CatalysisHub NEWSLETTER

The UK Catalysis Hub has created a thriving and successful network of catalytic scientists who are developing and promoting catalytic science in the UK. The Hub has succeeded in coordinating the community and is contributing to the development of new approaches and techniques in the field. It has provided substantial added value and is now recognised widely both in the UK and internationally. It will provide an excellent base for the future development of this crucial area of science in the UK.

"The Hub has demonstrated resilience in the current pandemic with the community coming together to support each other through webinars and training courses and we will continue these in more normal times. Our proposal round was very successful with a large number of high quality proposals submitted and we have funded an excellent portfolio of research. The next few months will hopefully see an easing of the lockdown and an increase in our ability to do research. We hope that all are keeping well and safe and we look forward to meeting in person when we can and discussing catalytic research face to face."
~ Professor Christopher Hardacre, Director

Events Highlights of 2020

COVID-19 has had a major impact on scientific network and dissemination due to travel restrictions and social distancing making face to face meetings and conferences unfeasible. The UK Catalysis Hub winter conference was held virtually and we worked on a vibrant programme of webinars, scientific discussions and other online events. The Catalysis Hub developed a webinar programme of monthly online seminars. Our first webinar: Cooperative Catalysis with Prof. Duncan Wass (Director, Cardiff Catalysis Institute) received a great deal of interest with an audience of over 200 people across the world. We have made the webinars available to watch online via our website, so they will be a future resource for the whole catalysis community.

UKCC 2020, 7 - 9 January 2020

The sixth UKCC conference took place at Loughborough University from the 7th - 9th January 2020.

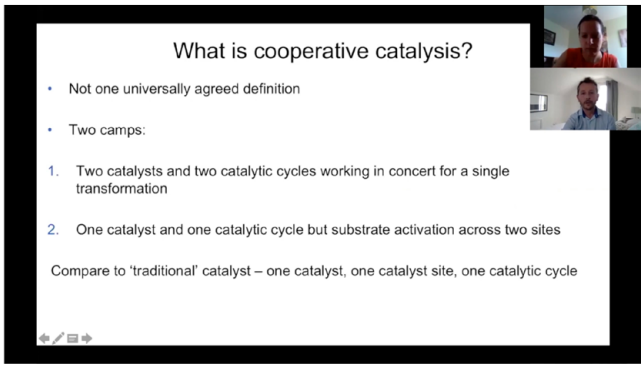
The conference was attended by over 200 delegates including academics, industrial researchers, experimentalists, theoreticians, and students.

Plenary speakers included: Duncan Wass (Cardiff University, UK), Johannes Lercher (Technical University of Munich, Germany), Angelika Brückner (Leibniz Institute for Catalysis, Germany), José Odriozola (University of Sevilla, Spain) and Stewart Parker (STFC, UK)

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.

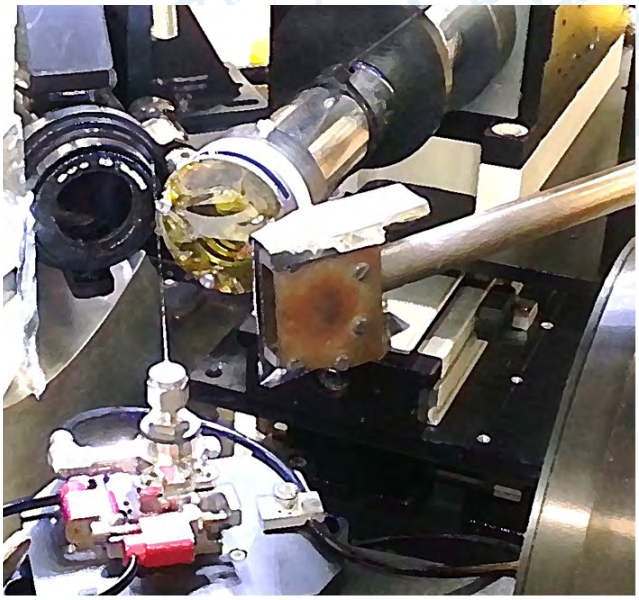
Webinar: Cooperative Catalysis with Prof. Duncan Wass (Director, Cardiff Catalysis Institute)
23 April 2020



Over the past decades, a key objective for both the homogeneous and heterogeneous communities has been to develop 'single site' catalysts, in the hope of achieving extreme precision in terms of catalyst selectivity. There have been notable successes so that, taking homogeneous catalysis as an example, the electronic and steric characteristics of a single transition metal site can be finely tuned by ligand design. However, more recently the limitations of what can be achieved with a single site are becoming apparent, and this approach is being surpassed in some areas by designing catalysts with multiple sites working in concert – so-called cooperative catalysis. This webinar discussed recent approaches in this area, from both the Wass group and more widely. Although the focus of the area to date has been in homogeneous catalysis, parallels to advances in heterogeneous catalysis are clear, often only separated by different nomenclature. Moreover, similar concepts have been accepted in biocatalysis for many years, making this an emerging field that can bring together many strands of the catalyst community.

Recording available to watch at https://ukcatalysishub.co.uk/new-webinar-cooperative-catalysis-with-prof-duncan-wass-director-cardiff-catalysis-institute/

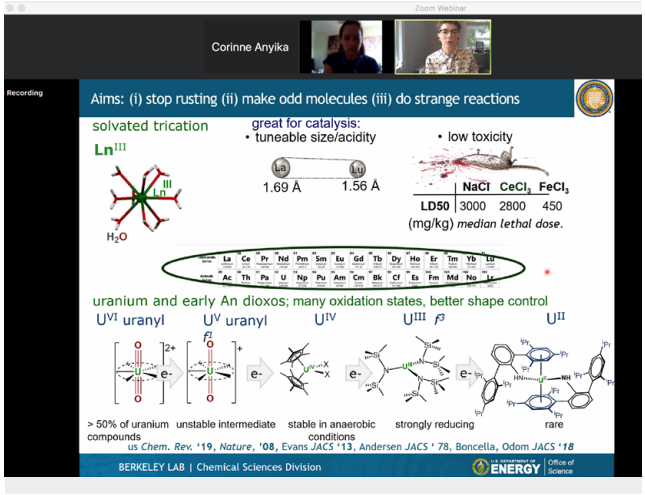
Webinar: Opportunities for studying catalytic materials with intense radiation sources; what, where, when and how.
28 May 2020



It was in 1836 that Jöns Jacob Berzelius provided the first, basic description of a catalyst and its properties. Both the breadth and depth of our understanding of catalysts and catalytic processes has clearly progressed a lot since then – to a large extent this has been enabled by catalyst characterisation, performed increasingly in real time as the catalyst performs its function. Despite these developments, designing a catalyst/catalytic process from scratch is still incredibly difficult. Fortunately, characterisation methods, particularly those using bright light sources (i.e. X-rays, Lasers etc.) and ways in which catalysts & catalytic process can be interrogated are constantly evolving. In this webinar Dr. Andrew Beale highlighted and discussed some recent exciting studies performed by his group and others and explained how the wider catalysis community can engage with and benefit from such developments. He concluded with an overview of some of the planned technical developments on the horizon and suggested where there might be future possibilities.

Recording available to watch at https://ukcatalysishub.co.uk/webinar-prof-andrew-beale-professor-of-inorganic-chemistry-dept-of-chemistry-ucl-finden-ltd/

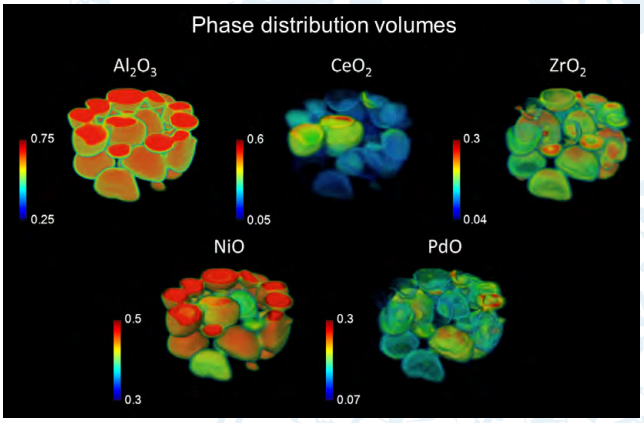
Webinar: F-block catalysts for the catalytic conversion of dinitrogen, carbon dioxide, and carbon oxygenates under mild conditions with Prof. Polly L Arnold (UC Berkeley)
23 June 2020



The subtleties of structure and bonding in compounds of the rare earths (Group 3 and the lanthanides) and actinides are still poorly-understood. However, their complexes can exhibit strong and tuneable Lewis acidity, high and tuneable reduction capacity, and the capacity for rapid ligand exchange reactions. Organometallic compounds of the lanthanides and actinides have begun to show many interesting small molecule activation reactions, and interest is increasing in their activity as catalysts, since the recognition that many rare earths are at least as abundant as iodine, and many are cheap and less toxic than iron.

Prof. Polly L Arnold demonstrated some new f-block organometallic complexes that have been designed to control a few different catalytic transformations. These included (a) the first homogeneous f-block catalysts for dinitrogen functionalization and a catalytic synthesis of secondary amines that uses reactive protons in the ligand, and (b) an exceptionally rapid catalyst that makes ultra-high molar mass cyclic polylactides that relies on the Lewis acidic Ln centre and the ligand's pendant Lewis basic group.

Recording available to watch at https://ukcatalysishub.co.uk/online-webinar-f-block-catalysts-for-the-catalytic-conversion-of-dinitrogen-carbon-dioxide-and-carbon-oxygenates-under-mild-conditions-with-prof-polly-j-arnold-uc-berkeley/



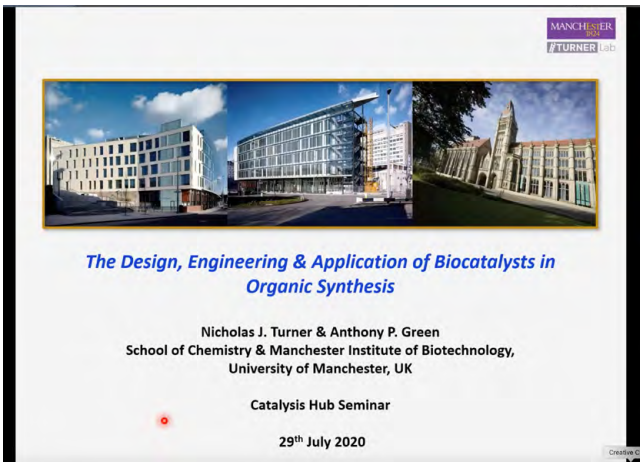
Webinar: X-ray diffraction computed tomography with Dr. Antony Vamvakeros
21 July 2020

Synchrotron X-ray diffraction computed tomography (XRD-CT) is a marriage between powder diffraction and computed tomography using a "pencil" beam approach. The spatially-resolved signals obtained with XRD-CT can reveal information that would otherwise be lost in bulk measurements, which opens up new possibilities in functional material characterization.

In this webinar, Finden Ltd research scientist Dr. Antony Vamvakeros presented results from key case studies where he and the team applied XRD-CT to track the evolving solid-state chemistry of complex functional materials and devices under operating conditions. The webinar also focussed on the recent technical advances in data acquisition, treatment and handling strategies, as well as bottlenecks/limitations of the technique and the potential routes to overcome them.

For more information and to watch the webinar visit – https://www.dectris.com/landing-pages/dectris-application-webinar-series-2020/

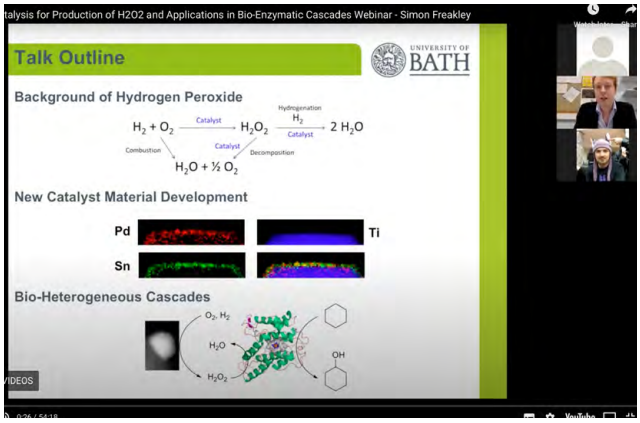
Webinar: The Design, Engineering & Application of Biocatalysts in Organic Synthesis
29 July 2020



A 40 minute seminar given by Dr. Anthony Green (Manchester) and Prof. Nicholas Turner (Manchester) presenting an overview of the current

state-of-the-art and challenges for future research.

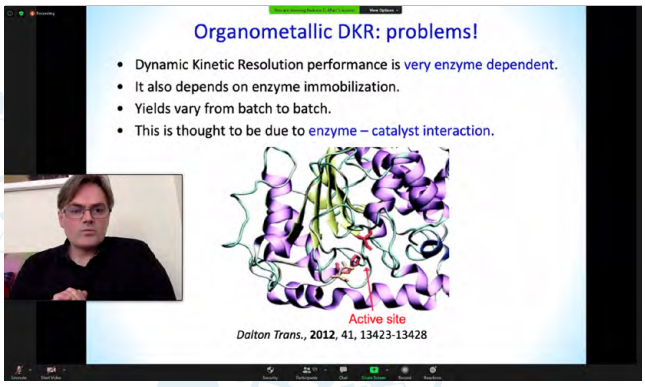
Webinar: Catalysis for Production of H2O2 and Applications in Bio-Enzymatic Cascades 27 August 2020



Dr. Simon Freakley (Bath) gave a seminar on production of H202. Hydrogen peroxide has a key role to play in developing clean chemical processes. The direct synthesis of hydrogen peroxide from H2 and O2 would represent an attractive atom efficient process which could be decentralised as an alternative to the large scale anthraquinone process. Pd based catalysts have been extensively studied for this reaction however selectivity remains a key challenge to prevent the over-hydrogenation or decomposition of the H2O2 to H2O. This webinar described his group's work on developing Pd based catalysts for the synthesis of H2O2 which reach high levels of selectivity in both heterogeneous and electrochemical systems. In addition, the development of one pot reaction cascades which combine enzymatic peroxygenases and heterogeneous H2O2 synthesis catalysts to achieve challenging oxidation reactions at mild conditions was discussed.

For more information and to watch the webinar visit – https://ukcatalysishub.co.uk/catalysis-for-production-of-h2o2-and-applications-in-bio-enzymatic-cascades/

Webinar: The Applied Catalysis Group (ACG) & UK Catalysis Hub Meeting 17 September 2020



A joint virtual meeting between the Applied Catalysis Group (ACG) and UK Catalysis Hub.

Speakers included:

Dr. Christopher Mitchell (SABIC) – Laboratory scale testing of formed catalyst particles For many heterogeneously catalysed processes, the final commercial application requires the use of formed catalyst particles in order to manage pressure drop, heat and mass transfer etc. It is therefore imperative that the performance of catalysts in their final form is evaluated relatively early in the development cycle. The presentation covered different approaches to the testing of formed catalysts at the lab scale, in particular the concept of a "pellet string" reactor.

Dr. Robert Parry (SRP Catalysts) – A look at Powder Hydrogenation Catalysts; Increasing the Catalyst performance Many of the catalysts handled and used industrially, will be formed to a shape like extrusions, tablets, spheres etc for use in continuously operated reactors. However powdered catalysts used in batch, slurry reactors are also widely used particular for Fine and Specialty chemicals. This presentation looked at a snapshot of catalyst manufacture, some tips on mixing and usage, reactor types and separation and catalyst reuse for subsequent batches. The necessity for improved activity and selectivity to the desired product, improved mixing, gas distribution and the relation to process scale up from lab and pilot plants, leads to many difficult questions. This short presentation attempts to elucidate the whole trouble-shooting field even down to purity of process gases, reactor types and feedstock purity and cost versus its catalyst poison profile. Examples of 3 applications for powdered catalysts are discussed.

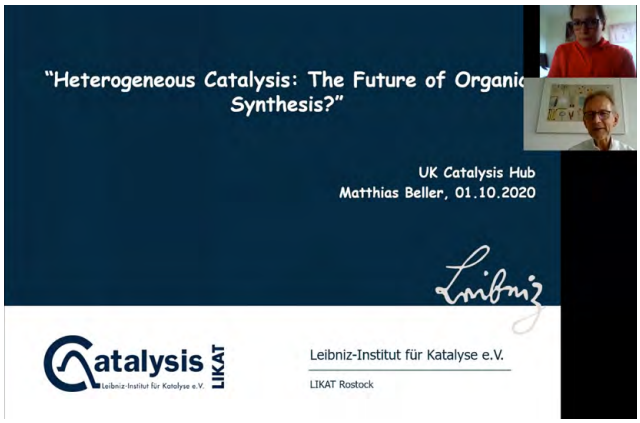
Dr. Andrew Marr (QUB) – Biocatalysis and Homogenous Catalysis: best kept apart, or stronger together? The rapid growth of biocatalysis research has provided many new technologies, and solved significant problems in chemicals synthesis. Examples can be found for which biocatalytic methods are a significant improvement over traditional routes. However, it is unlikely that biocatalysts will provide a cost-effective alternative to chemocatalysts in every case. This means that the ideal synthesis of a valuable target is likely to comprise a mixture of biocatalytic and chemocatalytic steps. It is therefore timely to examine the similarities and differences, the compatibilities and incompatibilities of the two approaches. In this lecture the growing relationship between biocatalysis and homogeneous catalysis will be highlighted, and we will consider the question: should biocatalysis and homogenous catalysts be kept apart, or are they stronger together?

Dr. Katherine Wheelhouse (GSK) – Catalyst selection in pharmaceutical manufacture

The types of reaction typically performed in pharma, how catalysts are selected from a performance and availability perspectives and the additional consideration of residual metals in the product.

Recording available to watch at https://ukcatalysishub.co.uk/the-applied-catalysis-group-acg-uk-catalysis-hub-meeting/

Webinar: Heterogeneous Catalysis: The Future of Organic Synthesis? 1 October 2020



Prof. Dr. Matthias Beller (LIKAT Rostock) gave a seminar on recent advancements in catalysis. Matthias Beller studied chemistry at the University of Göttingen, where he completed his PhD thesis in 1989. As recipient of a Liebig scholarship he then spent a one-year with Sharpless at MIT. Afterwards he worked in industry until 1995, when he moved to the TU of Munich as Professor for Inorganic Chemistry. In 1998, he relocated to Rostock to head the Institute for Organic Catalysis, which became in 2006 the Leibniz-Institute for Catalysis. The work of his group has been published in >1000 original publications, reviews and >158 patent applications have been filed / H-index: 127.

For more information and to watch the webinar visit – https://ukcatalysishub.co.uk/heterogeneous-catalysis-the-future-of-organic-synthesis/

Webinar: Microbial cell factories – engineering biology for chemicals production 27 October 2020

Prof. Nigel Scrutton (Manchester) spoke about biocatalyst engineering and engineering of microbial cell factories for chemicals production.

Biocatalyst engineering and the engineering of microbial cell factories for chemicals production has promised to deliver new routes to chemicals production. Major hurdles to scaled production of chemicals using microbial cell factories remain. Prof. Nigel Scrutton (Manchester) discussed a number of the current technical, scientific and economic challenges of chemicals production using microbial cell factories. The journey will move from automated strain engineering of the type that they have established in the Manchester Synthetic Biology Research Centre (SYNBIOCHEM) through to multiple scale-up challenges. De-risking of scale-up challenges is being met in the UK Future Biomanufacturing Research Hub (FutureBRH) together with industry partners. Selected examples were discussed and in particular, he summarised early commercial activities in the area of fuels production – work that has emerged from microbial strain engineering and scale-up in SYNBIOCHEM and FutureBRH.

Recording available to watch at https://ukcatalysishub.co.uk/microbial-cell-factories-engineering-biology-for-chemicals-production/.

Webinar: Chemocatalysis vs Biocatalysis: When do industry use which, and how can we bring them together? 19 November 2020

Dr. Amanda Jarvis (Edinburgh) & Dr. Samantha Staniland (Johnson Matthey) gave a joint webinar.

Dr. Amanda Jarvis – A brief introduction to artificial metalloenzymes

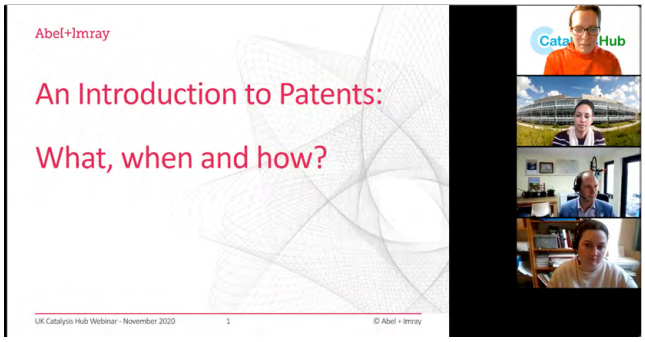
This talk introduced artificial metalloenzymes (ArMs) – biohybrid catalysts that aim to bring together the benefits of transition metal catalysts and enzymes. Using examples from our work, she illustrates how we can design and prepare ArMs, and their use to date in catalysis.

Dr. Samantha Staniland – Why biocatalysis?

This talk explored the pros and cons of biocatalysis vs. chemocatalysis from an industrial standpoint.

Recording available to watch at https://ukcatalysishub.co.uk/chemocatalysis-vs-biocatalysis-when-do-industry-use-which-and-how-can-we-bring-them-together/

Webinar: An Introduction to Patents: What, when and how? 23 November 2020



Abel + Imray hosted an "Introduction to Patents" webinar aimed at explaining what a patent is, why patents are relevant to you, as a chemist, and how you go about patenting an invention.

Obtaining adequate protection for your ideas from an early stage is crucial in order for you to get maximum benefit from your invention. The webinar provided an overview of patents and how to obtain patent protection in the UK, Europe and worldwide, with a particular emphasis on how to spot when you have a patentable invention, and when to starting thinking about filing a patent application.

Dr Tom Turner
Tom is a European and Chartered UK Patent Attorney and a Partner at Abel + Imray. Tom obtained a M. Chem. from the University of Durham, followed by a PhD from the University of Bristol under the supervision of Professor Paul Pringle. Tom's PhD research was in collaboration with Lucite International, and involved the development of new phosphine ligands for use with homogeneous palladium catalysts in industrial chemistry.

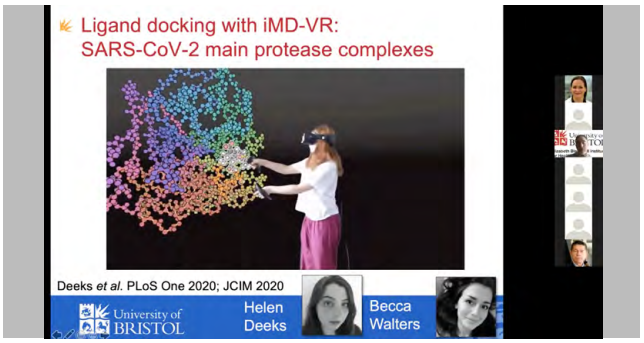
Tom's work on patents relates mostly to industrial chemistry, with a special focus on polymers, reactor technology, homogeneous and heterogeneous catalysis, and petrochemical processing. He is involved in drafting, prosecution and opposition work in the UK and Europe, and management of client portfolios around the world (including in particular other countries in Europe, the US, Australia and Canada). Tom regularly provides Freedom to Operate advice, coordinating searches for conflicting rights, reviewing UK and European patents and working with local attorneys to provide robust and pragmatic guidance. Tom's clients range in size from multinational chemical corporations to small start-ups, based in the UK and across Europe.

Dr Katy Pellow
Katy joined Abel + Imray in 2018 as a trainee Patent Attorney. Katy obtained a M. Chem. from Cardiff University before carrying out her PhD studies at the University of Bristol through the Chemical Synthesis Centre for Doctoral Training under the supervision of Professor Duncan Wass. During her PhD research, Katy developed transition metal catalysts for upgrading bioethanol to biobutanol, providing a sustainable route to advanced biofuel production.

Katy's patent work is mainly in the chemical field with a particular focus on industrial chemistry including petrochemical processing, lubricants, zeolites and polymers. Her work also encompasses pharmaceuticals, materials and formulation chemistry. Her day to day work covers patent drafting, prosecution and Freedom to Operate advice.

Recording available to watch at https://ukcatalysishub.co.uk/an-introduction-to-patents-what-when-and-how/

The UK Catalysis Hub Winter Conference 2020 7th & 8th December 2020



After careful consideration of the rapidly evolving situation with COVID-19 we decided it was best that the UK Catalysis Hub annual summer conference was postponed. Our conference took place on the 7th and 8th of December 2020 and was a virtual event. The event was attended by over 100 people via Zoom.

The conference included the presentation of the JMT Medal for Catalysis and a poster session showcasing work from the Hub postdocs.

Prof. Adrian Mulholland from the University of Bristol received the JMT Medal for Catalysis as person of outstanding achievement in catalysis for pioneering computational modelling of enzyme-catalysed reactions to reveal catalytic mechanisms and analyse the effects of protein dynamics. Read more about his award on page 8.

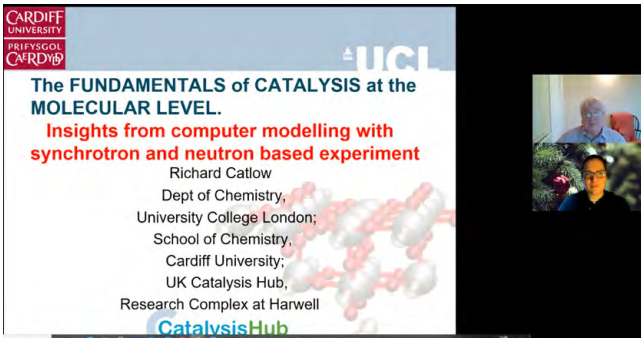
Speakers included: Prof. Dr. Johannes A. Lercher, (TUM), Dr. Marietjie Ungerer, Visiting Researcher, (Cardiff) and Prof. Johannes de Vries, (Rostock)

Highlights of the UK Catalysis Hub winter conference

also included the Poster Competition. First place went to Marco Tomatis (Manchester) for his poster - Life cycle assessment of novel catalysed treatment methods for fracking wastewaters: wet air oxidation. Second place to Aleksander Tedstone (Manchester) for his poster on Transition Metal Chalcogenide Bifunctional Catalysts for Chemical Recycling via Plastic Hydrocracking. Third place was taken by Hasan T. Imam (QUB) for a poster on Hiding the catalyst inside a (bio) material 'raincoat' for sustainable chemical transformations in water.

Recordings from the conference are available to watch at https://ukcatalysishub.co.uk/uk-catalysis-hub-virtual-conference-december-2020/

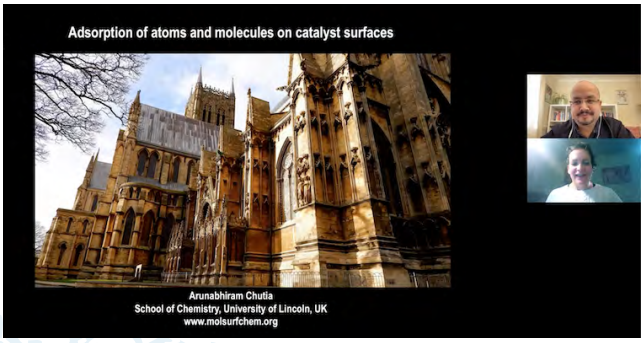
Webinar: The fundamentals of Catalysis at the Molecular level 14 December 2020



A seminar with Prof. Richard Catlow highlighting the use of computer modelling in conjunction with synchrotron and neutron techniques.

Recording available to watch at https://ukcatalysishub.co.uk/the-fundamentals-of-catalysis-at-the-molecular-level/

Webinar: Adsorption of atoms and molecules on catalyst surfaces: A theoretical perspective 25 January 2021

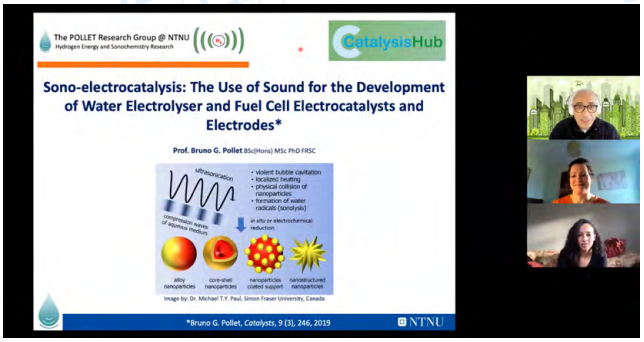


Adsorption of atoms and molecules is a fundamental process, which takes place on a catalyst surface before they dissociate, diffuse over the surface and recombine with other adsorbed species to form the final product. Therefore, understanding the local geometrical and electronic properties of the adsorbed species on the catalyst surface has been one of the topics of core focus.

In this talk, Dr. Arunabhiram Chutia (Lincoln) presented his group's studies on the adsorption properties of catalytically interesting atoms and molecules on catalyst surfaces using theoretical techniques in combination with experimental findings.

Recording available to watch at https://ukcatalysishub.co.uk/adsorption-of-atoms-and-molecules-on-catalyst-surfaces-a-theoretical-perspective/

Webinar: Sono-Electrocatalysis: The Use of Sound for the Development of Water Electrolyser and Fuel Cell Electrocatalysts and Electrodes 8 February 2021



Sono-Electrocatalysis Webinar with Prof. Bruno G. Pollet (NTNU).

Prof. Bruno G. Pollet (NTNU) presented research works undertaken over the years by the Pollet´s groups in Birmingham, Cape Town and Trondheim in the application of power ultrasound for the fabrication of electrolyser and fuel cell catalysts, electrodes and hydrogen production.

Recording available to watch at https://ukcatalysishub.co.uk/sono-electrocatalysis-the-use-of-sound-for-the-development-of-water-electrolyser-and-fuel-cell-electrocatalysts-and-electrodes/

JMT Award Winner Announced

The UK Catalysis Hub have named Prof. Adrian Mulholland from the University of Bristol as winner of the Sir John Meurig Thomas Catalysis Medal at the UK Catalysis Hub Winter Conference on the 7th of December 2020. Prof. Adrian Mulholland was selected from the nominations for top mid-career scientists working in the United Kingdom to win the medal for 2020.

Professor Chris Hardacre, UK Catalysis Hub Director said, "Adrian Mulholland has pioneered computational modelling of enzyme-catalysed reactions to reveal catalytic mechanisms and analyse the effects of protein dynamics. His work has shown how simulations complement experiments, in applications ranging from antibiotic resistance to enzyme evolution and design. He is a worthy winner of the JMT Medal."

The medal honours the achievements of Sir John Meurig Thomas, a distinguished professor in the field of catalysis who sadly passed away last year. 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.

Prof. Adrian Mulholland delivered a lecture on catalysis virtually to the UK Catalysis Hub Winter conference attended by over 100 people. He said on winning, "I am honoured to receive the Sir John Meurig Thomas Catalysis Medal. The award of the JMT Medal to a computational scientist demonstrates the real contribution that molecular simulation and multiscale modelling now make to understanding catalysts, in my case particularly enzymes, biological catalysts."

Prof. Adrian Mulholland gained his first degree from Bristol, where he was awarded the Garner Prize for graduating top of his year. He then worked at ICI Pharmaceuticals (now AstraZeneca), before doctoral studies with Graham Richards at Oxford University. It was during his doctoral studies that he began working on multiscale combined quantum mechanics/molecular mechanics (QM/MM) methods for modelling enzyme-catalysed reactions. He was awarded a Wellcome Trust Prize Travelling Research Fellowship to work with Prof. Martin Karplus at Harvard, and then in the School of Chemistry, University of Bristol. He was appointed as Lecturer at Bristol in 2000 and Professor in 2009. He was awarded an EPSRC Advanced Research Fellowship (1998-2003) and EPSRC Leadership Fellowship (2008-2014). As Chair of the Molecular Graphics and Modelling Society (2004-2008), he oversaw its conversion to a Registered Charity, and established the MGMS Silver Jubilee Award for Early Career Researchers. He plays a leading role in building the UK biomolecular simulation community, e.g. establishing and chairing the UK networks CCP-BioSim (ccpbiosim.ac.uk) and HECBioSim (hecbiosim.ac.uk). He is Chair of the CCP Steering Panel and of the Steering Group of the UK Catalysis Hub. He established (2015) and led BristolBridge, an interdisciplinary project funded by EPSRC to 'bridge the gaps' between engineering and physical sciences and antimicrobial resistance. He was Chair of the 2016 Computational Chemistry Gordon Research Conference. He has a strong interest in the application of high-performance computing (HPC) for biomolecular simulations. His recent work includes modelling of SARS-CoV-2 proteins as potential COVID-19 drug targets. His research is supported currently by the British Society for Antimicrobial Chemotherapy, BBSRC, EPSRC, MRC, BP, Janssen Pharmaceuticals and Oracle.

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

You can watch a recording of the JMT Prize announcement and Prof. Adrian Mulholland's JMT lecture at https://ukcatalysishub.co.uk/jmt-2020-award-winner-announced/

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 over the next five years.

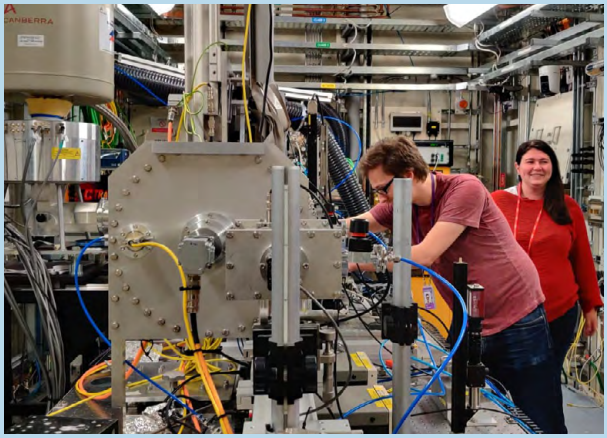
Dr. Martin Wilding - Experimental BAG Officer

Martin received his PhD from the University of Edinburgh where he studied mineral inclusions in natural diamond. Subsequently he focussed on the thermodynamics and structure of amorphous materials and liquids working in laboratories in both Germany and the USA before relocating in the UK.

Martin has worked extensively with colleagues at the Advanced Photon Source using high energy X-rays to determine the structure of refractory oxide liquids and molten salts. High energy X-ray diffraction and X-ray absorption spectroscopy has been used with novel, containerless sample environments that enable reactive liquid structures to be studied in both the stable and metastable, supercooled liquid regimes. Containerless techniques can combined with gas mixing and has been used to study iron bearing systems under controlled atmospheres.

He has also worked at both pulsed and reactor neutron sources, studying liquids and amorphous materials under extreme conditions, using quasialastic neutron scattering to determine the diffusion of sodium ions in molten carbonate and nitrate and using neutron diffraction with isotopic substitution (NDIS) to investigate the restructuring of solvents surrounding carbon nitride and graphene oxide nanoparticles. Most recently NDIS has been used to study the changes in liquid structure during the invert crystallisation of organometallic hybrid perovskites.

Martin now works as Experimental Officer for the Catalysis Hub and has taken over the management of the hub's BAG (Block Allocation Grant) beamtimes at the Diamond Light Source.



BAG at Diamond Light Source

Block Allocation Group (BAG) Programme Mode Application to Diamond Light Source

The UK Catalysis Hub BAG aims to provide members of the Hub network and all groups doing catalytic science in the UK with frequent and flexible access to B18, sending out two calls for proposals per cycle. One advantage of sending out two calls for proposals per cycle, is that our users can obtain beamtime on a rapid turnaround, which has been especially useful when additional measurements are required on a short timescale to finish pieces of work for publication.

We are committed to increasing the user base of XAFS in the catalyst community, and so in part the BAG works as a training scheme. The team at Harwell guides new users through the proposal and experimental stages, showing them the potential of XAFS for their projects and training them on the analysis of their data. We ask all PIs to name on their proposal a member of their group who will be responsible for the beamtime measurements and who will learn how to analyse the data.

The dates of calls for proposals are set by Diamond light source and will be sent to the Mailing list, for more information and to sign up for the mailing list visit https://ukcatalysishub.co.uk/bag-at-diamond-light-source/

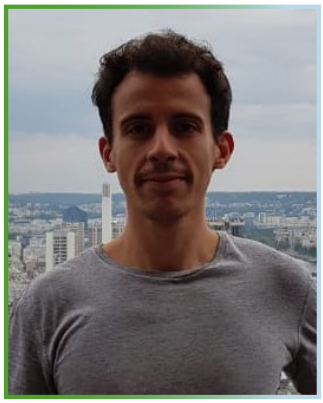
Contact Dr Martin Wilding - WildingM2@cardiff.ac.uk for more information.

Author:

Dr. Martin Wilding, UK Catalysis Hub

UK Catalysis Hub Phase II - Scientific Highlights

We now present some highlights which exemplifies the broad range of contemporary catalytic science enabled by the Hub programme and team.



Dr. Roberto Nolla Saltiel – Earth-Abundant Metals in Resource-Efficient Catalysis

In 2013, I obtained my BSc. Chemistry degree from UNAM (National Autonomous University of Mexico). During my research project, I focused on the study of new catalytic and stoichiometric reactions, mediated by Group 11 metal complexes. Of particular interest were the use of silver and gold metal centres as Lewis acids, enabling the substitution of nucleophiles on aliphatic halides and activated alkenes. Which can be used to selectively yield seven- and eight-membered ring lactones, and/or *2H*-chromenes, depending on the metal of choice.

Following this, I joined Prof. Deborah Kays' research group (University of Nottingham), where I carried out an MRes. (2014) and subsequently a PhD (2016). My primary interests during my postgraduate studies, included the stabilisation of highly reactive, low-coordinate metal centres. With particular attention towards new processes catalysed by environmentally benign and highly abundant elements. Examples of this, include use of *NNN* Group 1-Pincer complexes in the dehydrocoupling of $Me_2NH{\cdot}BH_3$, and the selective hydrophosphination of activated alkenes, catalysed by coordinatively unsaturated first row transition-metal complexes. In parallel, and heavily supporting my research, I routinely conducted single crystal XRD determinations for my metal complexes. A tool that has strongly driven my research.

Following completion of my PhD, in 2019 I joined Prof. Robin Bedford's group, as a Postdoctoral Research Associate. Where I study new synthetic strategies towards C-C bond formation, catalysed by first row transition-metal elements, with parallel interest in small molecule activation. Additionally, to this, I support other members of the group carrying out single crystal XRD determinations, providing further insight into their projects. Luckily and due to my interest in molecular crystallography, I have had the chance of co-supervising projects (collaboration with the Crystallography department), seeking to shed light in some mechanisms involving the spin-crossover characteristics of Fe(II)-bisphosphine complexes, targeting their potential use as single-molecule magnets (Figure 1).

Since I joined the group, I have had the opportunity of exploring a wide range of coordination/organometallic chemistry. Examples of this include careful tunning of bidentante phosphines based on a quinoxaline scaffold, for coordination of iron centres in iron catalysed Negishi cross-coupling processes. Development of new methodologies targeting the synthesis of new ligands based on the cyclopentadienyl moiety, for dinitrogen activation. Preparation of low-coordinate nickel(I) centres via comproportionation pathways and studies relating to the stabilisation of iron, cobalt and manganese by poorly donating ligands. One of my current challenges involves the characterisation of discrete low-coordinate metal centres, with potential use in our catalytic processes.

Research published:

[1] R. Nolla-Saltiel, A. Geer, L. Taylor, O. Churchill, E. S. Davies, W. Lewis, A. Blake, D. Kays, Hydrophosphination of Activated Alkenes by a Cobalt(I) Pincer Complex. *Adv. Synth. Catal*. 2020, 362, 3148–3157.

[2] R. Nolla-Saltiel, A. M. Geer, W. Lewis, A. J. Blake, D. L. Kays, Dehydrogenation of Dimethylamine-Borane Mediated by Group 1 Pincer Complexes. *Chem. Commun.* 2018, 54, 1825–1828.

[3] R. Nolla-Saltiel, E. Robles-Marín, S. Porcel, Silver(I) and Gold(I)-promoted Synthesis of Alkylidene Lactones and *2H*-Chromenes from Salicylic and Anthranilic Acid Derivatives. *Tetrahedron Lett*. 2014, 55, 4484–4488.

[4] R. Nolla-Saltiel, U. A. Carrillo-Arcos, S. Porcel, Silver Acetate Mediated Acetoxylations of Alkyl Halides. *Synthesis*, 2014, 46, 165–169.

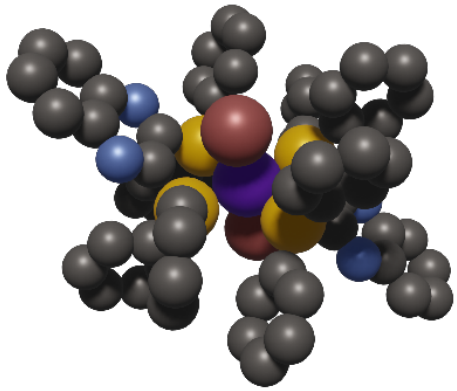
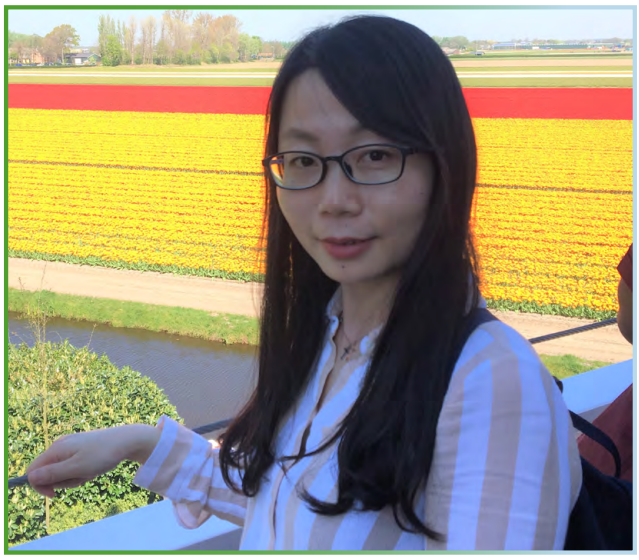


Figure 1. Molecular structure of $FeBr_2(QxPPh_2)_2$

Author:

Dr. Roberto Nolla-Saltiel, UK Catalysis Hub



Dr Xiaoxia Ou - Heterogeneous catalysis for environmental applications

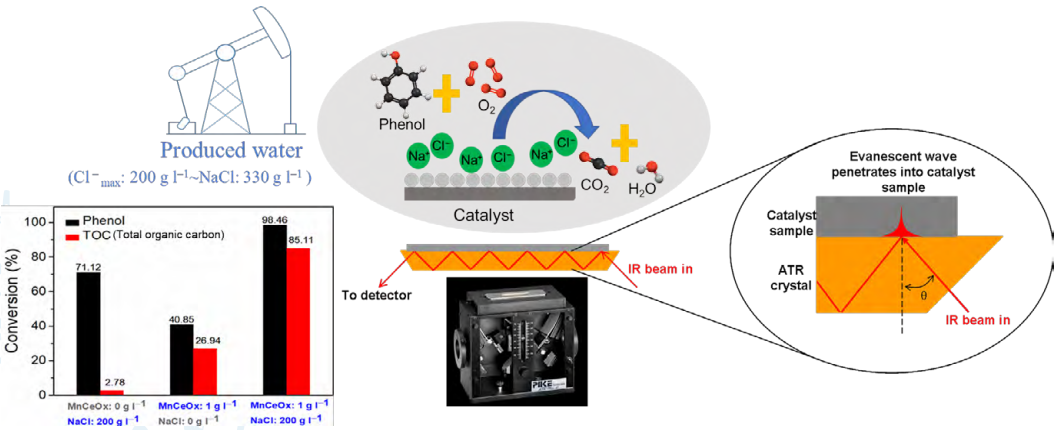
My research focuses on the field of porous materials and catalysis for environment and energy. Currently, I am working on high ionic strength wastewater treatment, specifically produced water treatment. Produced water is a major and environmentally devastating byproduct of oil and natural gas extraction, however, due to the presence of large amounts of catalyst poisons such as Cl^-, the application of catalysis for produced water treatment is lacking.

To explore the potential of catalytic wet oxidation (CWO) for produced water treatment, MnCeOx catalyst was tested in CWO of phenolic wastewater in the presence of NaCl. The catalyst was synthesised by the co-precipitation method and characterised by XRD, SEM-EDX, TEM, N_2 adsorption, XPS and H_2-TPR techniques. The effects of NaCl concentration, MnCeOx catalyst concentration, temperature, initial phenol concentration and O_2 pressure on CWO of phenol was evaluated in a batch reactor, and phenol concentration, total organic carbon (TOC) concentration and metal leaching were monitored. CWO of phenol over MnCeOx was also tested in a fixed-bed reactor and promoting effect of NaCl on phenol and TOC (total organic carbon) conversions were observed in both batch and continuous systems. Deactivation of MnCeOx catalyst was caused by carbon deposition during CWO of phenol, however, calcination was necessary for regenerating the spent catalyst used in the absence of NaCl, while a salt water wash under O_2 at the reaction conditions was effective to regenerate the catalyst used in the presence of NaCl.

To further understand the promoting effect of NaCl on phenol oxidation, adsorption/oxidation of phenol and the main aromatic intermediate products in CWO of phenol (i.e. phenol, catechol, hydroquinone and benzoquinone) on MnOx, CeO_2 and MnCeOx in the absence and presence of NaCl were investigated by *in situ* ATR-IR. What emerges from the ATR-IR results is that the effect of NaCl on CWO of phenol may be ascribed to (1) reduced adsorption strength of oxidation products and phenolates on catalyst surface; (2) promoted further oxidation of partial oxidation products; and (3) salting-out effect. In addition, it was found that Mn is responsible for oxidation of catechol while Ce is responsible for benzoquinone oxidation, thus the combination of Mn and Ce in the MnCeOx can be another good explanation for the improved phenol conversion over the mixed oxide compared to single oxides.

CuCeOx was synthesised by the co-precipitation method and tested in CWO of phenol in the absence and presence of NaCl in a batch reactor. Compared to MnCeOx, the catalytic activity of CuCeOx was lower. The promoting effect of NaCl on phenol oxidation on CuCeOx was also observed but severe copper leaching was found due to high salinity, which may cause more concerns on water toxicity.

Taken together, MnCeOx is a good chloride resistant catalyst with the potential for further exploration toward the application of CWO for practical produced water treatment.



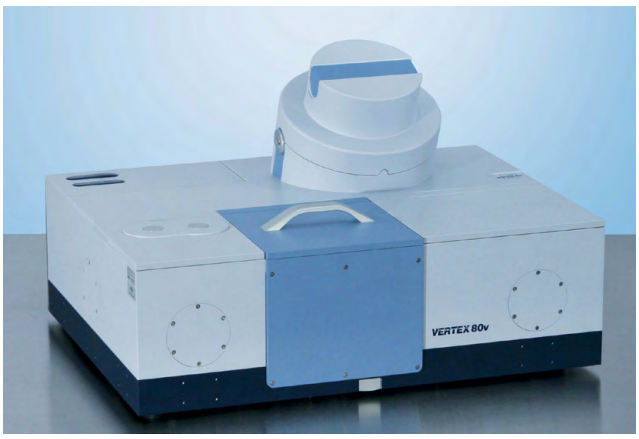
Author:

Dr Xiaoxia Ou, UK Catalysis Hub

UK Catalysis Hub Phase II - New Facilities and equipment

The UK Catalysis Hub works to contribute to the development of instrumentation and facilities on ISIS, Diamond and the Central Laser Facility, to enable new experimentation in catalytic science, with special emphasis on in situ studies of working catalysts. We have access to cutting edge facilities and equipment in Harwell.

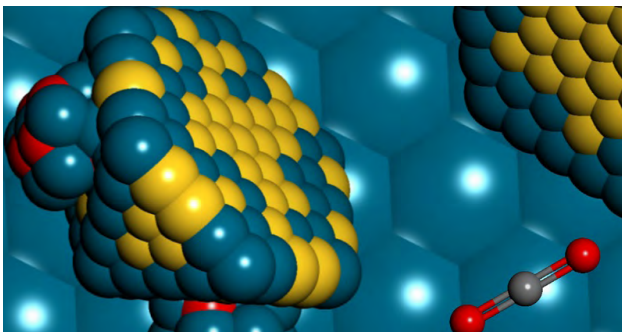
New facility for Time Resolved Spectroscopy in Catalytic Science



In collaboration with the Research Complex at Harwell and with funding from EPSRC The Hub is currently developing a new facility for time resolved IR including an ultrafast FTIR spectrometer with the capability to acquire data with a time resolution of millisecond (ms) to nanosecond (ns), a cell enabling data acquisition at high gas pressures, the capability to perform modulation excitation (ME) experiments using fast (ms) gas switching and a fast-response mass spectrometer to create a new facility for performing operando catalytic reactions for structure-activity relationship determination. This new capability coupled with the existing DRIFTS/FTIR capability currently available at RCaH will result in the establishment of a world leading suite of capability for studying dynamic catalytic systems, underpinning academic and industrial collaborations and will be made available nationally to all research groups working in catalysis and related areas using the Hub network which includes over 45 university groups. Indeed, external interest in such equipment will be strong as the techniques provide unique cutting edge capabilities for scientific advancements. This equipment will complement existing catalyst evaluation, and characterisation tools housed and at the Research complex at Harwell (RCAH) and UK Catalysis Hub. This capability will allow for the in situ & operando identification of adsorbed species on catalyst surfaces and for elucidating reaction intermediates and mechanisms in industrially relevant reactions under realistic conditions. The possibility to further exploit the application of the ME approach and to apply ultrafast (ultimately ns) to detect transient intermediate species represents an exciting opportunity to apply and develop beyond state-of-the-art approaches for determining structure-activity relationships in catalytic materials.

DRIFTS techniques have been at the forefront of catalysis research for several years, providing in depth information about the adsorbed species on the surface of catalysts essential for industrial applications. Although the technique is used widely throughout the catalysis community, technical limitations have restricted research in commercially relevant environments; in particular the use of DRIFTS cells with lower dead volumes and the monitoring of reactions at more realistic pressures (> 1 bar). Even when these technical limitations are overcome, there are still issues regarding the detection of intermediates and transients in the catalytic reaction. The setup(s) put forward in this application, based on the advances made at The Catalysis Hub, would allow for the in situ/operando reaction monitoring of high pressure reactions (notably for supporting research on important environmental challenges such as CO2-to-chemicals, hydrogen generation, electrocatalysis, ammonia synthesis and biomass upgrading) using fast scan technology, providing vital information on the mechanisms of a variety of reactions and materials under realistic conditions that is currently not possible with the equipment currently accessible in the RCAH and in the UK thus enabling an increased potential for innovative research.

In addition to the high-pressure capabilities provided by this equipment, bespoke sample cells have been developed by the UK Catalysis Hub that allow simultaneous acquisition of DRIFTS and XAFS data in collaboration with synchrotron facilities such as Diamond Light source whilst controlling environmental conditions of gas atmosphere and temperature.



UK Catalysis Hub Call for proposals 2020

The UK Catalysis Hub opened its Call for Projects in March 2020 and received 61 Proposals with 97 years PDRA time requested supported by over £850,000 funding from industry. The projects were of very high-quality science. All the funded proposals were aligned with the Hub's ethos, i.e. multi institution and multidisciplinary collaborative projects. This was an excellent outcome of the call and clearly shows the need for catalytic research and the interest of industry in the Hub, even in these uncertain times. The proposals were reviewed as per the procedure developed by the Hub since its outset in 2013 and included members from across the academic and industrial communities chaired by a member of the Hub's steering group.

The management group has been as flexible with the funding to support as wide a range of projects as possible and some projects have been offered short periods of funding or support from the Core PDRAs based in Harwell, in modelling, neutrons and synchrotron science, to enable projects to be tested or to bring the science to a point where further funding can be applied for. Overall, 29 projects have been funded.

The proposals received were of very high quality and each theme has a diverse portfolio of projects (see summaries below). It is worth noting the Hub is supporting a number of ECRs in this round including the core PDRAs on the Science 1 theme who have been involved in writing the proposals. A number of previous Hub postdocs have been successful in this round of funding as well as other ECRs in catalysis.

Science 1 – Optimising Predicting and Designing New Catalysts

Investigators	Title
Green (Manchester) Mulholland (Bristol) Catlow, Quesne (Cardiff) Heyes (Manchester)	Reengineering the active site of non-heame iron enzymes using an expanded genetic code
Hardacre (Manchester) Catlow, Mattam (Cardiff) Bowron (ISIS) Diaz-Moreno (DLS)	Modulation Excitation Neutron Scattering
Fey (Bristol) Lynam (York) Quesne (Cardiff) AZ CatSci	Integration, prediction and validation in enantioselective catalysis–proof-of-concept for an integrated workflow
Beale (UCL) Dann, Kondrat (Loughborough) Moreau	Elucidation of reaction and deactivation mechanisms of fresh and stabilized zeolites for End of Life Plastic (ELP) Pyrolysis
Regmi, Kine (MMU) Decarolis (Cardiff) Beale, Negahdar (UCL) Ronning (NTNU) AVS	Stable and economic iridium catalysts for renewable energy technologies
Kondrat, Buckley Christie (Loughborough) Catlow, Quesne, Decarolis (Cardiff) Hall (CCSL) Gianolio Aramini (DLS) Wells (Southampton)	Direct Hydrogenation of Captured Carbon Dioxide using a Heterogeneous Catalyst

Investigators	Title
Matam, Catlow (Cardiff) O'Malley (Bath) Van Veen (Warwick)	Sorbate Dynamics in Methanol to Hydrocarbon Catalysts
Davis (Oxford) Hutchings, Catlow (Cardiff) RFI	Protein Repair Catalysis
Vincent (Oxford) Freakley (Bath)	Cooperative Bio-Hetero Catalysts for Selective Hydrogenation
Gouget, McCullough (QUB) Wells (Southampton) Gibson (Glasgow)	Induction Heating After Treatment Solutions for Hybrid Vehicle Emissions Control
Gavriilidis, Sorensen (UCL) Blacker (Leeds) Catlow, Hutchings (Cardiff) JM	Changing the Philosophy of Catalyst Design: A Process Systems Orientated Approach

Science 2 – Catalysis at the water and energy nexus

Investigators	Title
Hardacre (Manchester) Davies, Hutchings, Catlow, Quesne, Delarmelina (Cardiff)	Removal of Low Concentration Pollutants from Potable Water
Regmi, Kine (MMU) Decarolis (Cardiff) Beale, Negahdar (UCL) Ronning (NTNU) Garbayo (AVS)	Stable and economic Iridium catalysts for renewable energy technologies
Mills, (QUB) Hardacre (Manchester) Brett (UCL)	Solar-driven, inexpensive, Photoelectrochemical Reactor for Treating High Ionic Strength Waste water
Wang (Lancaster) Howe, Kechagiopoulos (Aberdeen) Shi Ma (Tianjin) Lvu (Zhongtian Scie and Tech)	Photocatalysis in the water flow: mediator - free NAD(P)H regeneration for biotransformations
Hardacre (Manchester) Mattia, Exposito (Bath)	Treatment of microplastics in wastewater
Green (Manchester) Hardacre (Manchester) Catlow (Cardiff) Robertson (QUB)	Valorisation of Microplastics in Wastewater
Manyar, Gouget (QUB) Carlow (Cardiff) Hardacre (Manchester) Shell	Converting biomass derived VFAs into biofuels
McGregor (Sheffield) Nyugen (Leeds) 350 Solar Tech	Direct Catalytic Reduction of Carbon Dioxide with Water
Pordea, Morra (Nottingham) Marr (QUB) Vincent (Oxford)	Artificial heterobimetallic enzymes: Synthesis and application of [NiFe]-hydrogenase analogues.

Science 3 – Catalysis for Circular Economy and Sustainable Manufacturing

Academics	Title
Garforth, Fan, Hardacre, Partlett, Tedstone, Wilkinson, Yerokhin, Zhang, (Manchester) Davidson (Bath) Randvir (MMU)	Reframing plastic waste as a resource
Fairlamb, Wilson (York) Bourne Willans (Leeds) Beaumont (Durham) GSK	Sustaining pharma-relevant metal -catalysed cross-couplings: interrogation of metal catalysts using automated optimisation routines, rich data analytics and mechanistic studies
Wass, Sankar (Cardiff) Fan, Hardacre (Manchester) BP JM	Catalytic upgrading of carbon dioxide, hydrogen and small alcohols to liquids fuels
Buchard parsons, Lyall, Gobius Du Sart (Bath) Williams (Oxford) Mulholland (Bristol) Terill (DLS) Drochaid Oxford Engineering	From Rings to Polymers and Back Again: Catalytic Recycling of Waste Oxygenated Plastic
Papaioannou, Mutch (Newcastle) Gibson (Glasgow) McCue (Aberdeen)	CO_2 to MeOH: a supported molten-salt catalytic membrane reactor (CO_2MeOH)
Haigh (Manchester) Sankar (Cardiff) BP JM	Understanding wet impregnation synthesis for sustainable hydrogenation catalysts
Parlett,(Manchester/Diamond) Hondrow (Leeds) Evans (Aston) LuxferMEL	Catalytic cascade reactions for biomass valorisation
Pringle, Fey (Bristol) Hintermair (Bath) LiKat Bartlett (DLS) Evonik	-1-Rh–complexes of the super-π-acceptor fluoro-phosphite ligands: ligand design and operando studies of an industrially important class of hydroformylation catalyst
Jarvis, Wallace (Edinburgh) LiKat	Sustainable Syngas from engineered bacteria for next-generation catalytic hydroformylation

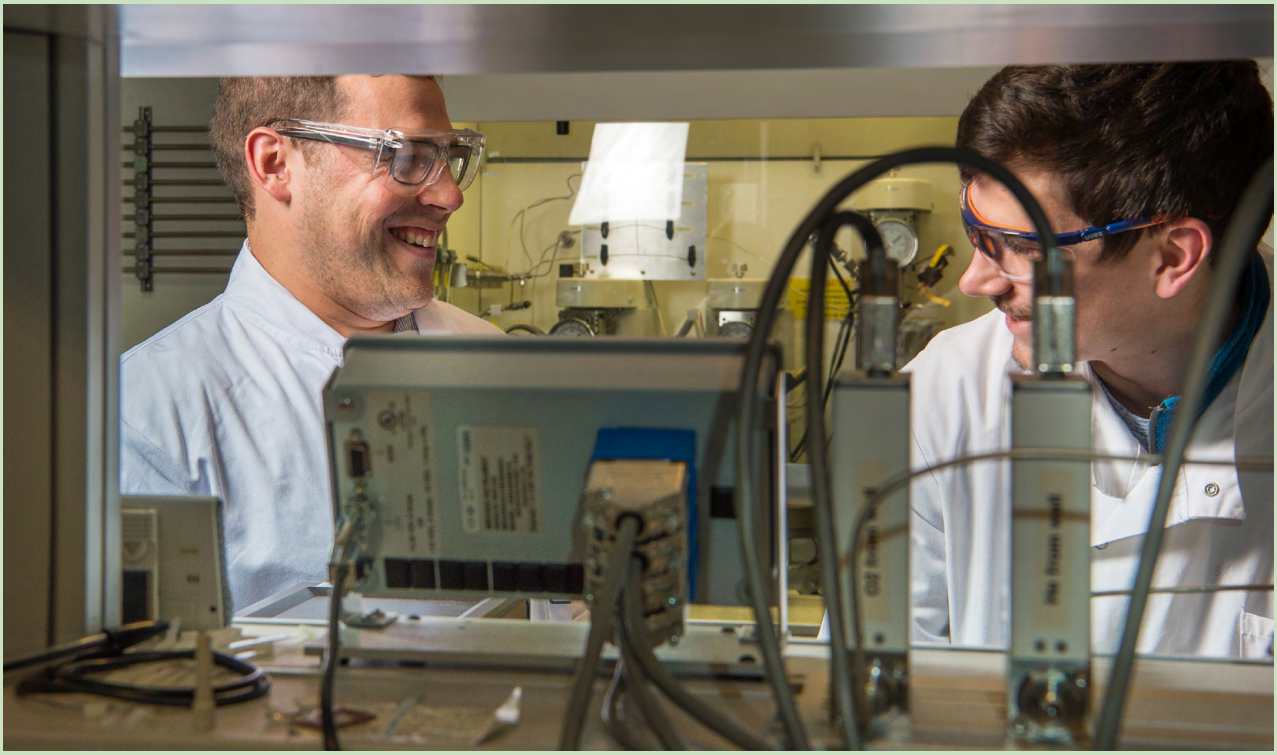
In addition one proposal was deemed to cross all the themes of the Hub and will be supported by all themes.

Cloud-enabled virtual collaboration for catalyst modelling for the circular economy

(Investigators – Mulholland, Bennie (Bristol), Green (Manchester), Jarvis (Edinburgh), Bouchard, Davidson (Bath), McGeehan (Portsmouth))

The call for proposals was a huge success and we look forward to this exciting and diverse portfolio of Projects getting started this year. The Hub is very happy to be able to support and enable cutting edge, collaborative research even is these difficult times.

Opportunities



New UK Catalysis Hub Research Associate position in Heterogeneous Catalysis

An 18-month Research Associate position in Heterogeneous Catalysis is available within the UK Catalysis Hub group at the University of Manchester at Harwell for an enthusiastic and highly motivated scientist. The post will deliver novel multifunctional catalytic materials design to facilitate multistep catalytic processes in one-pot.

You will undertake research in porous materials and catalysts development, for applications in biomass upgrading. The project, entitled Catalytic cascade reactions for biomass valorisation, is funded by the Engineering and Physical Sciences Research Council (EPSRC), as part of the UK Catalysis Hub. The position will be based at the Harwell Science and innovation campus, Oxfordshire, within the UK Catalysis Hub, and is available from March 2021, or soon thereafter, for 18 Months.

The project aims to deliver novel multifunctional inorganic catalytic materials, in which the location of different active species is precisely controlled, to dictate reaction pathways in multistep catalytic cascades. The project will be based within the research group of Dr Christopher Parlett and is supported through collaborations with by Dr Nicole Hondow (University of Leeds) and Dr Rob Evans (Aston University) with industrial support from Luxfer MEL. It is expected that there will be opportunities to conduct research within the collaborator's labs.

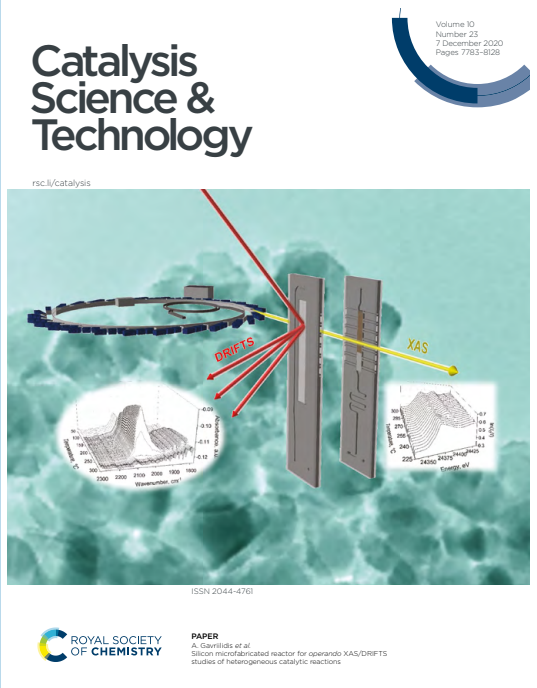
Closing date: 1st March 2021

Visit https://www.jobs.manchester.ac.uk/displayjob.aspx?jobid=19713 for more information and to apply.

Publications:

Silicon microfabricated reactor for operando XAS/DRIFTS studies of heterogeneous catalytic reactions

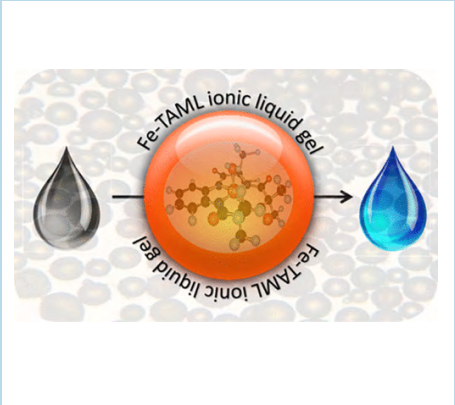
Venezia's et al paper on a microfabricated catalytic reactor for time- and spatially-resolved experiments using operando XAS/DRIFTS studies, has been highlighted on the journal's blog as a Catalysis Science & Technology Editor's Choice.: https://blogs.rsc.org/cy/2021/01/25/catalysis-science-technology-editors-choice-january-2021/?doing_wp_cron=1611592847.4686930179595947265625. It will be free to access until 26th April 2021.



Cover: Catalysis Science & Technology Publisher: Royal Society of Chemistry

Operando X-ray absorption spectroscopy (XAS), diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) and mass spectrometry (MS) provide complementary information on the catalyst structure, surface reaction mechanisms and activity relationships. The powerful combination of the techniques has been the driving force to design and engineer suitable spectroscopic operando reactors that can mitigate limitations inherent to conventional reaction cells and facilitate experiments under kinetic regimes. Microreactors have recently emerged as effective spectroscopic operando cells due to their plug-flow type operation with no dead volume and negligible mass and heat transfer resistances. Here we present a novel microfabricated reactor that can be used for both operando XAS and DRIFTS studies. The reactor has a glass–silicon–glass sandwich-like structure with a reaction channel (3000 μm × 600 μm; width × depth) packed with a catalyst bed (ca. 25 mg) and placed sideways to the X-ray beam, while the infrared beam illuminates the catalyst bed from the top. The outlet of the reactor is connected to MS for continuous monitoring of the reactor effluent. The feasibility of the microreactor is demonstrated by conducting two reactions: i) combustion of methane over 2 wt% Pd/Al2O3 studied by operando XAS at the Pd K-edge and ii) CO oxidation over 1 wt% Pt/Al2O3 catalyst studied by operando DRIFTS. The former shows that palladium is in an oxidised state at all studied temperatures, 250, 300, 350, 400 °C and the latter shows the presence of linearly adsorbed CO on the platinum surface. Furthermore, temperature-resolved reduction of palladium catalyst with methane and CO oxidation over platinum catalyst are also studied. Based on these results, the catalyst structure and surface reaction dynamics are discussed, which demonstrate not only the applicability and versatility of the microreactor for combined operando XAS and DRIFTS studies, but also illustrate the unique advantages of the microreactor for high space velocity and transient response experiments.

Read the full article at https://doi.org/10.1039/D0CY01608J

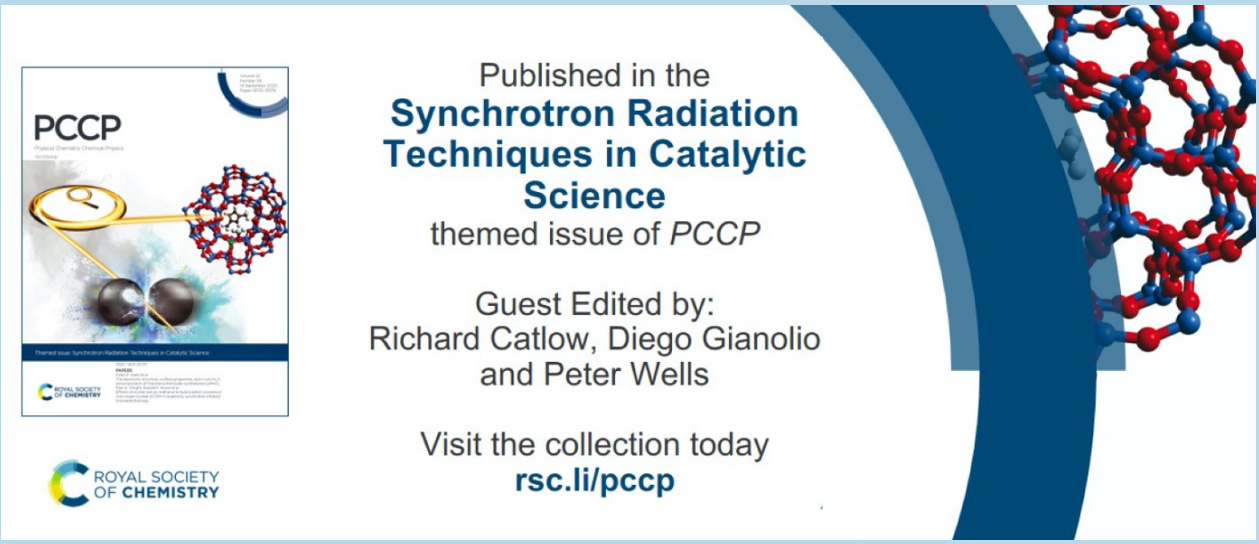


Graphical Abstract: Patricia C. Marr, Environ. Sci. Technol, Publisher: American Chemical Society

Designing Materials for Aqueous Catalysis: Ionic Liquid Gel and Silica Sphere Entrapped Iron-TAML Catalysts for Oxidative Degradation of Dyes

Collaborating with T. J. Collins of Carnegie Mellon, USA, A.C. Marr, P.C. Marr & co. (QUB) demonstrated the oxidation of contaminant dyes in water by H2O2 activated by ionic liquid silica gels and spheres containing Fe-TAML. No need to dissolve metal complexes or add pH buffers. A paper on the work, "Designing Materials for Aqueous Catalysis: Ionic Liquid Gel and Silica Sphere Entrapped Iron-TAML Catalysts for Oxidative Degradation of Dyes" was published in Environ. Sci. Technol. 2020. Read the full article at https://doi.org/10.1021/acs.est.0c04279.

Publications cont:



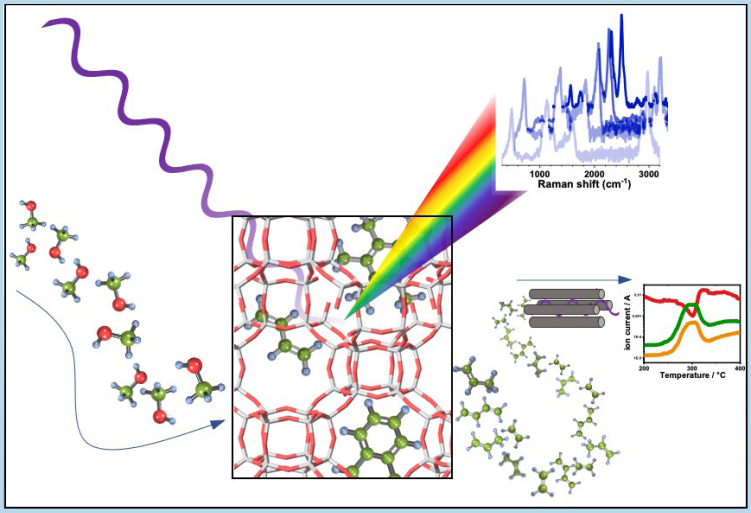
Cover: PCCP Published by the PCCP Owner Societies.

Synchrotron Radiation Techniques in Catalytic Science themed issue of PCCP

A number of UK Catalysis Hub members have been involved in the editing and are authors of articles in the themed collection of articles Synchrotron Radiation Techniques in Catalytic Science in PCCP. Guest Edited by: Richard Catlow (University College London and University of Cardiff), Diego Gianolio (Diamond Light Source), Peter Wells (University of Southampton)

Techniques employing Synchrotron Radiation (SR) have had a transformative effect on catalytic science. The unique properties of SR have led to entirely new opportunities in diffraction, spectroscopy, small angle scattering and tomographical studies of catalytic materials. Moreover, SR has been crucial in enabling the growth of in situ experimental studies of catalytic processes under realistic operating conditions.

Read the articles online at https://doi.org/10.1039/D0CP90186E



Graphical Abstract: Emma Campbell Publisher: Springer Nature

Insight into the effects of confined hydrocarbon species on the lifetime of methanol conversion catalysts published in Nature Materials

A new article has been published in Nature Materials with members of UCL and the UK Catalysis Hub. Authors included: I. Lezcano-Gonzalez, E. Campbell, A. E. J. Hoffman, M. Bocus, I. V. Sazanovich, M. Towrie, M. Agote-Aran, E. K. Gibson, A. Greenaway, K. De Wispelaere, V. Van Speybroeck and A. M. Beale. They report the combined results of an operando Kerr-gated Raman spectroscopic study with state-of-the-art operando molecular simulations, which allowed us to follow the formation of hydrocarbon species at various stages of methanol conversion. Read the article at DOI 10.1038/s41563-020-0800-y

Publications cont:

Synchrotron Radiation and Catalytic Science

An article by members of the UK Catalysis Hub has been published in Synchrotron Radiation News on the benefits of synchrotron to the catalysis community, the Block allocation group access to B18 and key catalysis research facilitated by synchrotron.

Photo credit: Dr. Josie Goodall Publisher: Taylor & Francis

Techniques employing synchrotron radiation (SR) have had a major and growing impact on catalytic science. They have made key contributions to our understanding of structural properties of catalytic systems and of structural changes during the operation of a catalytic process. They can also improve our understanding of electronic and vibrational properties, which can contribute to the understanding of mechanisms. SR techniques are now key components of the experimental tool box of the catalytic scientist.

Developments in sources, instrumentation, and data analysis techniques continue to extend the range and power of SR techniques in catalytic science. In this article, their growing impact is illustrated using a series of case studies based on work within the UK Catalysis Hub, a UK network of catalytic scientists, which has made extensive contributions to both the development and application of SR techniques in catalysis, especially using the facilities of the Diamond Light Source based on the UK Harwell Science and Innovation Campus.

Read it at https://doi.org/10.1080/08940886.2020.1701368

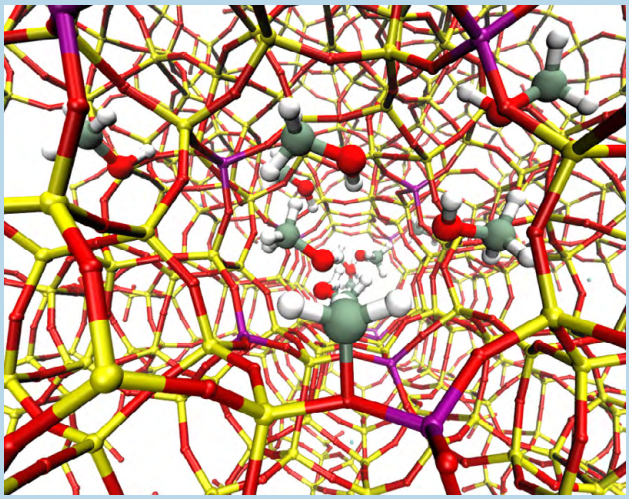


Image: Dr. Santhosh Matam Publisher: The Royal Society of Chemistry

Methanol loading dependent methoxylation in zeolite H-ZSM-5

An article was published by members of the UK Catalysis Hub including; Dr. Santhosh Matam, Stefan A. F. Nastase, Andrew J. Logsdail and Richard. A Catlow in Chemical Science.

In the article they evaluate the effect of the number of methanol molecules per acidic site of H-ZSM-5 on the methoxylation reaction at room temperature by applying operando diffuse reflectance infrared Fourier transformed spectroscopy (DRIFTS) and mass spectrometry (MS), which capture the methoxylation reaction by simultaneously probing surface adsorbed species and reaction products, respectively. Room temperature methoxylation is methanol loading dependent: the higher the methanol loading, the faster the methoxylation. Methanol load of ≥2 leads to methoxylation while no methoxylation is observed with ≤1 molecule per Brønsted acidic site.

Read more in Chemical Science at https://pubs.rsc.org/en/content/articlelanding/2020/sc/d0sc01924k#!divAbstract

Publications cont:

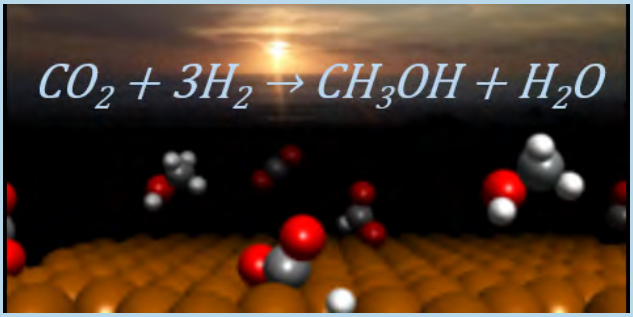


Image: Dr. Michael Higham

Mechanism of CO2 conversion to methanol over Cu(110) and Cu(100) surfaces

An article was published in Dalton Transactions authored by members of the UK Catalysis Hub including Michael Higham, Matt Quesne, and C. Richard A. Catlow.

Plane-wave Density Functional Theory (DFT) techniques were applied to investigate the mechanism of CO2 conversion to methanol over two low-index copper surfaces, namely Cu(110) and Cu(100). The calculations investigated several different mechanistic pathways, considering both formate (HCOO*) and hydrocarboxyl (COOH*) intermediates, as well as CO2 dissociation. For both of the two Cu facets investigated, the formate intermediate was found to be the favoured intermediate, although with close competition with the hydrocarboxyl intermediate, whilst the subsequent hydrogenation of CO after CO2 dissociation has taken place was found to have higher activation barriers. For both Cu(110) and Cu(100), a distinct metastable activated CO2 species was identified, in contrast to the most stable Cu(111) facet for which no such species was found. The present work will serve as a valuable benchmark study for future investigations on the mechanism of CO2 conversion to methanol over model Cu/ZnO catalysts which are representative of real industrial catalysts.

Read more at https://pubs.rsc.org/en/content/articlelanding/2020/DT/D0DT00754D#!divAbstract

Catalytic decomposition of NO2 over a copper-decorated metal–organic framework by non-thermal plasma

The UK Catalysis Hub collaborated on a project which resulted in an article published in Cell Reports Physical Science on 17 February 2021. The article's lead author is Dr Shaojun Xu of the Catalysis Hub at Cardiff University who was supervised by Professor Sir Richard Catlow at Cardiff and Prof Martin Schröder at Manchester. Many UK Catalysis Hub researchers and professors were involved.

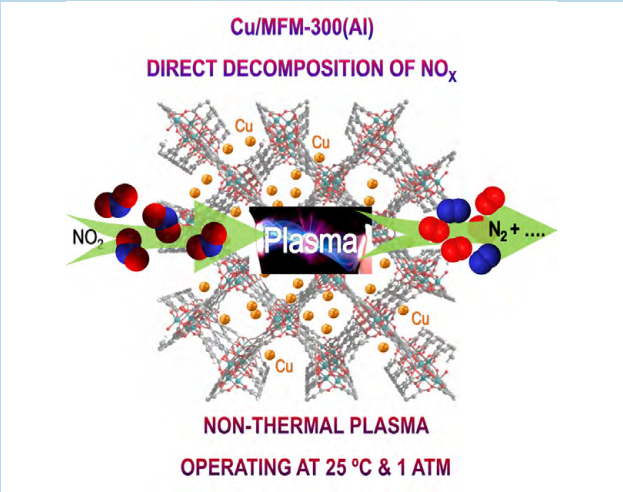


Image: Dr. Shaojun Xu

Nitrogen oxide causes significant effects on the environment and human health. Xu et al. report, to the best of their knowledge, the first example of nonthermal plasma-activated direct decomposition of NO2over stable and efficient metal-organic framework-based catalysts at room temperature and without the use ofNH3or other reducing agents.

Read the article at https://doi.org/10.1016/j.xcrp.2021.100349

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.

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Upcoming Events

UK Catalysis Hub Conference

20 - 22 July 2021
Harwell Campus, Oxfordshire

The UK Catalysis Hub Summer Conference 2021 will be held on **20th & 21st of July 2021** at Harwell Campus, Oxfordshire with a full day EDI event on the 22nd July.

Talks will be starting at lunchtime on the 20th July with a poster session on the evening of the 20th July followed by a dinner at a local venue. The lectures continue on the 21st July until lunchtime and the EDI event on the 22nd July.

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

New UK Catalysis Hub Webinars

The Applied Catalysis Group (ACG) & UK Catalysis Hub Meeting 2021

17 March 2021, 14:00 – 16:00 GMT

A joint virtual meeting between the Applied Catalysis Group (ACG) and UK Catalysis Hub based around the theme of applied characterization.

Speakers include:

Janelle Steves (GSK) - HTE in 3D

David Lennon (Glasgow) - Towards developing structure/reactivity relationships for elevated temperature operation of ultra-selective aniline synthesis catalysts

Ben Deadman (ROAR) - Reaction Characterisation at The Centre for Rapid Online Analysis of Reactions (ROAR)

Paul Collier (JM)

For more information and to register for FREE visit - https://www.eventbrite.com/e/the-applied-catalysis-group-acg-uk-catalysis-hub-meeting-tickets-136429848349

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

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.

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New 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.