upcoming External Events

ROYAL SOCIETY OF CHEMISTRY



27–29 March 2023
London, UK and online

Sustainable nitrogen activation

Faraday Discussion

Sustainable nitrogen activation Faraday Discussion – Open for poster abstracts

27 – 29 March 2023
London, United Kingdom

The upcoming Faraday Discussion on Sustainable nitrogen activation will take place in March 2023, to discuss sustainable routes to ammonia synthesis. Hear from expert speakers, network and explore one of the most important challenges in contemporary ammonia production.

For more information and to register visit https://www.rsc.org/events/detail/48190/sustainable-nitrogen-activation-faraday-discussion

IChemE-SCI Factories for the Future Symposium - Open for abstracts

28 March 2023
School of Chemical Engineering, University of Birmingham

The meeting will explore how future manufacturing plants will need to evolve as we strive towards net-zero carbon processes and respond to the depletion of traditional resources. Keynote lectures from academics and industrialists will cover multi-step synthesis and reactor design, process integration and control, catalysis and selectivity enhancement, the application of big data and machine learning, atom efficiency, sustainability and robotics.

For more information, including the speaker programme, and details on how to register, please visit the meeting webpage: https://www.icheme.org/membership/communities/special-interest-groups/catalysis/events/28-03-23-factories-for-the-future/

Posters and short talks: We are particularly keen to encourage early-career researchers to participate in the meeting and in addition to a poster session, have included slots in the programme for a series of short talks. Details on how to submit an abstract are included in the webpage above.

Chem4Energy Annual Conference – Sustainable Energy 2023

30 March – 2 April 2023
NWU Sports Village in Potchefstroom, South Africa

Chem4Energy is pleased to announce the 2023 conference on 'Materials and Processes for a Sustainable Energy Future'.

- The Chem4Energy annual conference has grown out of two collaborative UK-Africa consortium programmes and 2023 will see the third in this series of meetings, which focus in particular on:
- Highlighting the synergy between experiment and computation
- Offering opportunities for early career researchers to disseminate their work in oral and poster presentations – often their first conference talk!
- Allowing plenty of opportunity for discussion of the research

The Chem4Energy conferences aim to bring together local academic and industrial researchers and developers from Southern Africa with colleagues from Europe, the USA and further afield, to discuss the latest developments in clean energy materials and processes, build new collaborations, and influence and support future directions in the field of sustainable energy research.

Although contributions in all areas within the

Upcoming External Events cont.

Chem4Energy remit are welcome, particular themes of the 2023 meeting include: Homogeneous and heterogeneous catalysis for clean energy; CO2 capture and utilisation, Nanoparticles and surface processes, Materials for solar energy devices and High-performance computing in energy research.

For more information and to register visit https://natural-sciences.nwu.ac.za/chem-4-energy/home

Syngas Convention 4

2 – 5 April 2023
Conference Venue of the Graduate School of Business of the University of Cape Town, Cape Town, South Africa

The DST-NRF Centre of Excellence in Catalysis (c*change) at the University of Cape Town extends a cordial invitation to delegates from throughout the world to participate in the Convention 'Fuels and chemicals from synthesis gas: State of the art 4'. The meeting will be held from 2 to 5 April 2023 at the Conference Venue of the Graduate School of Business of the University of Cape Town right at the V&A Waterfront in Cape Town.

The Convention will focus on advancements in the production of synthesis gas and its conversion with a special focus on the activation of carbon dioxide.

Participants are encouraged to present their own work in the form of either an oral or a poster presentation. Themes on which papers are invited include synthesis gas production, Fischer-Tropsch and methanol synthesis as well as CO2 activation. The convention will in particular focus on: Modeling aspects heterogeneous catalysis, Catalyst synthesis and characterization, Product formation and selectivity, Deactivation.

For more information and to register visit https://syngasconvention.com

Harnessing non-covalent interactions for synthesis and catalysis Faraday Discussion

12 – 14 April 2023
York

Join us in York in April 2023 for this latest addition to our Faraday Discussion series. For over 100 years and 300 meetings, Faraday Discussions have led the conversation in the sciences lying between chemistry, physics and biology. Many Discussions have become landmark meetings in their field, with their unique format allowing for in-depth discussions and opportunities to establish new collaborations.

This meeting is for established and early-career scientists, post-graduate students and industrial researchers interested in non-covalent interactions. The meeting will bring together teams of physical and life scientists to discuss new developments in the understanding and control of the non-covalent intermolecular interactions that drive synthetic and catalytic processes.

Poster presentation opportunities are available to all, and we invite you to submit a poster abstract to make your contribution alongside leaders in the field.

For more information and to register visit https://www.rsc.org/events/detail/48165/harnessing-non-covalent-interactions-for-synthesis-and-catalysis-faraday-discussion

Dalton 2023

18 – 20 April 2023
Coventry, United Kingdom

Dalton 2023 is a conference that will bring together researchers from the full breadth of inorganic chemistry. The meeting is organised by the Royal Society of Chemistry Dalton Community and associated Interest Groups.

Inorganic Reaction Mechanisms Discussion Group

Coordination and Organometallic Chemistry Discussion Group

Inorganic Biochemistry Discussion Group

Main Group Chemistry Group

Oral and poster abstract submissions are now open. Abstract deadline 18 February 2023.

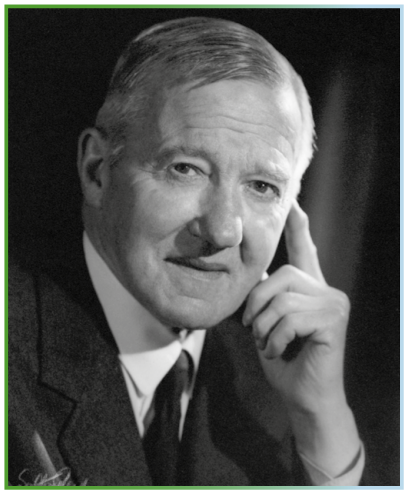
Speakers:
Saurabh Chitnis, Dalhousie University, Canada
Richard Kong, Cornell University, United States
Maxie Roessler, Imperial College London, United Kingdom
Jana Roithova, Radboud University Nijmegen, Netherlands
Jonathan Sessler, The University of Texas at Austin, United States
Richard Winpenny, University of Manchester, United Kingdom

For more information and to register visit https://www.rsc.org/events/detail/74994/dalton-2023

Upcoming External Events cont.

Save the date – Rideal 2023 'Catalysis for a Sustainable Future'

3 – 5 May 2023
University College London, London, United Kingdom



The Rideal Conference 2023 will be held at University College London, London, UK, from Wednesday 3rd – Friday 5thMay 2023 with the theme of "Catalysis for a Sustainable Future".

The conference brings together chemists, chemical engineers and physicists interested in the fundamentals and application of catalysis, and heterogeneous catalysis in particular.

Speakers include:
Michael Claeys (University of Cape Town, South Africa)
Chris Hardacre (University of Manchester, UK)
Amol Kulkarni (CSIR-National Chemical Laboratory, Pune, India)
Nora de Leeuw (University of Leeds, Leeds, UK)
Can Li (Dalian Institute of Chemical Physics, CAS, China)
Raj Natarajan (Indian Institute of Science, Bangalore, India)
Misbah Sarwar (Johnson Matthey Technology Centre, UK)
Susannah Scott (University of California Santa Barbara, USA)

One of the aims of the meeting is to allow young researchers and students a unique platform to get first-hand information from world-renowned scientists on topics of prime importance in catalysis. There are also many opportunities for young researchers and students to get involved and have a chance to have their work featured in the poster session.

For more information and to register visit https://www.rsc.org/events/detail/76022/rideal-2023

EuropaCat 2023 – Open for abstracts

27 August – 1 September 2023
Prague Congress Centre, Prague, Czech Republic

The 15th edition of the biannual congress of the European Federation of Catalysis Societies (EFCATS), EuropaCat will be held in August 2023 in the Prague Congress Centre, Prague, Czech Republic. The conference will be, for the first time, jointly organized by the catalysis societies of the Czech Republic, Hungary, Poland and Slovakia. Over the years, EuropaCat has become a traditional meeting place for scientists and researchers from academia and industry all over Europe. Consequently, it has developed into a forum to discuss important challenges in the field of catalysis and the related industrial areas and beyond.

We expect that the conference will attract over 1 500 participants from diverse fields of catalysis having academic as well as industrial background. We strongly encourage the participation of students, i.e. the future generation of scientists and researchers.

More information at https://www.europacat2023.cz/

PROFESSOR DAVID JACKSON MEETING

4 – 6 September 2023
University of Glasgow

A meeting to commemorate heterogeneous catalysis research at the University of Glasgow and the career of Professor David Jackson.

Plenary speakers: Gordon Kelly (Johnson Matthey), Lynn Gladden (University of Cambridge), Alan Allgeier (University of Kansas), Martin Lok (CataLok Consultancy)

Conference Organising Committee: Justin Hargreaves, David Lennon, Emma Gibson (UoG), Eric Gaigneaux (Universitse Catholique de Louvain), James McGregor (University of Sheffield), Simon Beaumont (Durham University).

More information at https://www.gla.ac.uk/schools/chemistry/research/catalysis/davidjacksonmeeting

Upcoming External Events cont.

Biocatalysis Faraday Discussion

22 – 24 May 2024
London

Join us for this edition of the Faraday Discussion series. The Faraday Discussions are unique international discussion meetings that address current and emerging topics at the forefront of the physical sciences.

This meeting is for established and early-career scientists, postgraduate students and industrial researchers working on various aspects of biocatalysis. It will be of interest to researchers working in the areas of enzyme design, protein engineering and catalyst optimization, both in industry and academia, and will provide the opportunity to identify opportunities and challenges, share expertise and advance knowledge at the frontiers of this rapidly developing area.

For more information and to register visit https://www.rsc.org/events/detail/75087/biocatalysis-faraday-discussion

HarwellXPS Thematic Summer School 2024

June 2024
'The Vale Resort' in South Wales, UK

HarwellXPS is hosting the 2024 Summer School for XPS at 'The Vale Resort' in South Wales, UK. This is a continuation of the long running workshop series run by CNRS in France, which concluded in 2022. This event is aimed at researchers from all stages, from XPS novices up to established experts – with concurrent sessions enabling delegates to pick and choose which sessions they wish to attend. Seminars will be delivered by world leading experts in the field including David Morgan (HarwellXPS/Cardiff University, UK), Mark Biesinger (Surface Science Western/ Western University, Canada), Emily Smith (University of Nottingham, UK) and Matthew Linford (Brigham Young University, USA) among others to be confirmed at a later date.

A general overview of the programme will be:
Day 1: Mixture of joint and spit sessions – Fundamentals for beginners, Advanced Experimental discussions for Advanced users
Day 2: New developments in software tools (mostly joint)
Day 3: Advanced material analysis – focus on new experimental methods to analyse batteries, catalysts, biological material and plastics
Day 4: Focus on good experimental and data analysis practices – ensuring reliable, repeatable science and discussing ISO standards
Day 5: Combining XPS/surface analysis with complementary techniques for further materials understanding

There will be a big focus on ensuring reliable and repeatable science throughout, and providing the attendees with the tools to do so.

The event will be attended by a number of industrial delegates, including XPS manufacturers and users alike.

Prices for attendance are subject to change, and nominally set at £650 students/750 postdocs/850 academics/1500 industry. The workshop is 5 nights and all accommodation, meals, daytime refreshment (tea/coffee etc), excursion (and karaoke) are included in the price, as is the large library of software tools and reference material provided to all delegates.

Attendance at these workshops is highly competitive, in order to ensure you receive notification as soon as registration is live, we encourage any interested parties to register an expression of interest via the link below.

For more information visit https://portal.harwellxps.uk/xps-school-interest

Upcoming External Events cont.

18th ICC – INTERNATIONAL CONGRESS ON CATALYSIS

14 – 19 July 2024
Lyon, France

The French catalysis community is honored to host the next International Congress on Catalysis, which will be held in Lyon on July 14-19, 2024.

All French academic laboratories related to catalysis, along with the majority of the industrial companies will contribute to a successful event. France's solid history in catalysis continues today thanks to a young generation of talented scientists in all major fields of catalysis. Building on these strong roots, the French catalysis community wishes to promote disruptive catalysis with the objective of building a better world. In a spirit of cross-fertilization between disciplines, worldwide societal challenges including the environment, energy, mobility, and the circular economy will be addressed through invited lectures and dedicated sessions in line with the main conference slogan "ROOTS AND WINGS FOR A BETTER WORLD".

As captured by our secondary slogan "BUILD YOUR ICC!", we would like to make the 18th ICC an opportunity for "participatory catalysis" by favoring interactions based on digital communication. Building a participatory ICC2024 is an early add-on prior to the conference. We are looking forward to meeting you in Lyon!

More information at https://www.icc-lyon2024.fr/

Database of expertise! Send your profile to be included in our featured list of experts

The UK Catalysis Hub is aiming to compile a database of expertise to help build the catalysis community and encourage collaboration.

If you wish to be included and have your profile featured in this list please send Corinne Anyika a summary of your expertise and up to 5 key words on your main interests.

Email corinne.anyika@rc-harwell.ac.uk with your profile summary.

Stay in Touch:
The UK catalysis Hub wants to hear your news. Please contact the project coordinator to be added to Hub emails, to contribute news articles, research highlights, events, details of talks and publications.

Project Manager: Dr Josie Goodall
Josie.goodall@rc-harwell.ac.uk or call (01235) 567870

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