

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.



“Over the past five years The Catalysis Hub has provided a successful and effective network for catalytic science in the UK, which has engaged the majority of the UK community and has advanced this key field of science both nationally and internationally. It has coordinated and developed the UK Catalysis community; it has established strong and enduring interactions with UK industry; and it is now widely known and recognised internationally.”
~ Graham Hutchings

Events Highlights of 2018

50 years of Synchrotron Radiation in the UK and its global impact 26 - 29 June 2018

The UK Synchrotron Radiation community led by the DIAMOND light source and Science and Facility Technology Council (STFC) decided to hold a major conference to mark the ‘50 years of Synchrotron Radiation in the UK and its global impact’ and asked Professor Samar Hasnain (Max Perutz Professor of Molecular Biophysics, University of Liverpool) and Professor Richard Catlow, FRS (Foreign Secretary of the Royal Society) to be the joint Chairs. This major conference was held in Liverpool in June 2018 attracting 175 speakers and delegates from 13 countries (Australia, Brazil, Canada, France, Germany, India, Japan, Netherlands, Spain, Sweden, Switzerland, UK and the USA).

Speakers included 12 Fellows of the Royal Society,

members of the US national academy of sciences, Chairman of the STFC, a Nobel prize winner and the President of the Royal Society.

The Ken Seddon OBE, Student Poster Prize was given to Ellie Dann, iCASE, UK Catalysis Hub.

Catalysis Hub Summer Conference 2018



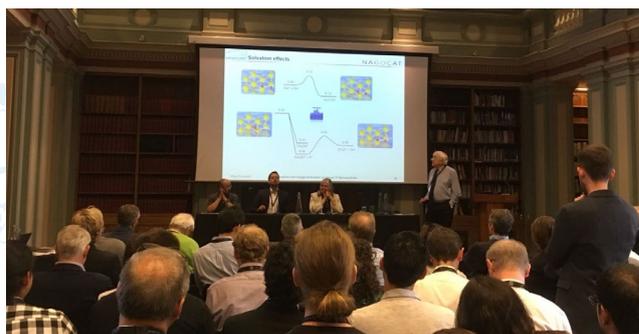
Our Summer Conference on the 19 - 20 June 2018 was attended by over 160 scientists and engineers across the breadth of catalysis; heterogeneous, homogeneous and bio, bridging the disciplines of chemistry engineering and biology.

There were many informative and entertaining talks and presentations. Speakers included: Prof. Andrew Weller (Oxford), Prof. Helen Hailes (UCL), Dr. Pawel Plucinski (Bath), Dr Natalie Fey (Bristol), Dr. Antoine Bucharth (Bath), Dr. Jeremy Titman (Nottingham), Dr. Stephen Mansell (Heriot-Watt University), Dr. Thomas Farmer (York), Prof. John Blacker (Leeds), Dr. Arthur Garforth (Manchester), Prof. Valentine Ananikov (Zelinsky Institute of Organic Chemistry), Prof. Ben Davis (Oxford).

The first day finished with a busy poster session, ECR networking session and conference dinner. The ECR networking event on the 19th June provided the opportunity for early career scientists involved in the UK Catalysis Hub to interact and establish networks with a variety of professionals from a range of sectors related to scientific research at a career workshop. Dr. Victoria Richards, Dr. Philip Bennett, Dr. Rebecca Melen and Dr. Katie Renouf kindly led the workshop sessions with discussions into their careers in academia, patent law, editing and fire investigations.

Posters were presented by: Tamsin Bell, Dr. Sofia Diaz-Moreno, Dr. Charlie Fehl, Yunhu Gao, Dr. Alex Grigoropoulos, Dr. Michael Higham, Dr. Zhigang Hu, Dr. Hasan Tanvir Imam, Dr. Patricia Marce Villa, Clare F. Megarity, Giorgio Morello, Dr. Yaroslav Odarchenko, Dr. Mary Ortmayer, Dr. Bruno Pinho, Dr. Sumesh Kureppadathu Raman, Dr. Scott Rogers, Dr. Kevin Vincent, Lei Wan, Dr. Constantinos D. Zeinalipour-Yazdi and Liyun Zhang. During the conference dinner Dr. Andrew Bourne, Associate Director, Universities, EPSRC spoke about the future of funding for the sciences sector and the importance of collaboration in driving it forward.

Faraday Discussion - Designing Nanoparticle Systems for Catalysis 16 - 18 May 2018



Nanoparticles are ubiquitous in many heterogeneous catalysts and the Faraday Discussion focussed

on concerning key aspects of their synthesis characterisation and use. The discussions explored the modern methods being used to design, synthesise and characterize nanoparticles and how these bridge across the disciplines of physical science and chemical engineering. The core aim of this discussion meeting was to develop a fundamental understanding of these crucial aspects of catalytic science, especially relating to nanoparticle synthesis and its use in catalytic reactions, knowledge of which is essential for the design of new catalysts.

The event was attended by 124 scientists from a broad spectrum of backgrounds and experience levels. Delegates came from Belgium, Brazil, China, Denmark, France, Germany, India, Israel, Italy, Japan, Latvia, Netherlands, Russian Federation, Singapore, South Africa, South Korea, Spain, Sweden, Turkey, UK and USA.

A poster session took place with Miss Julia Pimonova, Southern Federal University, Russian Federation and Mr Said Said, University of Oxford winning poster prizes.

Rideal Conference 2018



The Rideal Conference took place on the 26th – 28th March 2018. The event was attended by over 60 scientists and engineers across the breadth of catalysis; heterogeneous, homogeneous and bio, bridging the disciplines of chemistry engineering and biology. Attendees traveled from a number of countries to attend the meeting including; Belgium, Germany, Italy, Greece, Japan, The Netherlands, Switzerland and the USA.

There were many informative and entertaining talks and presentations. Plenary speakers included: Joris Thybaut (Ghent), Wataru Ueda (Kanagawa), Gianfranco Pacchioni (Università Milano-Bicocca), John Woodley (DTU) and Angelika Brückner (LIKAT Rostock).

This year there were three poster prizes awarded to Dr. Santhosh Kumar Matam, Mr. Charan Kuppili and Dr. Ines Lezcano-Gonzalez. The prizes given were a year's subscription to the Reaction Chemistry & Engineering journal, a year's subscription to the Molecular Systems Design & Engineering journal,

a year's subscription to the Catalysis Science & Technology journal courtesy of the RSC and a £50 Amazon voucher courtesy of Finden Ltd.

The first day finished with a busy poster session and the second with a conference dinner sponsored by Johnson Matthey at The Crown & Thistle, Abingdon. At the dinner Professor Martyn Twigg spoke about the great influence of Sir Eric Rideal on the development of catalysis.

Papers from the last "Rideal Conference" were published in Topics in Catalysis (Editors-in-Chief Freund and Somorjai), 2016, Volume 59, issue 8 -9 <https://link.springer.com/journal/11244/59/8/page/1>. This will be repeated for Rideal 2018 and the paper will be published in Topics in Catalysis based on the conference and with kind collaboration of Springer.

The Catalysis Hub sponsored the accommodation and travel for the plenary speakers. Twigg Scientific & Technical Ltd kindly provided the conference USB sticks containing a digital version of the program and Springer sent along some journals.

UK Catalysis Conference 2018



The fourth UK Catalysis Conference took place at Holywell Park, Loughborough over 3rd - 5th January 2018. The meeting was an opportunity for catalytic scientists and engineers from across the UK's academic and industrial communities to interact and network over the whole spectrum of Catalysis ranging from Organocatalysis, Biocatalysis, Homogenous catalysis and Heterogeneous catalysis with over 190 registered participants.

The UKCC 2018 featured 4 plenary talks and 72 oral presentations as well as 47 posters covering a wide range of catalytic science. In addition, there were two additional themed symposiums entitled "Polymerisation Catalysis" and "Dial-a-Molecule: Catalytically".

Plenary speakers included: Adrian Mulholland (Bristol University, UK), Louise Olsson (Chalmers University of Technology, Sweden), Moniek Tromp (University of Amsterdam, Netherlands) and Karen Wilson (RMIT University, Melbourne, Australia).

There were four poster prizes given to: Martin Chan - Chemical Looping Epoxidation of Ethylene, Arron Deacy - Heterodinuclear Catalysts of the form

LZnMXn for use in polymerization catalysis, Andrew Hall - Insights into Homogeneous Catalysis by FlowNMR Spectroscopy and Terri-Louise Hughes - Total Neutron Scattering of Aromatic Sorbates in ZSM-5.

The conference was very grateful for sponsorship for the event from the IChemE, RSC, Quantachrome UK, BP, Avantes, GPE, MI micromeritics, STREM Chemicals Ltd, Springer, SciMed, Dial-A-Molecule, Hiden Analytical, Johnson Matthey, Sabic, Catalysis Science & Technology Journal and supported by the UK Catalysis Hub.

International Conferences & Visits:



A UK Russia Seminar on Catalysis that was held in Moscow on 24-28 September. The seminar aimed to address the key problems facing society at present and to identify areas of catalysis where a much deeper scientific collaboration can be set up going forward. This was followed up with Professor Valentine Ananikov, Zelinsky Institute of Organic Chemistry visiting the UK for the UK Catalysis Hub Summer Conference and a visit to the Cardiff Catalysis institute.



Prof Bowker gave a Plenary at the 3rd Syngas Convention in Cape Town, South Africa in March 2018 on the Hub work on CO₂ conversion to methanol entitled "*Methanol Synthesis from Syngas derived from Fossil Fuels or Renewables*" and also at The Mason Symposium, Stanford University, California in May 2018 "*Much Ado about Methanol: the pivotal role of methoxy and formate in methanol synthesis*"

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. Read more about ECR experiences at the UK Catalysis Hub over the following pages.



Investigating molecular diffusion in porous solids using quasielastic neutron scattering (QENS)

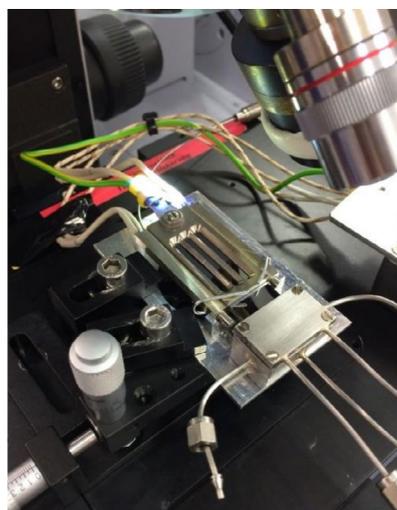
In 2015 I joined the ISIS Neutron and Muon Source after leaving my hub-funded UCL postdoctoral position at the Research Complex at Harwell. I now work as an instrument

scientist within the molecular spectroscopy group, pursuing my own research and helping visiting users of ISIS from universities and industry. A major part of my role within the hub was to encourage and facilitate neutron experiments throughout the Catalysis Hub collaboration. This provided me with a broad experience of neutron techniques across many instruments at ISIS and the Institut Laue-Langevin in Grenoble. In many ways my role has not changed, and I continue to collaborate with hub members, predominantly investigating molecular diffusion in porous solids using quasielastic neutron scattering (QENS). This low energy spectroscopy was introduced to me during my time with the Catalysis Hub, and illustrates the benefits of being located on the RAL campus. Easy access to experts in neutron and x-ray techniques facilitates data interpretation and ensures efficient exploitation of the facilities, using both familiar and previously unappreciated techniques.

Working in the Research Complex was a great way to meet people and learn about their science. People are constantly visiting so you get to pick up on trends and talk to all kinds of researchers. It doesn't always lead to natural collaborations but it does make for an interesting place to work. I've been interested in the development of methods to allow *operando* spectroscopy which provides information from the active phase of the catalyst as it is working since my Ph.D. It's really the only way to be sure that the measurement is relevant. During my time at the hub I built silicon microreactors that allowed

IR spectroscopy under elevated temperatures and pressures in collaboration with the Gavriilidis group at UCL.¹ The small volumes required make these reactors inherently safer and allow greater flexibility in control of the reaction. The spectroscopy proved challenging, but the approach of bringing an analytical tool to an optimised reactor, rather than designing a compromised reactor suited to measurement is the gold standard for *operando* measurement. This thread continues at ISIS and I recently measured the diffusion of propane in ZSM-5 pores whilst in equilibrium with a flowing gas phase using QENS.² This is the first time that QENS has been reported measuring an adsorbed gas phase in equilibrium with a flowing gas and opens up a range of possibilities for *in situ* measurement. A new niobium sample holder was developed and this has since been used by Catalysis Hub members for their experiments. Expanding the range of conditions that are possible to achieve increases the problems that can be addressed and I hope to continue helping to solve problems for catalytic science.

1. I. P. Silverwood, N. Al-Rifai, E. Cao, D. J. Nelson, A. Chutia, P. P. Wells, S. P. Nolan, M. D. Frogley, G. Cinque, A. Gavriilidis, and C. R. A. Catlow, *Rev. Sci. Instrum.*, 87 (2016) 024101
2. I. P. Silverwood and V. García Sakai, *Chem. Eng. Sci.*, 186 (2018) 116-121



Silicon microreactor in preparation for measurements on the IR beamline at Diamond Light Source

Author:

Dr Ian Silverwood, ISIS Neutron and Muon Source



The UK Catalysis Hub: Beamtime memories

I joined the Hub team at Harwell in September 2013 as one of the first batch of Hub PDRA's in phase 1 of the enterprise, and spent an enjoyable four years there. The time in the Hub gave me the chance to learn new techniques, work with a bunch of different people and on a wide variety of projects. It was a fantastic experience. The open discussions in the office from science to politics, between professors, PDRA's and students alike was a breath of fresh air!

I worked on two main projects, firstly developing a combined XAFS-DRIFTS set up for operando studies of catalytic reactions, secondly, using XAFS to characterise catalysts *in situ* during non-thermal plasma hybrid catalytic reactions.^{1,2} These projects let me gain experience in new techniques and also work with different groups in the UK, mainly UCL, QUB and Manchester. Learning X-ray Absorption Spectroscopy was a main focus of my time and so many sleepless nights were spent (and will no doubt continue to be spent) on B18. Working on side projects, I also got to do some time at ISIS and the Central Laser Facility. All those sleepless nights will no doubt stand me in good stead over the next few months.

Helping out on the BAG, then stepping in as PI for the last two years has been a fantastic experience, not just the involvement in papers, which has definitely helped my career, but the exposure to a wide variety of chemistry projects and learning how to organise the chaos has been invaluable. Also, the people I had the chance to work with, from professors to students, has given me a great network of friends and colleagues. The camaraderie is something else, I'll treasure all the beamtime memories, from working on some of the most dangerous experiments you could imagine to raking through the bin for samples I'd accidentally thrown out and that crazy drive to the Swiss Light Source.

My time in the hub and the great people I've worked with has been a fantastic help in my career, and in no small way has helped me gain my current position. I moved back to Scotland in August 2017 to start a three year Lord Kelvin Adam Smith Fellowship in the School of Chemistry at the University of Glasgow. It is great to be home, but I hope to keep in touch and continue working with many of those I met during my time in the Hub.

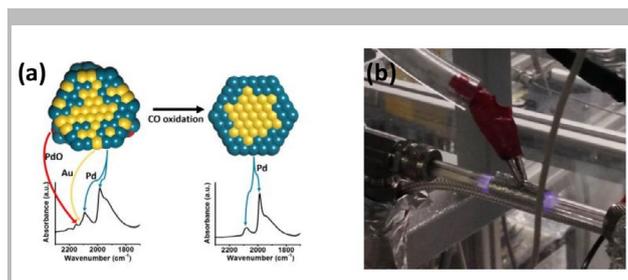


Fig 1 (a) Results from the XAFS-DRIFTS study on AuPd/Al₂O₃ under CO oxidation, (b) non-thermal plasma-catalytic hybrid reactor set up used to study CH₄ oxidation over Pd/Al₂O₃.

References:

1. E. K. Gibson, A. M. Beale, C. R. A. Catlow, A. Chutia, D. Gianolio, A. Gould, A. Kroner, K. M. H. Mohammed, M. Perdjon, S. M. Rogers, and P. P. Wells, *Chem. Mater.* (2015) 27, 3714–3720
2. E. K. Gibson, C. E. Stere, B. Curran-McAteer, G. Cibir, Diego Gianolio, A. Goguet, P. P. Wells, C. R. A. Catlow, P. Collier, P. Hinde, C. Hardacre, *Angew. Chem. Int. Ed.* (2017) 56, 9351-9355



Author:

Dr Emma Gibson, LKAS Research Fellow, University of Glasgow

Understanding Catalysts and Catalysis

Mastering the design and preparation of new materials to out-perform existing catalysts is a widespread ambition amongst scientists researching catalysis. It requires new basic knowledge to control the chemical phenomena occurring at the catalyst/reactant interface during the catalytic turn-over. The application of *in situ* techniques at synchrotrons and other large-scale facilities, together with computational approaches, have made significant contributions to the current scientific landscape. I became fascinated by this research line very early in my career and made it my primary interest. My aim is to contribute to fundamental scientific knowledge that can help solve the energy challenges mankind is facing nowadays. Currently I am a beamline scientist at DLS and my membership in the UK Catalysis Hub has been pivotal for producing impactful research outcomes.

As an example, I have recently carried out research aiming to electro-reduce carbon dioxide, a well-known greenhouse gas, into more valuable molecules. In a previous study¹ I found that the reactivity of Fe oxides can be tuned by the interaction with the carbon support such that it catalyses the C-C coupling, which is one of the biggest challenge in the CO₂ reduction. It was therefore natural to dig deeper into the structural features that cause the selectivity of the catalyst towards the C2 rather than the C1 product or the parasitic hydrogen evolution reaction (HER). Sandra Krick Calderon, a DLS visiting PhD student from FAU Erlangen-Nürnberg in Germany, prepared the samples for this project directly on site, using the catalysis hub laboratory facilities. The samples were first characterized *ex situ* by means of X-ray absorption near edge structure (XANES) spectroscopy at the B18 beamline of DLS within the BAG proposal call followed by *in situ* spectroscopic measurements. Through this work, which involved a

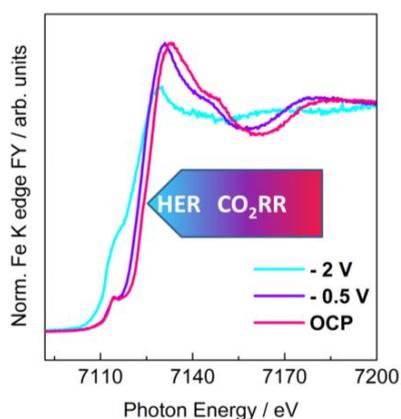


Figure 1: Fluorescent Yield-mode Fe K edge XANES spectra of carbon supported ferrihydrite at different potential during cyclic voltammetry. The edge shift reveals the redox chemistry involved in the activation and selectivity changes. More details on this study are in ref. [2].

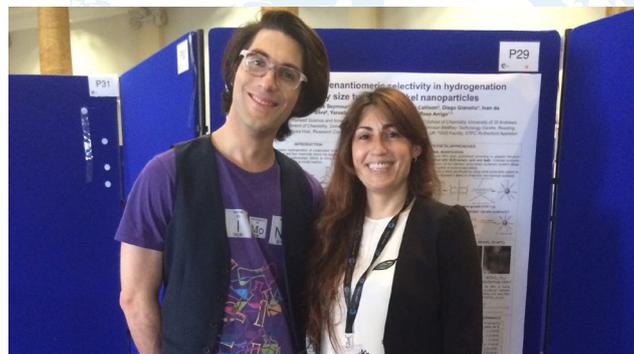


Figure 2: Simone Gallarati (left) and Rosa Arrigo (right) presenting their poster at the Faraday Discussion: “Designing Nanoparticle Systems for Catalysis” held in London on May 2018.³

large team of scientists, it was possible to clarify the nature of the Fe sites responsible for the C-C coupling as well as the structural transformation that leads to the change in selectivity (Fig 1). This is a major scientific breakthrough, which was published recently.²

In collaboration with Prof. Georg Held, many DLS visiting students from the University of Reading have benefited from the UK Catalysis Hub facilities for sample preparation, off-line samples characterization and also catalytic testing. Alex I. Large and Jake Seymour have received great support from the team there (June Callison, Josie Goodall, Garth Harris, Sadie Primmer) to develop various skills across the multidisciplinary field of catalysis. Simone Gallarati’s project “Tailored synthesis of Ni nanoparticles for enantiomeric selective hydrogenation” (Fig 2) was a project carried out at DLS as part of its one-year industrial placement programme. The vicinity of the UK Catalysis Hub to DLS has sped up the process of producing important results, which were recently presented at the Faraday Discussion on “Designing Nanoparticle Systems for Catalysis”.³ This top class environment offers a unique experience for students and PDRAs to learn and become the next generation of scientists.

References:

- [1] R. Arrigo, M. E. Schuster, S. Wrabetz, F. Girgsdies, G. Centi, J-P. Tessonnier, D. S. Su, R. Schloegl, *ChemSusChem*, 2012, 5, 577-586.
- [2] C. Genovese, M. E. Schuster, E. K. Gibson, D. Gianolio, V. Posligua, R. Grau-Crespo, G. Cibin, P. P. Wells, D. Garai, V. Solokha, S. Krick Calderon, J. Velasco Velez, C. Ampelli, S. Perathoner, G. Held, G. Centi, R. Arrigo, *Nature Communications* 2018, 9, doi:10.1038/s41467-018-03138-7. [Included in the editor highlights and featured as behind the paper].
- [3] R. Arrigo, A. Logsdail, L. Torrente-Murciano, *Highlights from Faraday Discussion on Designing Nanoparticle Systems for Catalysis*, London, UK, May 2018, *Chemical Communications*, 2018, DOI: 10.1039/C8CC90324G.

Author:

Dr Rosa Arrigo, BLB07 Beamline Scientist, Diamond Light Source



The UK Catalysis Hub: Developing research skills

My involvement with the UK Catalysis Hub started with my employment as a core post-doctoral researcher within environment theme in 2013. Over the following 4 years I had the opportunity to be involved in several research programs that focussed on novel synthesis of heterogeneous catalysts utilising supercritical fluids and ionic liquids. These research programs, as is the nature of research within the catalysis hub, involved many different collaborators from a range of UK academic institutions. In addition, I was able to take advantage of the unique opportunities provided by the research complex at Harwell and its proximity with UK central facilities, such as Diamond Lightsource and ISIS neutron source. Consequently, I have been able to develop skills in a range of advanced catalyst characterisation studies such as X-ray absorption spectroscopy and elastic and inelastic neutron techniques in tandem with knowledge on catalyst synthesis and design.

Along with many valuable research skills, the UK catalysis hub has provided a great opportunity to build friendships and collaborations with experts in catalyst characterisation, synthesis and theoretical modelling. The biannual meetings along with the UK Catalysis Conference has provided me with an opportunity to interact with the broader catalysis community and open my eyes to a range of different existing research.

A consequence of these opportunities has been several publications (including; Nature, 2016, 531, 83 and Science, 2017, 355, 1399) and presentations at conferences (including; Faraday Discussions Designing New Heterogeneous Catalysts and Catalysts for Fuels) that I am very proud of and that have help advance my career in academia. One particular example of studying single-site Au catalysts by in situ x-ray absorption spectroscopy (see Figure) exemplifies the collaboration between catalyst design, advanced characterisation and complimentary theoretic calculations enabled by

the UK Catalysis Hub.

To date, I am an author on 46 journal publications and 2 international patents. In October 2017 I took up a position as Lecturer in Inorganic Chemistry at Loughborough University and have spent the last year has been spent developing teaching skills and building the foundations of a research program. I remain interested in studying catalyst synthesis and characterisation, particularly the evolution of metal nanoparticles from parent oxide structures and the local structure and catalytic properties of promoters and poisons. Collaborative research grants and studentships through Diamond Lightsource and the Royal Society have seen me boarding my research interests into energy storage and photoactive materials. My involvement with the UK Catalysis hub remains strong with regular visits to the research complex and Diamond Lightsource in addition to being part of the steering group. I look forward to being part of the continued success of the UK Catalysis Hub.

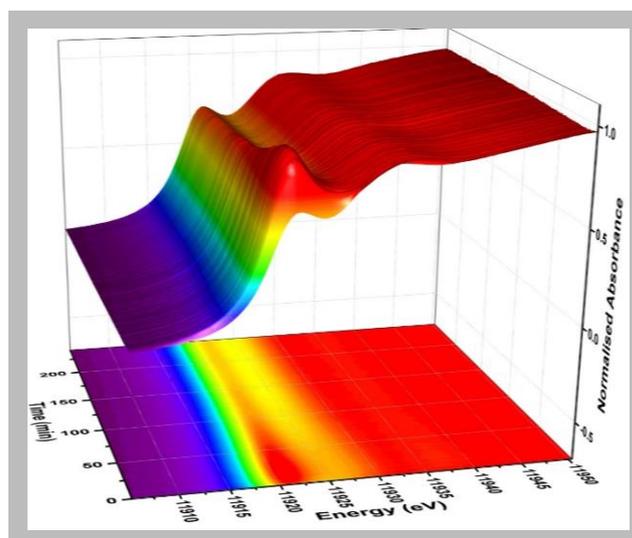


Figure 1: Change in XANES of Au/C catalysts during reaction: An example of successful research with the catalysis hub

Author:

Dr Simon Kondrat, Lecturer in Inorganic Chemistry, Loughborough University



A journey into understanding catalytic processes using electronic structure calculations

I joined the UK Catalysis Hub (UKCH) on the 19th September 2013 as a research associate and remained there until the 31st January 2018. I thank Prof. C. Richard A. Catlow for his invitation to work with him at the UKCH because of which I had the opportunity to explore the exciting avenues of heterogeneous catalysis. I especially appreciate the numerous stimulating scientific discussions, which we had at Research Complex at Harwell, or during my visits to University College London and Cardiff University. During my stay at the UKCH, the main area of my study involved understanding catalytic processes on metal and metal oxide surfaces using electronic structure calculations. The fundamental aspects of these studies such as chemical bonding, electron transfer phenomenon and the mechanisms of chemical reactions on catalyst surfaces greatly fascinated me.¹⁻⁵

The unique research environment at the UKCH strongly encourages the early career researchers to engage in collaborative projects and discuss science with other researchers based in different institutes and universities across the UK and abroad to explore challenging ideas. As a computational chemist, it also gave me the wonderful opportunities to not only employ quantum mechanical tools to understand how catalysts work at the atomic level, but also to join my experimental friends and colleagues to perform experiments at the ISIS Neutron and Muon Source. In this regard, our studies on the interaction of organic molecules on metal surfaces for example formate species on the low index copper surfaces using Density Functional Theory (DFT) and Inelastic Neutron Spectroscopy (INS), in collaboration with Dr. Ian P. Silverwood and Dr. Stewart F. Parker, is worth mentioning (Figure 1). In several other studies my experimental colleagues and I worked closely together to explore many other interesting topics, which I truly loved working on.

The four and half years of my stay at the UKCH was one of the best times of my research career and the afternoon tea/cake times (Figure 2), the friendly discussions in the office or over a dinner/lunch in the pubs in Oxford, Abingdon and/or Chilton village will remain some of the most beautiful memories of my life. The UKCH gave us the opportunities to not only work very closely with many renowned scientists but also to meet very good friends who over the time became my close collaborators. I strongly believe that the exposure, which I received during this period played a crucial role in making my next stop at the School of Chemistry, University of Lincoln as a senior lecturer. I eagerly look forward to interacting further with scientists at UKCH and working closely on interesting projects in the very near future.

References:

- (1) Phys. Chem. Chem. Phys. 2017, 19, 27191
- (2) Faraday Discussion 2018, 2018, 123
- (3) Surface Science 2016; 653, 45
- (4) ACS Catalysis 2017, 7(4), 2266
- (5) Chem. Comm. 2016, 52(14), 2897.

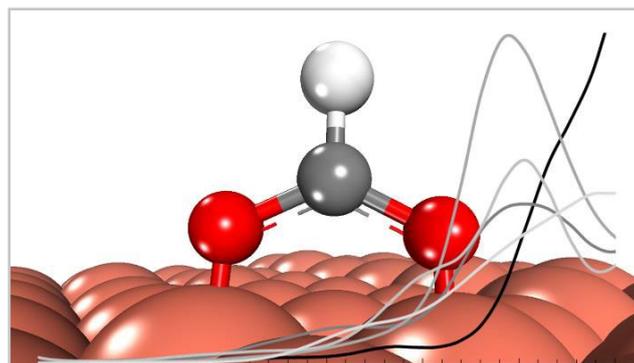


Figure 1. A graphical abstract of our study on the interaction of formate species on low index copper surfaces. (Ref: Surf Sci. 2016, 653, 45.)

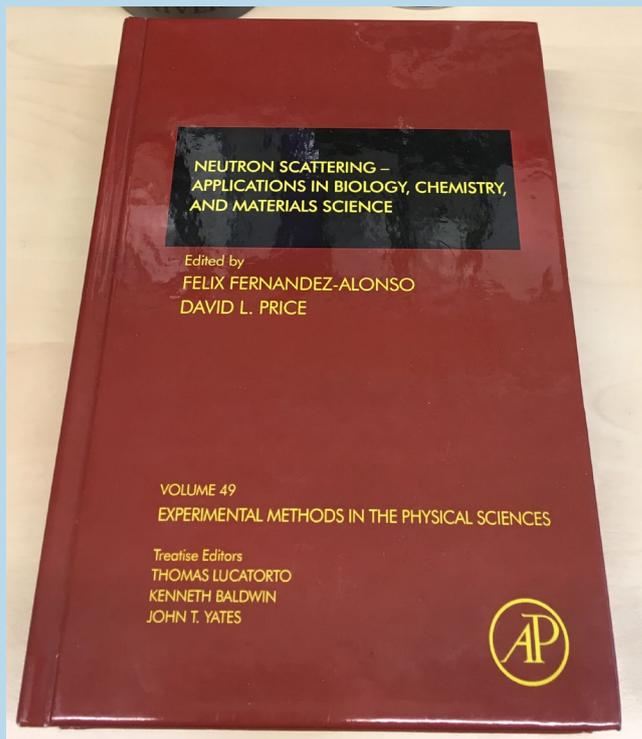


Figure 2. During a cake/coffee break at the UKCH.

Author:

Dr Arunabhiram Chutia, Senior Lecturer, Molecular SurfChem Group, School of Chemistry, University of Lincoln

Publications:

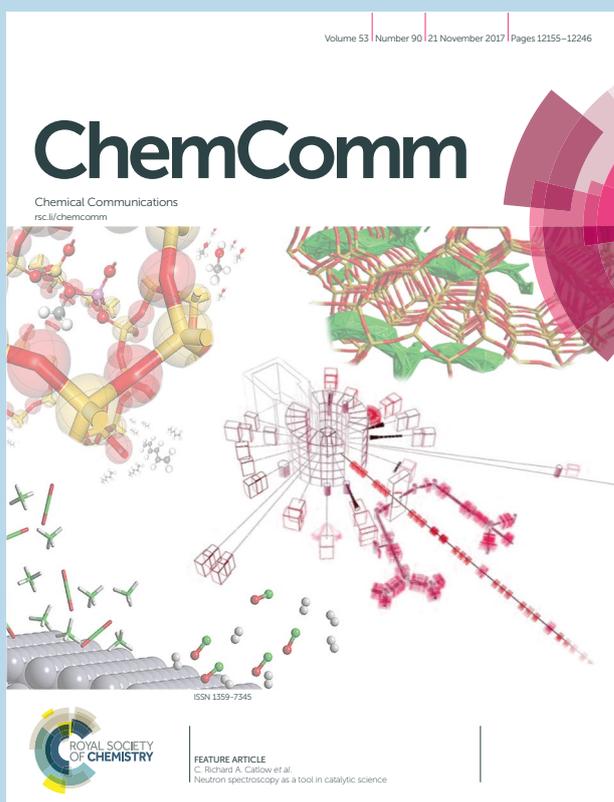


Cover image: This article was published in *Neutron Scattering – Applications in Biology, Chemistry, and Materials Science*, Felix Fernandez-Alonso and David Price, Eds. (Volume 49 in *Experimental Methods in the Physical Sciences*), ISBN 9780128053249, Academic Press, 2017

Neutron Scattering – Applications in Biology, Chemistry and Materials Science Book

In Collaboration with Johnson Matthey, ISIS Neutron and Muon source and the catalysis community the UK Catalysis Hub spearheaded the publication of a special issue of PCCP on “Neutron scattering in catalysis and energy materials” (*Phys Chem Chem Phys* 18, 2016) which was edited by UK Catalysis Hub scientists (Silverwood, Parker and Catlow).

Following from this the UK Catalysis Hub has collaborated to publish a book titled, “Neutron Scattering – Applications in Biology, Chemistry and Materials Science”. The book provides an in-depth examination of the applications of neutron scattering in the fields of physics, materials science, chemistry, biology, the earth sciences, and engineering, looking at advances in instrumental, experimental and computational techniques over the past quarter-century. The book includes contributions from Prof. Richard Catlow and Dr Alexander O’Malley.



Cover image: Alex O’Malley
Published by The Royal Society of Chemistry

Neutron spectroscopy as a tool in catalytic science

An article was published in the *Chemical Communications* journal co-authored by Dr Alexander O’Malley, Dr Stewart Parker and Prof Richard Catlow on neutron spectroscopy and the role of these techniques in advancing the field of catalysis. There is a brief introduction to the basic principles of the techniques and then the authors discuss their use in the study of three key catalytic systems: the behaviour of hydrocarbons confined in zeolite catalysts; the methanol-to-hydrocarbons process; and methane reforming. They demonstrate the importance of neutron spectroscopy in understanding established catalytic processes, but also consider its role in the design of future catalytic systems.

The article titled, “*Neutron spectroscopy as a tool in catalytic science*” was published in *Chem. Commun.*, 2017,53, Pages 12164–12176 , DOI: 10.1039/C7CC05982E.

Publications cont:

Directed aqueous-phase reforming of glycerol through tailored platinum nanoparticles

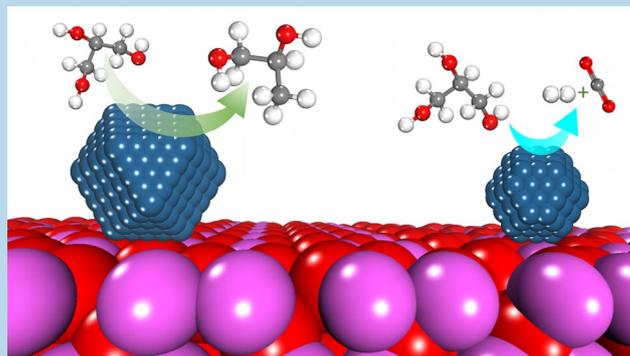
An article was published in *Applied Catalysis B: Environmental* authored by members of the UK Catalysis Hub including; J.Callison, N.D.Subramanian, S.M.Rogers, A.Chuti, D. Gianolio, C.R.A. Catlow, P.P.Wells, N.Dimitratos.

Highlights include:

- Demonstration of how Pt NP size can be tuned by changing the temperature of colloidal reduction.
- The influence of Pt NP size on the selectivity profile of the APR of glycerol.
- Mechanistic insight into reaction pathways and the influence of Pt NP size.

Sustainable technologies require both renewable feedstocks and catalysts that are able to direct their conversion to specific products. They establish a structure-activity relationship for the aqueous phase reforming of glycerol over 2% Pt/Al₂O₃ catalysts, whereby the reaction pathway can be controlled to produce either hydrogen or 1,2-propanediol as the main product. Using the colloidal synthesis method, the reduction temperature was altered to produce Pt nanoparticle catalysts supported on Al₂O₃ with varying Pt particle size. The catalytic activity of the samples for the APR of glycerol resulted in a higher conversion of glycerol (34%) for the larger Pt particle size of ~ 3.5 nm, producing the liquid 1,2-propanediol as the major product with a yield of 12.5%, whereas smaller particles of ~ 2.2 nm gave hydrogen as the main product (5.5% yield). This work demonstrates how the APR of glycerol can be tuned to yield both valuable liquid and gas products using tailored Pt nanoparticles.

The article was published in *Applied Catalysis B: Environmental*, Volume 238, 15 December 2018, Pages 618-628, <https://doi.org/10.1016/j.apcatb.2018.07.008>



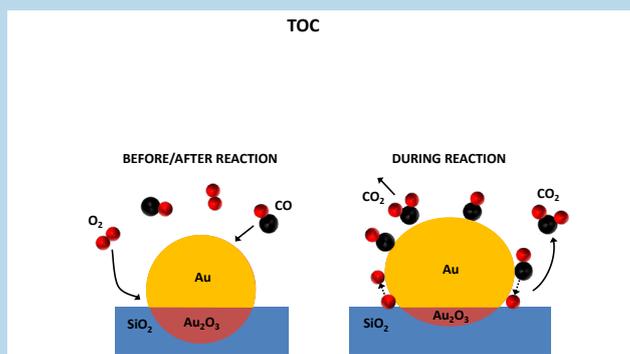
Graphical abstract: Suggested sites for differing reaction pathways in the APR of glycerol by Dr Arun Chutia

CO oxidation over supported gold nanoparticles as revealed by operando grazing incidence X-ray scattering analysis

An article was published in *Faraday Discussions part of the Designing Nanoparticle Systems for Catalysis collection* authored by Yaroslav Odarchenko, David J. Martin, Thomas Arnold and Andrew M. Beale

The mechanism of carbon monoxide oxidation over gold was explored using a model planar catalyst consisting of monodisperse gold nanoparticles periodically arranged on single crystal SiO₂/Si(111) substrates using a combination of Grazing Incidence Small Angle X-ray Scattering and Grazing Incidence X-ray Diffraction (GISAXS/GIXD) under reaction conditions. It is shown that nanoparticle composition, size and shape change when the catalyst is exposed to reactive gases. During CO oxidation, the particle's submergence depth with respect to the surface decreases due to the removal of gold oxide at the metal-support edge, meanwhile the particle 'flattens' to maximise the number of the reaction sites along its perimeter. The effect of the CO concentration on the catalyst structure is also discussed. Results support the dual catalytic sites mechanism whereby CO is activated on the gold surface whereas molecular oxygen is dissociating at the gold-support interface.

The article was published in *Faraday Discuss.*, 2018,208, 243-254, DOI: 10.1039/C8FD00007G



Graphical abstract:

Call for new projects

Call for Business Interaction Vouchers (BIV) funding

Introduction

The aim of the UK Catalysis Hub Business Interaction Vouchers scheme is to encourage and support those initial steps towards collaboration between academic partners and industrial partners within the UK Catalysis Hub Networks.

It is expected that the vouchers will help resource small, confidence-building measures between an academic partner and an industrial based partner with the view that they will deliver more significant future outcomes – for example:

- A longer-term relationship
- Improved interaction
- New research technology transfer projects

Eligibility

Either partner – industry or academic – can initiate the application but funds will only be paid to the academic partner. Conversely, academic partners need an industry partner who is contributing either in cash or in-kind to the same value as the requested BIV in order for the application to be eligible.

Value

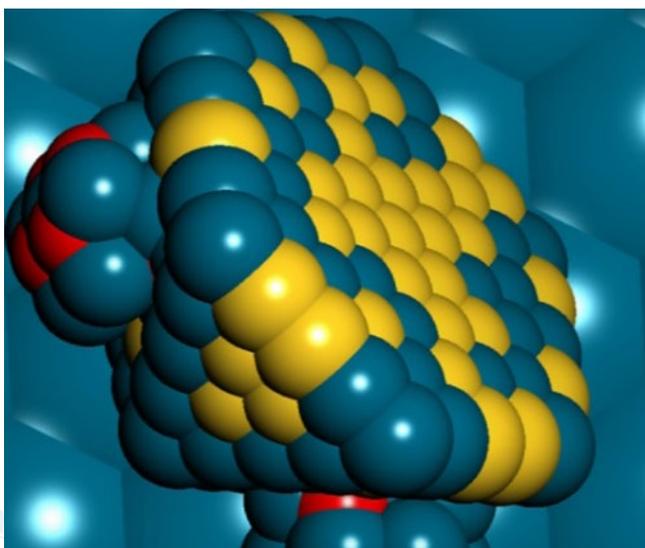
Vouchers can be requested up to the value of £10,000, including VAT, but can be for smaller amounts – as required by the objectives and type of the interaction.

Example activities for BIV

This is by no means an exhaustive or prescriptive list but example activities that would be likely to be supported when combined in a well-defined short term project are:

- Short term visits to learn how process/equipment works
- Short term visit for training purposes – either academic to industry or vice versa
- Short term data gathering and/ or analysis – especially if it is being done to support a future proof of concept proposal
- Meeting or series of meeting to discuss areas of technical overlap/ collaboration/ establish specific challenge areas
- More specific technology transfer activities/ sharing of information and expertise to address specific technical challenges

For more information visit www.ukcatalysishub.co.uk/interaction/Business_Interaction_Vouchers_BIV



The Catalysis Hub is keen to offer support to research proposals that are complementary to the scope of the UK Catalysis Hub programme. Please contact us, via the management group, at the earliest possible stage in proposal development so that we can work with you to ensure that any support we offer is fully integrated and meaningful. This may not be possible at a late stage.

Upcoming Events

STFC B4I Chemical Event by The Knowledge Transfer Network

17 October 2018
Centre for Process Innovation, Wilton,
TS10 4RF

Bridging for Innovators (B4I) Funding Now Available to Support UK Industry in Boosting Productivity: Chemical Industry Roadshow

About the Funding: Bridging for Innovators (B4I) is a programme run by STFC* to support UK industry to overcome challenging product, manufacturing or process performance. Accessing unique laboratories and engaging with world class researchers, you will develop projects that address your specific challenge and help you make a step-change to your business.

Why should you attend?

- Discussing your challenge with world leading scientists
- Understand how to access leading edge

research infrastructure

- Hear government strategies, grand challenges and funding opportunities for the chemical industry
- Networking with other chemical companies
- Facility tour at CPI's state of the art facilities (see uk-cpi.com)

Who should attend?

Companies who need to overcome challenging problems that restrict their potential productivity and competitiveness

Technical and Business development staff

Lead Scientists

Engineers involved in the chemicals or process industries sector.

Visit for the event website <https://www.eventbrite.co.uk/e/stfc-b4i-chemical-event-registration-49082052741> for the full agenda and more information.

International Winter School on INNOVATIVE CATALYSIS AND SUSTAINABILITY

7 -11 January 2019
Bardonecchia, Torino, Italy

The International Winter School on INNOVATIVE CATALYSIS AND SUSTAINABILITY, organized by the Group of Catalysis (GIC) of the Italian Chemical Society in collaboration with the European Federation of Catalysis Societies (EFCATS), that will take place in Bardonecchia (Torino, Italy) from 7th to 11th of January 2019.

The School is addressed to young researchers (PhD students and post-docs) working in the field of catalysis. It will be organized as an informal forum for discussing the latest advances and the future of the field. Focus will be on the current scientific, social and economical challenges of the catalytic community in the current strive to move from fossil fuels to a more renewable-energy driven society, through the prism of 5 pivotal molecules that are at the roots of many current production routes: hydrogen, ammonia, methane, olefins/biomass and carbon dioxide.

The School venue is Bardonecchia 'The Queen of the Piedmont Alps', which was the protagonist of the Winter Olympics in Turin 2006, hosting the

snowboard races and one of the Olympic villages. Taking advantage of the beautiful location and programme schedule attendants will have the opportunity to get together, discuss their cutting edge research among peers and mentors and enjoy Bardonecchia ski resort and winter sport facilities.

Highlights:

- Lectures by international scientists
- Groups activity on soft skills
- Poster and Q&A sessions
- Contest on communication/dissemination skills
- Round table: "The role of catalysis in the new society" with invited members from major Editorial boards from Journals in catalysis
- Free time every day for open-air activities

Key dates:

Registration: October 15th

Early payment: November 2nd

For more information, please refer to the School website:

www.nis.unito.it/ics2019/index.html



UK Catalysis Conference 2019 (UKCC)

9 -11 January 2019
Holywell Park,
Loughborough,
Leicestershire

The meeting will provide an opportunity for catalytic scientists and engineers from across the UK's academic and industrial communities to interact and network over the whole spectrum of Catalysis ranging from Organocatalysis, Biocatalysis, Homogenous catalysis and Heterogeneous catalysis.

The scientific programme will be organised around the following all aspects of catalysis: Organo/Biocatalysis, Heterogeneous Catalysis, Homogeneous Catalysis and Engineering.

We are pleased to announce that our plenary speakers in 2019 will be Nora de Leeuw (Cardiff University, UK), Sabine L Flitsch (University of Manchester, UK), Andreas Jentys (Technical University of Munich, Germany) and Freek Kapteijn (Delft University of Technology, Netherlands).

Please note that the early bird registration fee will be £410 for PDRA, Academic, Industry & Government registrations and £340 for PhD student and Emeritus registrations. The deadline to register with the earlybird

registration price will be Friday 9th November. Following this the price will be £480 and we will not be able to guarantee on-site accommodation (although accommodation will still be included).

The conference registration fee includes the conference, two nights accommodation at nearby Burleigh Court (including breakfast and dinners), the abstracts, coffee/tea, lunches and access to the lectures and poster session. Accommodation will be arranged for participants upon registration by the UKCC team. The conference registration fee includes the conference, two nights accommodation at nearby Burleigh Court (including breakfast and dinners), the abstracts, coffee/tea, lunches and access to the lectures and poster session. Accommodation will be arranged for participants upon registration by the UKCC team.

A number of bursaries of £100 for early career researchers, excluding PhD students, are available to assist with participation in the UKCC2019. These will be awarded to staff within 10 years of the award of their PhD and will be prioritised by the researcher giving an oral presentation then a poster presentation in registration date order.

Abstract submission is now available with a final deadline for submission of 30th September 2018, 23:59.

Visit <http://events.manchester.ac.uk/event/event:e4y-jhjab6we-q9k8yc/uk-catalysis-conference-2019> for more information and to register.



Catalysis: Fundamentals and Practice Summer School 2019

15 - 19 July 2019
University of
Liverpool, UK

On-line registration is now open for the next EPSRC/Liverpool Summer School in Catalysis with the support of the EPSRC, the UK Catalysis Hub and the SURCAT groups of the RSC.

The Summer School will:

- Provide an introduction to the fundamental aspects of catalysis
- Broaden and update the knowledge base in catalysis.
- Describe some of the frontier developments occurring in catalysis today.
- A forum for discussion and the formation of new professional contacts.

Topics:

- Basis of Catalysis and Chemical Engineering
- Sustainability and renewables
- Catalysis in Bio-Tech
- Discovery
- Process Development
- Catalysts
- Catalyst Characterization

REDUCED REGISTRATION FEE FOR PHD STUDENTS

Applications must be received before 31st May 2019.

For more information visit the website:

www.liverpool.ac.uk/chemistry/events/catalysis-summer-school-2019

Future Publications

Acknowledgements

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

“UK Catalysis Hub is kindly thanked for resources and support provided via our membership of the UK Catalysis Hub Consortium and funded by EPSRC (grants EP/K014706/1, EP/K014668/1, EP/K014854/1EP/K014714/1 and EP/M013219/1)”

When publishing work performed at the Research Complex please also include the following text (replacing X and 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 Coordinator of all Publications arising from Hub Projects.

Stay in Touch:

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

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