# CatalysisHub NEWSLETTER

The UK Catalysis Hub is 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 UK has some outstanding researchers in the field of Catalysis, and it is a vital field for UK industry with a major role to play in the creation of new or improved processes and solving global challenges. Catalysis will be critical in issues including sustainability, energy, green fuels, $CO_2$ utilisation and water.

Building on The UK Catalysis Hub's previous initiatives, we will draw academics and institutions together to further enable cross-disciplinary research, and create a critical mass of activity which will enhance the international standing of the UK catalysis community and address the major challenges faced by the UK through scientific excellence." ~ Graham Hutchings

## £14 million investment into the UK's Catalysis Hub

A new £14 million investment into the UK's Catalysis Hub that will support a nationwide research programme was announced on the 8th October by the Engineering and Physical Sciences Research Council (EPSRC), which is part of UK Research and Innovation (UKRI).

Professor Lynn Gladden EPSRC's Executive Chair, said,

*"Catalysis is important for UK and global industry, generating £50 billion a year for the UK economy, as well as intellectual property for big and small UK companies and universities.*

*"This further funding for catalysis research will help our research communities and industries develop new products and processes that will bring economic and social benefit to the UK. We have to maintain our research capability to keep our nation productive and resilient."*

## UK Catalysis Hub New Grant


The EPSRC has funded UK Catalysis Hub for a further 5 years starting 1/12/2018. The hub will continue to have a physical centre at the Research Complex at Harwell (Oxfordshire) and will co-ordinate a collaborative research program across the UK with 25 universities directly involved in projects and over 45 involved in a wider network across the catalysis community.

The Research Complex houses the Hub's cutting edge catalysis facilities in a vibrant an innovative research environment across the physical and biological science disciplines. The Research Complex location on the Harwell campus offers key collaborations with the UK's cutting edge major facilities including Diamond Light Source, ISIS Neutron and Muon Source, and the Central Laser Facilities, all of which stimulate the development of new techniques and advancements in understanding.

Industry has committed over £800K in kind support to the program and the large scale facilities have co-funded two PDRA positions and 7 studentships.

### The four new interrelated themes of the hub are:

**Core**

**Optimising, Predicting and Designing New Catalysts**

**Catalysis at the Water Energy Nexus**

**Catalysis for the Circular Economy and Sustainable Manufacturing**

### New Objectives for the UK Catalysis Hub

(i) **To deliver an ambitious and adventurous scientific programme,** coordinating the work of UK scientists in catalytic science in fundamental areas relating to catalysis for the circular economy and sustainable manufacturing.

(ii) **To maintain an effective and clear management structure** with strong scientific leadership for a coordinated UK catalysis research programme that cuts across traditional boundaries in catalytic science.

(iii) **To sustain a staff, resource and equipment base** allowing a platform for internationally leading catalytic science on the Harwell/RAL campus.

(iv) **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.

(v) **To publish a substantial volume of high quality scientific papers** in major international journals.

(vi) **To train a cohort of postgraduate research students** associated with catalytic science in the Centre.

(vii) **To contribute to a visitors' programme** for both national and international scientists.

(viii) **To contribute to training and dissemination events**, including a high profile annual meeting associated with the UK Catalysis Hub.

(ix) **To promote knowledge transfer and exchange** between academic catalytic scientists, industry and other stakeholders.

(x) **To sustain and further develop the UK Catalysis Hub** as a world leading centre for catalytic science through establishing international collaborations of the highest calibre.

# The future of the Catalysis Hub

## Vision

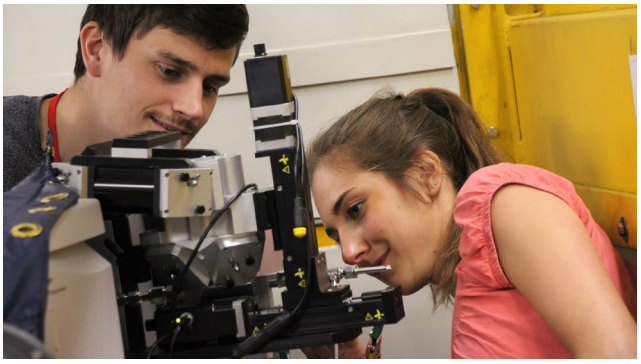
The vision of the Hub is to lead and coordinate catalytic science in the UK and to achieve the maximum impact for the field both nationally and internationally. Its physical hub in the Research Complex at Harwell will continue to be a focal point for catalysis in the UK and internationally. We will expand its highly successful series of conferences and workshops and will further promote dissemination and outreach by publication where appropriate of journal special issues and monographs. The success of the Hub structure will, however, enable a more ambitious future programme, in which we plan to give strong emphasis to the following key strategic areas:

**Career and skills development of ECR catalytic scientists**

The field is fortunate in having a large number of talented early career academic and industrial researchers. The Hub can play an important role in contributing to their skills base and where appropriate to the effective coordination of their programmes.

**Building international collaborations**

As we have noted, the Hub has a rapidly developing international profile. We now have the opportunity to build strategic partnerships particularly relating to the role of catalytic science in global challenges. Our plans include new collaborative programmes with the developing world, in view of the high relevance of catalytic technologies to several of the UN SDGs, where we will also aim to develop consortia for projects under GCRF.



**Deeper engagement with industry**

The Hub has broadened the relationship between academic and industrial catalytic science providing a basis for even stronger interactions in the future. In particular, we will work with industry to ensure that UK catalytic science is closely aligned to the Industrial Strategy.

# Community Development for Early Career Researchers

The UK Catalysis supports ECRs where our regular conference series has allowed interaction and liaison, especially for those new to the field or to the UK and where our funding streams have assisted some ECRs in developing their programmes. The Hub has supported early career researchers from eight institutions to collaborate with Hub scientists through the affiliate researcher scheme. In addition it has housed a successful team of graduate students (currently thirteen, past six) who have responded well to the scientific environment of the Harwell campus.

## UK Catalysis Hub: From small beginnings

I began my PhD at the UK Catalysis Hub in 2013, part funded by the ISIS neutron source, studying the behaviour of hydrocarbons in zeolite catalysts. To begin with it was a rather quiet place with two research fellows in Nikos Dimitratos and Peter Wells helping myself and two other PhD students (Cath Brookes and Wilm Jones) and Scott Rogers, then a Masters student. As a team, people guided and supported each other through their first beamtimes (a nerve-racking experience for anyone!), first conference presentations and the first of many publications that we're all very proud of!

The Hub then expanded rapidly with an influx of new students and post-docs, many of whom helped me so much during the earliest stages of my career, and have gone onto great success. Catalysis research also showed it was here to stay, becoming a significant part of the research output from the national facilities at Rutherford Appleton Laboratories. I'm very pleased to have contributed to that output from the ISIS neutron source.

Throughout my time at the Hub I've been offered unique opportunities for collaboration with the many groups who pass through, and are associated with the centre, carrying out studies I never thought I would. I was also given many some very special opportunities for travel both to conferences and research visits (related to zeolite science, catalysis and neutron scattering) all over the world. I also made friends for life in this group of young people "growing up" together over the 4 years of doing a PhD, and all the emotional highs and lows that can bring.

With the help and guidance of the great expertise across a range of fields (particularly from my PhD supervisor Richard Catlow, and ISIS supervisor Stewart Parker), I was able to perform experiments and publish research that I'm incredibly proud of, which lead to my being awarded a Ramsay Memorial Fellowship - a two year independent junior fellowship in chemical sciences at Cardiff University, and now my recent appointment as a Whorrod Fellow in Sustainable Chemical Technologies at University of Bath, where I now have the opportunity to start my own research group (exciting but also rather terrifying at the same time..).

I feel very lucky to have been based at the Catalysis Hub - with its resources, outstanding expertise and position as a physical base for the numerous research institutions within the Hub network. All of these made a huge difference to the quality of research I've been able to carry out, and my chances of becoming (hopefully one day!) a future leader in studying the materials and chemical phenomena that I care about the most. I look forward to keeping a very strong, close relationship with the Catalysis Hub throughout my career, for all it has done for me and for the opportunities it brings. Thank you!

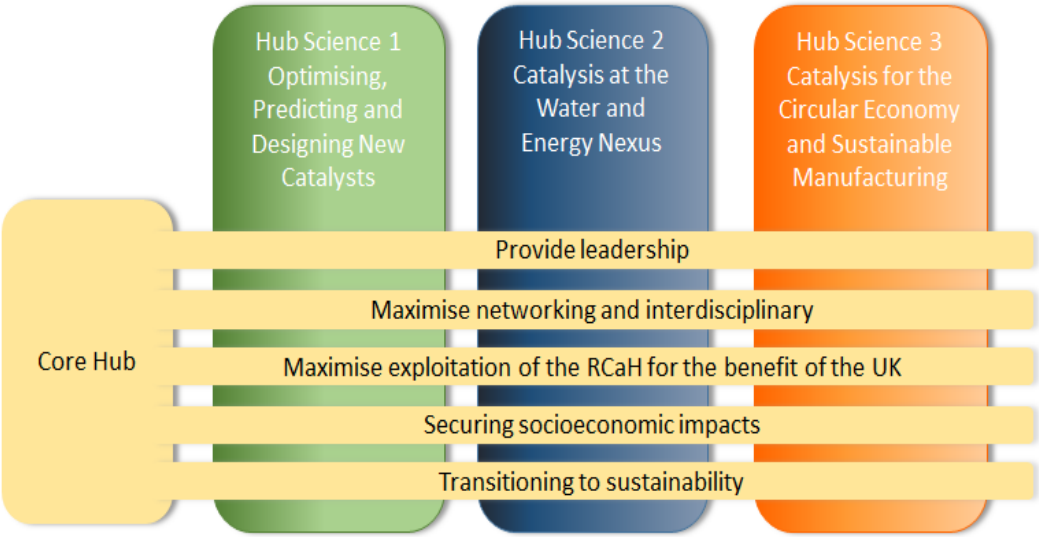

## Author:

Dr Alexander O'Malley, Whorrod Fellow, Bath

## New projects in scientific research coming with the new grant in 2018

The hub will continue to be focused around four themes coordinated by a core theme. The scientific themes are:

- Optimising, Predicting and Designing New Catalysts
- Catalysis at the Water Energy Nexus
- Catalysis for the Circular Economy and Sustainable Manufacturing




### Core

The CORE will coordinate all the Hub activities and interaction with the UK catalysis community and ensure technique development at the Harwell Hub through two science workpackages. The core programme will provide the key management and governance for the scientific programmes operated by the Hub. This will involve a matrix structure as set out in the schematic diagram, with the core programme developing and building the community; ensuring strong academic-industrial interactions and international engagement and promoting dissemination and outreach, thereby facilitating and connecting the work within the proposed new Hub Science themes (see Figure); in addition the existing Biocatalysis Theme (EP/M013219/1.) will continue until 31/03/2020 with 7 projects and the Hub Core will ensure the new themes interact fully with this existing theme. Over the next five years, the structure, programme and activities of the core component of the Hub will therefore comprise:

### High throughput and improved sample environments for catalysis at central facilities

One of the major successes of the UK Catalysis Hub has been to increase the efficient and effective use of the facilities at the Harwell campus for catalytic research. With the Diamond Light Source, through the Block Allocation Group (BAG) time on the core XAFS beamline (B18), the Hub has rapidly expanded the user base for X-ray absorption studies over the last five years. The Hub has also encouraged its network to use neutron scattering; a number of groups associated with the hub are now regular users of neutron scattering at ISIS, with a large growth in the use of quasielastic measurement for interrogating diffusion processes. In recent years, the Hub's interaction with the Central Laser Facility (CLF) has resulted in the first in situ catalytic studies being performed in the CLF. One outcome from these fruitful collaborations with the facilities on the Harwell campus, is the realisation that we are pushing the capacity of these facilities. In addition, we recognise that there is a drive for improved sample environments to push the boundaries of in situ/operando measurements. This five-year plan aims to provide high throughput sample environments for both in situ and ex situ XAFS analysis, reactive gas environments for Quasielastic Neutron Scattering and an in situ spatially resolved plug flow reactor for neutron diffraction of liquid phase heterogeneously catalysed reactions with combined liquid phase

composition analysis. Also, we will build a plug-flow reactor to be used initially in conjunction with optical microscopy platforms such as confocal and fluorescence lifetime imaging and eventually with super-resolution techniques such as SIM, STED and STORM.

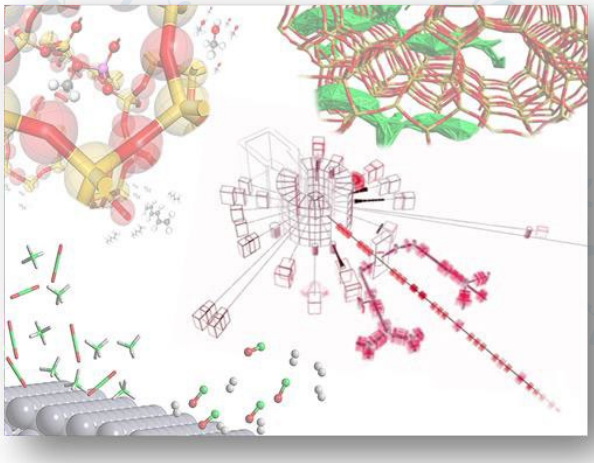
## Data analysis, processing and curation

In order to understand the nature of materials and processes relevant to catalysis and other applications, a wide range of experimental and computational simulation techniques need to be deployed and their data and information combined into single coherent models. For this to be possible the various techniques need to become more accessible to the non-experts and the data need to be recorded, combined and exchanged seamlessly. To this end, we propose to develop a Catalysis Data infrastructure and a Catalysis Research Workbench to enable further and easier exploitation of stored experimental data and assist in the characterisation or structure solution of catalytic compounds by integrating experimental and computational techniques.

## Optimising predicting and designing new catalysts

Understanding of catalysts and catalytic processes at the molecular level is vital for optimising existing catalytic processes and developing and designing new systems This theme will primarily be based on the Harwell campus and we will build on phase 1 of the UK catalysis Hub with a powerful combination of technique development around the world class facilities on the campus and with adventurous new applications embracing the full range of catalytic science and engineering. This will create a world leading programme of catalytic science and engineering, exploiting to the full the unique opportunities opened up in development of synchrotron, neutron and laser science.

## Optimising, Predicting and Designing New Catalysts



**The work packages are:**

- **Future developments in catalysis using synchrotrons;**
- **Novel applications of neutron scattering in catalysis;**
- **Future developments in catalysis using lasers;**
- **New areas and opportunities for catalysis;**
- **Integrating catalysis through cascade processes;**
- **Modelling in catalytic science;**
- **Changing the philosophy of catalysis design.**

Catalysis underpins so many of the key processes that are required for the well-being of society. Without effective catalysts life as we currently know it would not be possible. Designing new and improved catalysts is a key requirement to enable our life quality to be enriched further. Based on the initial success of the first phase of the Hub programme on design we now set out an adventurous programme in seven work packages that cover all aspects of the design of new catalysts. In line with the Hub philosophy all the work packages will utilise expertise across a wide spectrum and from several universities. The nature of the problems are such that they focus on major catalyst design problems that require the real depth and breadth of expertise we have at our disposal. The new programme will continue our successful work with major facilities with a growing emphasis on exploitation of laser facilities including XFEL technology. Computational modelling will remain a major component of our programme with new directions in modelling hybrid systems and in engaging with data curation and processing. We will also initiate new themes including exploratory high risk projects and our science will have a strong engagement with chemical engineering.

## Catalysis at the Water and Energy Nexus


**The work packages are:**

- **Treatment of High Ionic Strength Waste Water;**
- **Catalytic treatment to reduce biofouling of membranes;**
- **Energy-efficient catalytic advanced oxidation processes for water and waste water treatment;**
- **Catalytic transformations in and with water;**
- **Energy and fuels from waste water;**
- **Life cycle sustainability assessment;**
- **Modelling.**

Severe water shortages in parts of the world have been increasing over the last 20 years due to the increased usage in agriculture, changes in the climate, increases in the global population and utilisation in industrial processes and it is estimated that over 660m people do not have access to clean water. The issue of water supply is now as much of a challenge of developing more sustainable energy supplies and these are intimately linked. Catalysis is a key underpinning technology to address the issues of clean water, more efficient utilisation/valorisation of water systems and the use of water as a reaction medium or reagent. Significant research experience has been built up through the energy and environmental themes of phase 1 of the UK Catalysis Hub but without having a clear focus on water. EPSRC has recognised that there is a clear priority across government and the Research Councils in the area of water. The Hub model provides a unique opportunity to tackle this wide area through experimentation coupled with the incorporation of life cycle analysis and simulation science. The proposed work programme brings together aspects of the energy, environment and biocatalysis themes of the Hub in phase 1 into a coherent new theme which addresses the use of catalysis in the usage, valorisation and treatment of water in the chemical and energy industries. In particular it aims to provide catalytic solutions to enable energy efficient catalytic processes using water as a reagent or solvent for fine chemical production, utilisation of waste water as a resource for chemicals and fuels as an alternative to waste water treatment, increasing the efficiency of waste water treatment for produced waters from across the energy and chemical industries and, importantly, life cycle and sustainability assessment of these processes.

There is a clear link between energy and water as noted by the recent report by the US Department of Energy and the learned societies and due to changes in climate and progressive droughts across the globe, the more efficient utilisation of water has become as important as the transition from a fossil fuel based economy to one which is more sustainable. For example, significant amounts of water is used in the transformation of energy, for example, it is estimated that 1.8 L kWh-1 is required in thermal power plants and 2.5 L L-1 is used to extract crude oil. Moreover, not only is water required for energy conversion and transmission, significant amounts of energy are used to source and purify water as well as to move it and treat it for recycle. As an example, in the latter, the utilisation of solar energy for purification of waste water has been extensively studied, particularly using UV radiation, and Scientific theme 2 will address some of the disadvantages of the current approaches, including the need to use visible light, as well as employ the technology for less traditional applications.

# Catalysis for the Circular Economy and Sustainable Manufacturing

A Traditional linear approach to production and consumption (take, make, dispose) is unsustainable. New circular approaches (make, use, return) are growing in influence and importance with global economic growth and urbanisation. Advances in catalysis central to the circular concept of "*keeping the molecules in play*". Using waste $CO_2$, plastics recycle/reuse, bio-based resources, non toxic and abundant additives, and elimination of waste from processes all rely on new catalytic science.

Within industry, closed-loop, circular value chains and sustainable manufacturing are increasingly recognised as vital to future innovation and growth. So far, technical aspects of the Circular Economy have lagged behind the political capital. This new theme will put UK catalytic science and engineering at the centre of the transition to a Circular Economy. This then will use the application of catalysis in developing circular and sustainable molecules, materials and processes across the chemicals and chemistry-using industries. In particular, the seven work packages aim to provide catalytic solutions that will (in the words of Dow Chemical's Chief Sustainability Officer) "keep the molecules in play". In order to realise the circular economy, more sustainable manufacturing processes are required and there is an imperative need to develop new catalysts and catalytic processes across a diverse range of the chemicals, materials and pharmaceuticals supply chains.

**The program focuses on the following areas:**

- **New cooperative catalysts for C-C bond forming reactions from $CO_2$;**
- **Activation of C-O bonds for valorisation of bio-derived feedstocks;**
- **Using and understanding sustainable catalytic oxidation processes in flow;**
- **Earth-abundant metals in resource efficient catalysis;**
- **Keeping platform molecules in play: catalytic chemical recycling of polymers;**
- **New sustainable polymer architectures for high performance plastics;**
- **Optimising bio-based platform molecules: establishing diformyl furan as a bio-based platform for polymers**

## Pathways to Impact

The goals of developing new catalytic processes for more effective use of water and energy, waste minimisation and material reuse and reduction in gaseous emissions which are main themes of Phase 2 of the UK Catalysis Hub are strongly aligned with EPSRC's Prosperity Outcomes Framework (2016 – 2020) and will have impact in the following areas:

- **Society and Environment:** contributing towards environmental sustainability through reduced waste, increased energy and water efficiency and increased utilisation of bio-sourced materials.
- **Economic:** through increases in R&D productivity and industrial capability.
- **People:** through delivery and training of highly skilled researchers in all areas of catalytic science and engineering.
- **Outreach and Engagement:** contribute to dissemination of the new methodologies and processes developed to the academic and industrial communities and increased public awareness and understanding of the scientific, engineering, economic and societal issues associated with catalytic processes.

To maximise the impact of Phase 2 of the UK Catalysis Hub project we have identified key objectives and deliverables for each area that will be monitored closely by the management group and reported to the external advisory board and industrial advisory panel who will also advise on impact activities. Impact is an integral part of the project and will be managed by the project manager (Josie Goodall) who will spend 25% of her time on developing these activities in conjunction with the management group. In addition, each RA will spend 5% of their time on impact activities and advocacy for Central facilities techniques and their application to catalysis. The timeline for the pathway to impact and the related deliverables are included on the workplan.

**Society and environment** – Objective: Development of catalytic processes which will lead to advances in sustainable manufacturing and efficient use of water and energy leading to greener and cleaner processes and products, improving the well-being of those employed in the relevant sectors and the general populations who are affected by the environmental impacts of the energy, water and manufacturing sectors.

**Economic – Objective**: To increase productivity of catalysis based R&D and to implement new catalytic processes to address sustainable manufacturing, for example, in an industrial setting.

**People – Objective:** To deliver the new generation of highly skilled researchers in catalytic science and engineering

**Outreach and Engagement** - Objective: Inclusive approach to improve visibility of the proposed research amongst the wider research community and engage with the general public to promote benefits to the whole community.

### More Information:

Please visit our website at www.ukcatalysishub.co.uk or contact the project coordinator to be added to Hub emails, to contribute news articles, research highlights, events, details of talks and publications.

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