

# 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.



### Events Highlights of 2019

Royal Society Discussion: Science to enable the circular economy  
24 - 25 June 2019

Scientific discussion meeting organised by Professor Matthew Davidson, Professor Richard Catlow FRS, Professor Adrian Mulholland and Professor Graham Hutchings CBE FRS. For society to be sustainable, realising circular flows of molecules and materials will be fundamental to delivering the circular economy. This meeting brought together scientists and engineers to highlight efforts to meet the formidable challenge of 'keeping the molecules in play' by addressing important global challenges such as using waste carbon dioxide, harnessing biotechnology and eliminating plastics pollution. Meeting papers will be available in a future issue of Philosophical Transactions of the Royal Society A.

"The last year has been a highly successful first year of phase II of the Catalysis Hub and has demonstrated the reach and impact of UK catalytic research. The coming months will be more difficult given the challenges of the Covid-19 virus. Meetings are moving online and research projects may be delayed; however, we will continue as much as possible to develop the Hub's plans and activities. One of these is the new call for proposals and we hope that you are gearing up for the submission of a new tranche of exciting projects."  
~ Professor Christopher Hardacre, Director

UK Catalysis Hub – FELIX: Free Electron lasers for the Catalysis Community  
18 July 2019



The FELIX facility in Nijmegen, the Netherlands is based on a suite of free electron lasers (FELs) that

generate high-intensity, ultrashort pulses of widely tunable radiation. The facility has numerous end-stations covering a wide array of scientific experiments as well a space for user-provided kit to be installed. The FEL light properties can be altered and optimised to match individual experiments and the facility operates in a reliable and professional manner, providing strong hands-on user support. EPSRC supports the use of the facility by UK scientists via a National Research Facility grant and supports new users of the facility via the FLUENCE grant. Catalysis has been identified as one of the potential areas where new activity on FELIX might flourish. FLUENCE is investigating the potential of, and need for, a UHV Catalysis end-station. FLUENCE would like to identify scientists who might benefit from such a facility.

The meeting provided the catalysis community with an opportunity to learn about the; Accelerator Driven Light Sources for the UK community, The FELIX Facility, FLUENCE: Facilitating access for UK scientists to FELIX, Opportunities with, and limitations of, IR and THz Lasers at RAL, FLUENCE Catalysis and AstroScience Initiative, Laboratory Surface Astrophysics at FELIX and Bridging the gap between catalysis and facilities.

Speakers included; Prof. Peter Weightman, University of Liverpool, Dr B. Redlich, Radboud & FELIX, Dr. Michele Siggel-King, University of Liverpool, Prof. Mike Towrie, CLF, Prof. Martin McCoustra, Heriot-Watt University, Dr. Sergio Ioppolo, Queen Mary University London and Dr. Andrew Beale, UCL & Harwell.

### Clean Transport, 9 October 2019



The third UK Emission Control Workshop took place on the 8-9th October at the Research Complex in Harwell, Oxfordshire. The programme included an interactive workshop with an open forum for technical discussion about the current challenges facing the automotive industry and experts from industry and academia came together to share knowledge and ground-breaking technologies with colleagues from around the UK. Topics included; research and the challenges of future regulation in a multi-pronged approach, investigating advanced

combustion regimes, alternative fuels, and next-generation emissions control technology.

### Plastics - Water Industry Event, 23 October 2019

The UK Catalysis Hub organised a joint event with KTN for the water industry held in Manchester. The meeting took place to bring together experts from the UK Catalysis Hub, UK academics, UK water utility companies and members of KTN in water research. The event focussed on the challenges that water companies face in treating water and wastewater: to see where there are commonalities and what outliers might exist in certain regions and catchment areas in the UK. There was much discussion of the research in the UK Catalysis Hub and UK, the issues facing water companies, challenges and future perspectives on possible solutions. The event also featured a lively brainstorming session to generate new research ideas. It was a very successful event and the UK Catalysis Hub aims to roll out similar events to other sectors next year.



### Reactive Plasmonics Meeting, November 2019

Although photosynthesis underpins life on earth, photochemical technologies are yet to make an impact on our modern lives. Meanwhile photovoltaics is a mature and successful industry that shares a common theme with photochemistry – both rely on energetic electrons and holes; in the former to generate electrical power and in the latter to drive redox reactions. The EPSRC funded Reactive Plasmonics Project, led by King's and Imperial, explores the science of hot carriers generated by light absorption within metals and semiconductors. Remarkably, metals sustain electrons and holes at temperature of many thousands of degrees Kelvin, while the host material remains near ambient conditions. This phenomenon activates a variety of thermodynamically unfavourable electronic and chemical processes with applications in photodetection, sensing and catalysis. The UK Catalysis Hub and Reactive Plasmonics Group held a joint workshop to try to find synergies between the two research areas. The programme included presentations from the Reactive Plasmonics project members and Prof. Richard Catlow, a tour of the facilities and interactive breakout sessions

on Photocatalysis and CO<sub>2</sub>, Reaction Pathway, Particle Size or different scales in catalysis and plasmonics. Throughout the day there was much discussion about possible areas of interaction and collaboration between the academic groups.

UKCC 2020, 7 - 9 January 2020



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

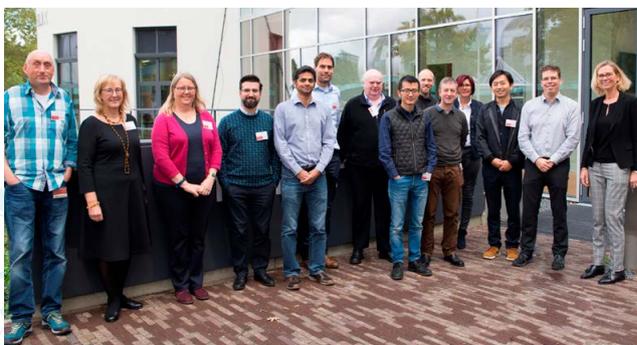
The conference was attended by over 200 delegates including academics, industrial researchers, experimentalists, theoreticians, and students.

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.

#### International Conferences & Visits:



The 3rd FLUENCE Workshop at FELIX took place from the 1st - 2nd October 2019 in FELIX, Nijmegen, the Netherlands. FELIX, HFML and Radboud staff and FLUENCE members came together to the workshop on the new FELIX facilities. The day

included: facility talks from the FELIX and High-Field Magnet Laboratory, a tour of FELIX and High-Field Magnet Laboratory, scientific talks: highlights from FELIX and Magnet Lab, discussions on ideas for the facility with experts from FELIX, access to FELIX and FELIX staff & users and a dinner on the Monday evening. UK Catalysis Hub member Andrew Beale from UCL gave a talk on Structure-activity relationships in catalytic materials; an interest of the UK Catalysis Hub.



Recently Professor Brent Melot, from the University of Southern California, spent a three-month sabbatical visiting the UK Catalysis Hub. Prof Melot's group is interested in elucidating design principles for the development of new functional materials. His solid-state materials chemistry group has worked extensively on magnetoelectric multiferroics, Li-ion batteries, and photovoltaics, but used this research visit to expand a nascent project on heterogeneous catalysts. In particular, the Melot group has been studying the catalytic properties of transition metal phyllosilicate clays. The layered topology of these materials makes them interesting model catalysts because the crystallites adopt sheet- or scroll-like morphologies in a highly reproducible way, which limits the number of exposed facets and potential active sites.

Prior to visiting the Hub, Melot had limited formal training in the characterization of heterogeneous catalysts. During his visit, he spent time learning how to perform temperature-programmed desorption experiments to characterize the Lewis acid/base character of the phyllosilicate clays and how to accurately model the materials using DFT calculations. Being able to interact with world-class experts in both experiment and computation was a primary reason for Melot to visit the Hub for this stay. By the end of his visit, Melot and the group of Richard Catlow had determined that the phyllosilicates show activity for CO<sub>2</sub> reduction under fairly mild conditions. This collaboration is ongoing, with Melot providing samples to Catlow's group to further evaluate the selectivity and conversion of the catalysts and inelastic neutron scattering experiment planned for early 2020.

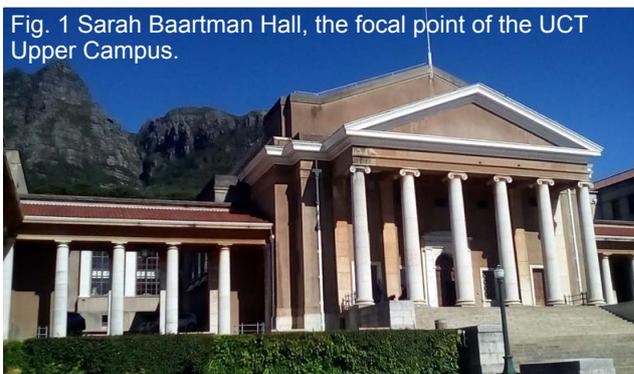


Fig. 1 Sarah Baartman Hall, the focal point of the UCT Upper Campus.

### Dr. Michael Higham Report on visit to the University of Cape Town - START Project

From 05/11/2019 to 19/12/2019, Michael Higham, a postdoctoral researcher in computational catalysis (Cardiff University), visited the University of Cape Town to forge new collaborations with Prof. Michael Claeys and his research group. The GCRF START project, which is supporting Michael's research, intends to promote closer cooperation between researchers in the UK and across Africa on ambitious research projects that will enable valuable contributions to be made towards solving real-world problems, especially those of concern to developing nations. Research exploring new catalytic technologies for clean fuel, such as CO<sub>2</sub> conversion to methanol, and Fischer-Tropsch synthesis to convert CO to hydrocarbons, are particularly active fields of research within the START Energy Materials community, addressing challenges in both alleviating the impact of pollution from fossil fuels, and paving the way towards more sustainable fuels by enabling CO<sub>2</sub> recycling. Such technologies are especially attractive to developing nations where existing infrastructure can be more easily adapted to enable widespread use of sustainable liquid combustion fuels, compared to electricity generated from clean, renewable sources, which requires significant new infrastructure investment.



Fig. 2 View facing South-East across Cape Town from the UCT Upper Campus; the Helderberg Mountains are visible in the background.

As part of his secondment, Michael was able to attend the 15th C\*Change Symposium, held from 08/11/2019 to 10/11/2019 at the Krystal Beach Hotel, at Gordon's Bay, near Cape Town. The C\*Change group, of which Prof. Claeys is director, is a Centre for Excellence in

Catalytic Research, supported by the South African Department of Science and Technology and the National Research Foundation of South Africa. Based at the UCT Department of Chemical Engineering, C\*Change comprises three main areas of research, all of which being connected to both environmental challenges and issues specific to South African industries: syngas conversion, paraffin activation, and olefin valorisation. Researchers in Prof. Claeys' group form part of the syngas conversion community, with many of the projects underway overlapping with Michael's current projects investigating copper-based catalysts for CO<sub>2</sub> conversion to methanol, thus providing a broad scope for collaborative experimental and computational studies.



Fig. 3 View facing West from UCT accommodation at Forest Hill; Devil's Peak, at the North-East end of the Table Mountain range, is clearly visible.

During his secondment, Michael worked with UCT researchers Dr. Mohamed Fadlalla, Dominic de Oliveira, and Christopher Mullins, starting two new projects that will combine computational modelling studies with detailed experiments to provide valuable insights into two different systems. The first project, in collaboration with Dominic, concerns that origin of experimentally observed adsorption-induced magnetisation changes in Ni particles under Fischer-Tropsch synthesis conditions; it is intended that the complementary computational studies will reveal which adsorbates are responsible for the corresponding observed magnetisation changes, and a qualitative model linking these changes to adsorbate surface coverage will be developed. The second project, in collaboration with Mohamed and Christopher, concerns the activity and selectivity of bimetallic alloy transition metal catalysts for CO<sub>2</sub> hydrogenation; it is intended that the computational studies will provide rational explanations for experimentally observed catalyst selectivity and will provide valuable insights into the relation between the alloy surface structure and composition, and observed activity.

These latest projects represent a part of the next chapter in a long history of collaboration between UK and South African researchers, and it is hoped that this international partnership between catalytic communities will result in scientific discoveries that offer solutions to global problems, applicable to both developing nations and the wider community.

### Author:

Dr. Michael Higham, UK Catalysis Hub

## 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 Willinton Yesid Hernández Enciso: Development of time-resolved Kerr-gate Raman spectroscopy for studying the evolution of molecular species in catalytic processes with lasers**

I received my PhD in Chemistry from the University of Seville (Spain) in 2010, working on the design and characterization of heterogeneous catalysts for the Preferential Oxidation of CO in presence of hydrogen (PROX reaction), under the supervision of Prof. José Antonio Odriozola and Dr. Miguel Ángel Centeno.

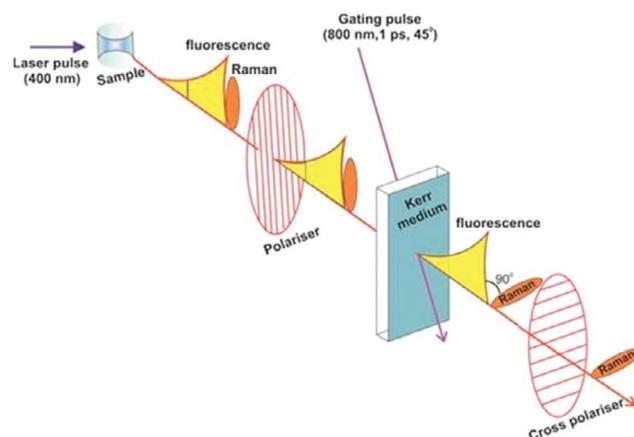
Since my PhD I have had the great opportunity to explore different research topics (for instance: diesel-exhaust-gas treatment, catalytic oxidation, hydrogen generation, biomass valorisation, among others), always focussed on the rational design and preparation of heterogeneous catalysts, as well as the establishment of relevant structure-to-activity relationships. This professional and life adventure has given me the opportunity to work and learn in diverse research teams and institutions, including IRCELYON (in France), ICIQ (in Spain) and Ghent University (in Belgium). In addition, during the last three years I worked as a Research Scientist for the chemical company, Solvay, in the research center located in the city of Shanghai, China. This last job experience allowed me to understand a bit better about the research needs and demands associated to the investigation and development in the chemical industry context.

Since February 2020 I joined the UK Catalysis Hub as PDRA associated to Cardiff University, under the supervision of Prof. Richard Catlow and Prof. Andrew Beale. In this new role I will be involved in the utilization of laser-related techniques (especially the so-called Kerr-gated Raman spectroscopy) as a dynamic characterization tool for interrogating catalysts under operation conditions. To me, this is a wonderful opportunity to explore in more detail the application of In situ and Operando spectroscopic characterization techniques, and to learn and interact with highly skilled

and recognized researchers on this topic.

Examples of research published:

1. J.P. Zhao, W.Y. Hernández, W.J. Zhou, Y. Yang, E.I. Vovk, M. Capron, V. Ordonsky, Selective Oxidation of Alcohols to Carbonyl Compounds over Small Size Colloidal Ru Nanoparticles. *ChemCatChem*, 12, (2020), 238.
2. D. Wu, W.Y. Hernández, S. Zhang, E.I. Vovk, X. Zhou, Y. Yang, A.Y. Khodakov, V.V. Ordonsky, In Situ Generation of Bronsted Acidity in the Pd-I Bifunctional Catalysts for the Selective Reductive Etherification of Carbonyl Compounds under Mild Conditions, *ACS Catal.*, 9, (2019), 2940.
3. W.Y. Hernández, D. Lopez-Gonzalez, S. Ntais, C. Zhao, A. Boréave, P. Vernoux, Silver-modified manganite and ferrite perovskites for catalyzed gasoline particulate filters, *Appl. Catal. B*, 226, (2018), 202.
4. W.Y. Hernández, J. Lauwaert, P. Van Der Voort and A. Verberckmoes, Recent advances on the utilization of layered double hydroxides (LDHs) and related heterogeneous catalysts in a lignocellulosic-feedstock biorefinery scheme, *Green. Chem.*, 19, (2017), 5269.
5. W.Y. Hernández, K. De Vlieger, P. Van Der Voort, A. Verberckmoes, Ni-Cu hydrotalcite derived mixed oxides as highly selective and stable catalysts for the synthesis of  $\beta$ -branched bioalcohols by the Guerbet reaction, *ChemSusChem*, 9, (2016), 3196.
6. W.Y. Hernández, A. Hadjar, A. Giroir-Fendler, P. Andy, A. Princivale, M. Klotz, A. Marouf, C. Guizard, C. Tardivat, C. Viazzi and P. Vernoux. Electrochemically-assisted NO<sub>x</sub> storage-reduction catalysts, *Catal. Today*, 241, (2015), 143.



Scheme 1. Schematic representation of Kerr-gated Raman spectroscopy setup (adapted from Central Laser Facilities website <https://www.clf.stfc.ac.uk/Pages/Kerr-Gated-Raman-Spectroscopy.aspx>). This technique allows the collection of high-quality Raman spectra while suppressing the undesired background associated to fluorescence.

### Author:

Dr. Willinton Yesid Hernández Enciso, UK Catalysis Hub

## UK Catalysis Hub Phase II - Facilities and equipment list

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. See our equipment list below.

### 1. Spectroscopy

#### a. DRIFTS Setup



Diffuse Reflectance Infrared Fourier Transform

Spectroscopy is an infrared technique ideal for research on catalyst surfaces. It allows the chemical and structural evaluation of all types of solid surfaces (including non-transparent, highly absorbing

materials, coatings and roughened surfaces).

An infrared beam focused onto a fine particulate material can interact with it in several possible ways. It can be absorbed, reflected from the surface or penetrate the particles before being scattered. Diffuse reflectance results from the penetration of the incident radiation into one or more particles and subsequent scattering from the sample matrix.

The advantages of DRIFTS over conventional FTIR methods include the following: (i) DRIFTS is fast and non-destructive since the sample can be analysed as is or in powdered form, (ii) It is well suited to the analysis of strongly absorbing materials which are characterized by very low signals and sloping baselines when investigated in transmission mode, (iii) It requires little or no sample preparation.



Our Drifts setup consists of an Agilent Cary 680 FTIR spectrometer with an MCT detector, gas delivery system, a Harrick reaction chamber with high pressure dome, a Praying Mantis

Diffuse Reflection Accessory and a Hiden Analytical mass spectrometer. The sample is filled (either pure or mixed with an IR transparent matrix (e.g. KBr)) in a sample cup and placed inside the reaction chamber. The IR beam is directed into it by the Praying Mantis accessory, a highly efficient diffuse collection system

which minimizes the detection of the specular component. The IR radiation interacts and is reflected off the surfaces of the particles, resulting in the light being diffused or scattered as it moves through the sample. This scattered energy is directed to the detector in the spectrometer by the output mirror. The altered IR beam is recorded by the detector as an interferogram, which is then used to generate a spectrum.

#### Specifications

The specifications listed below are the limits of the instrumentation. These are dependent on several factors including gases used, type of windows and O-rings and conditions such as vacuum.

- Temperature: RT – 910°C
- Pressure: 10<sup>-6</sup> Torr – 34 bar
- Gases available: He, N<sub>2</sub>, Ar, H<sub>2</sub>, 10% O<sub>2</sub>, 10% CO, 10% CH<sub>4</sub>, 10% NH<sub>3</sub>
- Organic liquid injection using heated lines

#### b. The da Vinci arm



The da Vinci arm is a unique articulated opto-mechanical accessory designed for analysing samples outside the sample compartment.

The sampling head is configurable for diffuse and specular reflectance.

It facilitates a small sampling spot size, which allows analysis with high spatial resolution.

The optics involved in the working of the da Vinci arm is as follows: the optics in the sample compartment directs the IR beam through the arm to the sampling spot which is some sample, the light reflected back from the sample is directed towards the detector. Our Da Vinci arm is principally used for measurements with x-rays in conjunction with IR.

**c. Dewar Transmission / Reflection Accessory Cell**



The transmission cell (Harrick cell) allows for transmission-mode measurements of solid samples at between  $-196^{\circ}\text{C}$  –  $350^{\circ}\text{C}$  in a controlled environment and is ideal for the investigation of catalytic and other solid-gas chemical reactions.

The cell is made from 316 stainless steel, with a Dewar incorporated into the accessory for low temperature operation. Gases can be flown through the cell and it can be used with vacuum down to  $10^{-6}$  Torr. It is equipped with low voltage heaters for heating the sample.

The cell can also be reconfigured for near-normal ( $12^{\circ}$ ) specular reflection with a Variable Angle Reflection Accessory.

**d. Gas Cell**



This is a temperature-controlled cell which can be used for both static and flow applications. It is made of stainless steel, is thermally isolated and has a path length of 10 cm. The maximum operable temperature of

the cell is defined by the o-ring material. O-rings available with us include Kalrez (Temperature limit  $260^{\circ}\text{C}$ ) and viton (Temperature limit  $260^{\circ}\text{C}$ ).

**e. Linkam Cell**



The Linkam Cell is designed to study catalytic reactions at high temperature and pressure. The cell works in reflectance mode. The samples are mounted on ceramic

fabric filters placed inside a ceramic heating element, capable of heating samples from room temperature up to  $1000^{\circ}\text{C}$  very quickly, up to 5 bar pressure. The stage body is water cooled to keep it at safe temperature.

The cell can be used with a variety of gases, including corrosive gases. Lid windows made of several different materials can be used to adapt the cell to brightfield and Raman microscopy techniques as well.

**f. Agilent MP-AES**



The Agilent MP-AES 4100 is a benchtop microwave plasma atomic emission spectrometer based on a robust magnetically excited microwave plasma

excitation source. It is used for simultaneous multi-analyte determination of major and minor metal. MPAES employs microwave energy to produce a plasma discharge, which eliminates the need for sourcing gases in remote locations.

Atomized sample passes through the plasma, promoting the electrons to excited state. Light emission from the electrons is directed to a wide range, low noise CCD detector, measuring the intensity of each emission line and background simultaneously while providing excellent detection limits and precision.

The instrument in the Catalysis Hub is set up to run inorganic and organic samples with general detection limits between  $\sim 100$  ppb – 10%, depending on element.

Along with the MP-AES, an Anton Paar Multiwave 3000 is available for digestion of solid samples. Generally, samples are digested using Aqua Regia at temperatures and pressures up to  $310^{\circ}\text{C}$  and 115 bar.

**2. Reactors**

**a. Parr Flow Reactors**



Continuous flow reactors permit easier automation of sequential and parametric changes in temperature, flow rate and time. The amount of product hence is a function of time and not the size of the reactor, thus increasing safety since only small amounts of materials are present at any given time.

They also bring about improved mixing and heating, and as a result, higher selectivity. They are used in a variety of industries and applications. Their length to diameter ratio can be varied to study the effect of catalyst bed length.

The Catalysis Hub has 2 flow reactors with a gas delivery system allowing a mixture of up to 3 gases with flow rates up to 100ml/min each. Liquid feed can also be pumped in using an HPLC pump. Reactions can run at up to 600°C and 69 bar. The outlet of the reactors can be connected to either GC or GCMS for inline analysis. A liquid catch pot with chiller is also used to trap out water and low boiling point products for further analysis.

#### b. Parr Stirred Batch Reactors



Parr's high pressure stirred batch reactors are microreactors designed to provide as many features of larger vessels as possible in the limited space available. They are ideal for liquid phase reactions involving expensive materials and materials with limited availability. They are also useful when hazardous

materials are involved in the reaction and there is the need to limit the reactants or products to a minimum for safe waste disposal.



They can be easily converted from one size to another by simply exchanging the cylinder and corresponding fittings.

The Catalysis Hub has 3 batch reactors two 50ml and one 100ml that can be operated up to 200 bar and 350°C. A liquid sampling valve is incorporated to allow samples to be taken throughout the reaction time.

#### c. Catlab



The CATLAB system is a modular benchtop analysis system for comprehensive in-situ catalyst characterization, kinetic and thermodynamic measurements. The system is designed for both isothermal and temperature programmed studies of catalytic systems. The system consists of (i) a CATLAB microreactor module, which is a fast response, low thermal mass furnace, and (ii) a

Hidden Analytical QIC-20 dynamic sampling mass spectrometer, which is a compact benchtop gas analysis system for continuous analysis of gases and processes at pressures up to atmosphere.

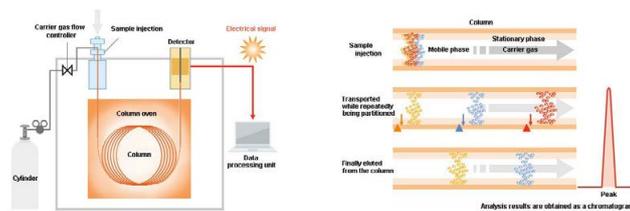
The CATLAB uses Gas Adsorption Chromatography to directly determine metal surface areas for metals. It also allows the determination of surface coverages as a function of temperature and calculate the resulting adsorption isotherms. It can also be used to study energetics, kinetics and reaction mechanisms of catalytic systems using temperature programmed techniques up to 1000°C.

The system has an integrated pulse valve to allow pulsed chemisorption studies, 8 flow channels with varied flows between 3 – 500 ml/min and is suitable for use with corrosive gases.

### 3. Chromatography

#### a. Gas Chromatography

Gas chromatography is an analytical technique applicable to gas, liquid and solid samples, thus offering the possibility to separate and quantify each component of a mixture of compounds. Typically, the sample solution is injected into the instrument, wherein it is transported into a column (separation tube) by a gas stream (carrier gas). The various components are separated inside the column. The detector measures the quantity of the components that exit the column. While measuring a sample with an unknown concentration, a standard sample with known concentration first is injected into the instrument. The data obtained enables the identification and quantification of the components present in the sample.



#### b. Agilent GCMS

The Agilent 7890A GC System is a state-of-the-art gas chromatograph that provides superior performance for all applications. Its performance is defined by the use of advanced electronic pneumatic control (EPC) modules and high-performance GC oven temperature control. Each EPC unit is optimized for its intended use with a specific inlet and detector option. The GC oven temperature control of the 7890A oven allows for fast and precise temperature ramping. The overall thermal performance provides optimal chromatography including peak symmetry, retention time repeatability, and retention index accuracy. The combination of precise pneumatic

and temperature control leads to extremely precise retention time reproducibility, which is the basis for all chromatographic measurement. Agilent's proprietary Capillary Flow Technology provides reliable, leak free, in-oven capillary connections that stand up to repeated GC oven cycling over time. provide gains in productivity and data integrity for routine analyses via 2-dimensional heart cutting, detector splitting, and column back flushing. It also has advanced built-in capabilities to monitor system resources (counters, electronic logs and diagnostics).

The system at the Catalysis Hub includes MS, FID and TCD detectors to allow a wide range of analysis. Incorporated vici valves allow the system to be used for online testing combined with our flow reactors.

#### 4. ChemBET



The Quantachrome ChemBET pulsar is an automated flow chemisorption and reactivity analyser.

The chemisorption of reactive gases such as CO, hydrogen etc. on the catalysts depends on the formation of chemical bonds between the surface

atoms of the solid and the gas molecules, and the dissociation of the gas molecules. Chemisorption studies can be used to evaluate the active surface area of a catalyst, which is distinct from the total BET surface area (active plus non-active).

Temperature Programmed Reduction, or Reaction, (TPR) is simply an experiment in which the amount of reduction is monitored as a function of temperature. The temperature is raised in a linear fashion so that a suitable detection system can record a characteristic reduction profile or fingerprint of the sample being tested. If the reactive gas is oxidizing (such as one containing oxygen), one can perform Temperature Programmed Oxidation.

In an analogous manner, gases that were previously adsorbed during a chemisorption study can be desorbed by once again ramping the temperature to sufficiently high values to break the chemical bonds holding the gas molecules (or atoms) on the surface of the catalyst. This type of analysis is called Temperature Programmed Desorption (TPD).

The ChemBET Pulsar can be used to perform low-cost automated TPR, TPO, TPD analyses up to 1100°C, as well as manual or automated pulse titrations (i.e. injection and peak detection) for metal area/

dispersion measurements. It also offers the capability to perform BET surface area measurements. It is compatible with H<sub>2</sub>, O<sub>2</sub>, CO, CO<sub>2</sub>, N<sub>2</sub>O, SO<sub>2</sub>, NH<sub>3</sub>, N<sub>2</sub>, Ar, Ke and He.

#### 5. Quantachrome Surface Area Analyser



At low temperatures, non-reactive gases (nitrogen, argon, krypton, etc.) are physisorbed by the surface. Through gas physisorption, the total surface area of the sample can be calculated by the BET method.

The Quadrasorb EVO is a versatile high throughput gas adsorption instrument.

4 samples can be analysed simultaneously. It operates by measuring the quantity of gas adsorbed onto or desorbed from a solid surface at some equilibrium vapor pressure by the static volumetric method. To obtain the data, a known quantity of adsorptive gas is admitted or removed in and out of a sample cell containing the solid adsorbent at a constant temperature below the critical temperature of the adsorbate. As adsorption or desorption occurs the pressure in the sample cell changes until equilibrium is established. The quantity of gas adsorbed or desorbed at the equilibrium pressure is the difference between the amount of gas admitted or removed and the amount required to fill the space around the adsorbent (void space).



Microporous samples are measured with Nitrogen or argon in volume-pressure range 0.001 to slightly less than 1. Low surface area samples are measured with krypton in volume pressure range  $4 \times 10^{-5}$  to slightly less than 1.

The volume-pressure range can be reduced to BET surface area (single and/or multipoint), Langmuir surface area, adsorption and/or desorption isotherms, pore size and surface area distributions, micropore volume and surface area using an extensive set of built-in data reduction procedures in the associated QuadraWin software.

The setup includes a FloVac Degasser that allows preparation of up to 6 samples in a single heated

zone. Needle valves allow careful control of flow rate to avoid elutriation (blowing out) of fine powders.

## 6. Solar Simulator



High pressure Xe arc lamps make excellent artificial sources to simulate sunlight. The high colour temperature of the xenon lamps (6050 to 6350 K) is a close match to the solar temperature. This results in similar spectra in the UV and VIS although the lamp has some Xe emission lines in the near IR.

Our LOT Quantum Design solar simulator is a 150W Xe light source. It includes filters to filter the Xe lamp to match various atmospheric conditions and thus match well with standard spectra. The matching is better in the UV and VIS than in the IR.

## 7. Metrohm pH Titrator



This is an intelligent potentiometric titrator and synthesis controller. Our titrator setup consists of a Metrohm 902 Titrando, a "dosino" dosing unit, a magnetic stirrer with base plate, and is controlled by a Tiamo 2.3 software interface.

## 8. Vapourtec



This is a cost-effective reactor for gas-liquid reactions, offering the possibility to control reaction temperature and feed in gas with the same coil tube reactor.

Liquid is fed through the coil and gas is fed through a separate connection at the desired pressure from a regulated supply.

The reactor can be used in two different ways:

- Pre-dissolving the gas into the liquid before the reaction.
- Performing the reaction in the reactor itself by feeding in the gas as it is consumed by the reaction.



## Publications:

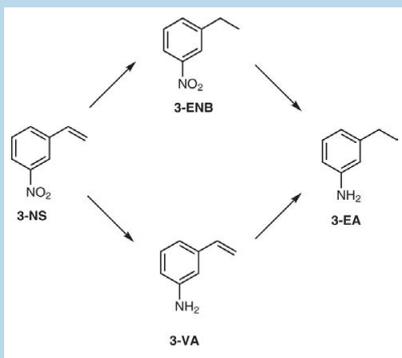


Image: The desired chemoselective hydrogenation of 3-NS to form 3-VA, and the associated side products 3-ENB and 3-EA. *Nature Catalysis*, volume 2, pages 873–881

### Tuning of catalytic sites in Pt/TiO<sub>2</sub> catalysts for the chemoselective hydrogenation of 3-nitrostyrene

An article was published in *Nature Catalysis* co-authored by Margherita Macino, Alexandra J. Barnes, Sultan M. Althahban, Ruiyang Qu, Emma K. Gibson, David J Morgan, Simon J. Freakley, Nikolaos Dimitratos, Christopher J. Kiely, Xiang Gao, Andrew M. Beale, Donald Bethell, Qian He, Meenakshisundaram Sankar and Graham J. Hutchings.

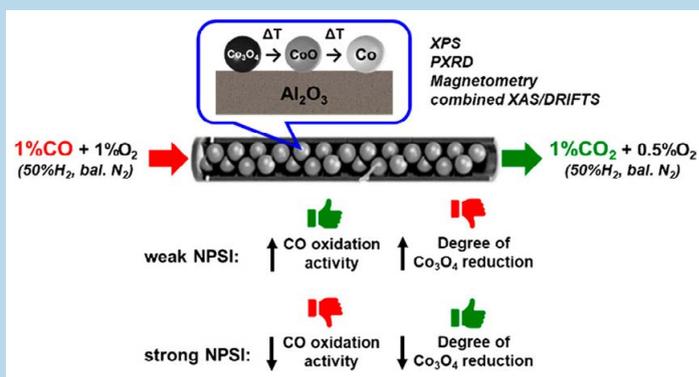
The article titled, “*Tuning of catalytic sites in Pt/TiO<sub>2</sub> catalysts for the chemoselective hydrogenation of 3-nitrostyrene*” can be found in *Nature Catalysis*, volume 2, pages 873–881. The catalytic activities of supported metal nanoparticles can be tuned by appropriate design of synthesis strategies. Each step in a catalyst synthesis method can play an important role in preparing the most efficient catalyst. Here they report the careful manipulation of the

post-synthetic heat treatment procedure—together with control over the metal loading—to prepare a highly efficient 0.2 wt% Pt/TiO<sub>2</sub> catalyst for the chemoselective hydrogenation of 3-nitrostyrene. For Pt/TiO<sub>2</sub> catalysts with 0.2 and 0.5 wt% loading levels, reduction at 450 °C induces the coverage of TiOx over Pt nanoparticles through a strong metal–support interaction, which is detrimental to their catalytic activities. However, this can be avoided by following calcination treatment with reduction (both at 450 °C), allowing them to prepare an exceptionally active catalyst. Detailed characterization has revealed that the peripheral sites at the Pt/TiO<sub>2</sub> interface are the most likely active sites for this hydrogenation reaction.

### Impact of Nanoparticle–Support Interactions in Co<sub>3</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub> Catalysts for the Preferential Oxidation of Carbon Monoxide

An article was published in *ACS Catalysis* co-authored by Thulani M. Nyathi, Nico Fischer, Andrew P. E. York, David J. Morgan, Graham J. Hutchings, Emma K. Gibson, Peter P. Wells, C. Richard A. Catlow and Michael Claeys.

Different supporting procedures were followed to alter the nanoparticle–support interactions (NPSI) in two Co<sub>3</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub> catalysts, prepared using the reverse micelle technique. The catalysts were tested in the dry preferential oxidation of carbon monoxide (CO-PrOx) while their phase stability was monitored using four complementary in situ techniques, viz., magnet-based characterization, PXRD, and combined XAS/DRIFTS, as well as quasi in situ XPS, respectively. The catalyst with weak NPSI achieved higher CO<sub>2</sub> yields and selectivities at temperatures below 225 °C compared to the sample with strong NPSI. However, relatively high degrees of reduction of Co<sub>3</sub>O<sub>4</sub> to metallic Co were reached between 250 and 350 °C for the same catalyst. The presence of metallic Co led to the undesired formation of CH<sub>4</sub>, reaching a yield of over 90% above 300 °C. The catalyst with strong NPSI formed very low amounts of metallic Co (less than 1%) and CH<sub>4</sub> (yield of up to 20%) even at 350 °C. When the temperature was decreased from 350 to 50 °C under the reaction gas, both catalysts were slightly reoxidized and gradually regained their CO oxidation activity, while the formation of CH<sub>4</sub> diminished. The present study shows a strong relationship between catalyst performance (i.e., activity and selectivity) and phase stability, both of which are affected by the strength of the NPSI. When using a metal oxide as the active CO-PrOx catalyst, it is important for it to have significant reduction resistance to avoid the formation of undesired products, e.g., CH<sub>4</sub>. However, the metal oxide should also be reducible (especially on the surface) to allow for a complete conversion of CO to CO<sub>2</sub> via the Mars–van Krevelen mechanism. The article titled, “*Impact of Nanoparticle–Support Interactions in Co<sub>3</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub> Catalysts for the Preferential Oxidation of Carbon Monoxide*” can be found in *ACS Catalysis*, 2019, 9, 8, 7166–7178, <https://doi.org/10.1021/acscatal.9b00685>



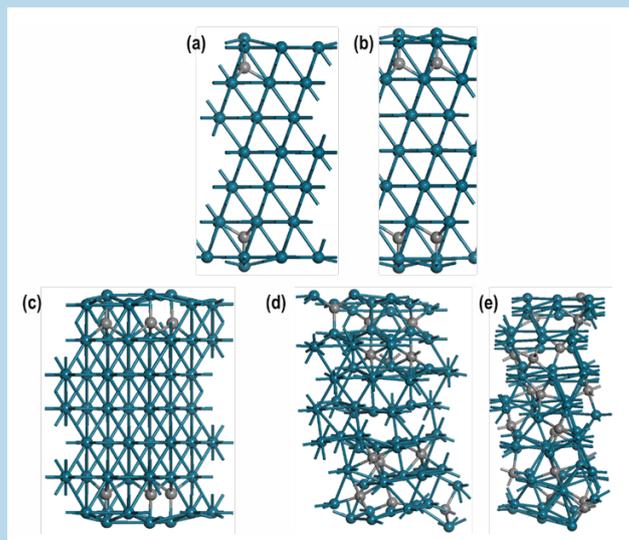
Graphical Abstract by Thulani Nyathi, *ACS Catal.* 2019, 9, 8, 7166–7178

## Publications cont:

### Carbideisation of Pd Nanoparticles by Ethene Decomposition with Methane Production

An article was published in *Chem Cat Chem* authored by members of the UK Catalysis Hub including; Wilm Jones, Peter. P. Wells, Emma K. Gibson, Arunabhiram Chutia, Ian P. Silverwood, C. Richard A. Catlow and Michael Bowker.

In the presence of oxygenated organic molecules pure Pd, which is widely used in chemicals processing and the pharmaceutical industry, tends to defunctionalise and dehydrogenate such molecules to H<sub>2</sub>, CO and surface/bulk carbon, in the form of a palladium carbide. They investigated the formation of this carbide by ethene adsorption using a variety of techniques, including pulsed flow reaction measurements, XAS and DFT calculations of the lattice expansion during carbideisation. These experiments show that two main reactions take place above 500 K, that is, both total dehydrogenation, but also disproportionation to methane and the carbide, after which the activity of the Pd is completely lost. They estimate the value of x in PdC<sub>x</sub> to be 0.28 (±0.03), and show by computer modelling that this fits the lattice expansion observed by XAFS, and that there is charge transfer to C from Pd of around 0.2–0.4 e.

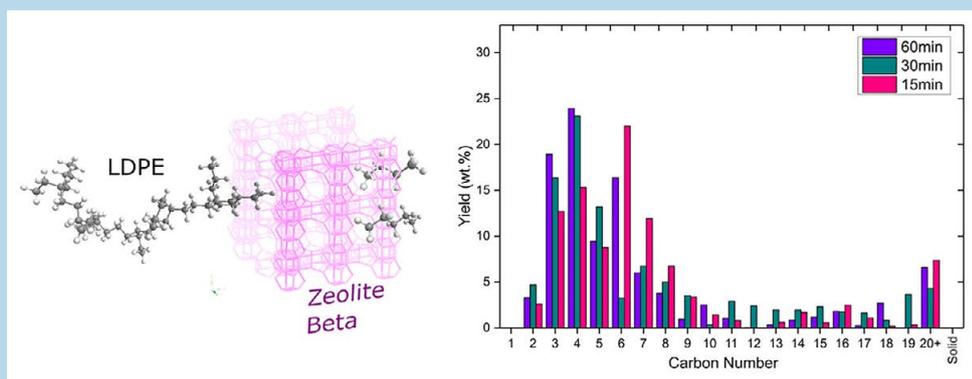


Pd(111) surface with (a) 2 C-atom (0.357 wt%), (b) 4 (0.711 wt%), (c) 6 (1.063 wt%), (d) 12 (2.105 wt%), and (e) 18 (3.124 wt%). Image by Dr Arunabhiram Chutia, *Chem Cat Chem*, Volume11, Issue 17, September 5, 2019, Pages 4334-4339

The article was published in *Chem Cat Chem*, Volume11, Issue 17, September 5, 2019, Pages 4334-4339, <https://doi.org/10.1002/cctc.201900795>

### Catalyzing the Hydrocracking of Low Density Polyethylene

An article was published in *Industrial & Engineering Chemistry Research* authored by Abdulrahman Bin Jumah, Vanithasri Anbumuthu, Aleksander A. Tedstone and Arthur A. Garforth.



Graphical abstract by ? *Ind. Eng. Chem. Res.* 2019, 58, 45, 20601-20609

The hydrocracking of squalane and low density polyethylene (LDPE) into low molecular weight hydrocarbons has been demonstrated with the use of bifunctional zeolite catalysts, Pt-impregnated USY and Beta, with selectivity toward isomers of C<sub>4</sub>–C<sub>6</sub> alkanes. Quantification of liquid and gaseous products via GC-FID and GC-MS demonstrated that appropriate catalyst selection can yield >95% conversion of polymer to fluid products at mild reaction conditions of 330 °C and 20 bar of H<sub>2</sub> and short reaction times of <15 min in a batch system. Zeolite Beta exhibits marked selectivity toward C<sub>4</sub> hydrocarbons, and its efficacy in this reaction is related to its acidic and structural properties. The appropriate selection of reaction time, temperature, and Pt-loading are discussed. The article was published in *Ind. Eng. Chem. Res.* 2019, 58, 45, 20601-20609, <https://doi.org/10.1021/acs.iecr.9b04263>

## Publications cont:

### Detection of key transient Cu intermediates in SSZ-13 during NH<sub>3</sub>-SCR deNO<sub>x</sub> by modulation excitation IR spectroscopy†

An article was published in *Chemical Science* authored by members of the UK Catalysis Hub including; Alex G. Greenaway, Adrian Marberger, Adam Thetford, Inés Lezcano-González, Miren Agote-Arán, Maarten Nachtegaal, Davide Ferri, Oliver Kröcher, C. Richard A. Catlow and Andrew M. Beale.

The small pore zeolite Cu-SSZ-13 is an efficient material for the standard selective catalytic reduction of nitrogen oxides (NO<sub>x</sub>) by ammonia (NH<sub>3</sub>). In this work, Cu-SSZ-13 has been studied at 250 °C under high conversion using a modulation excitation approach and analysed with phase sensitive detection (PSD). While the complementary X-ray absorption near edge structure (XANES) spectroscopy measurements showed that the experiments were performed under cyclic Cu<sup>+</sup>/Cu<sup>2+</sup> redox, Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) experiments provide spectroscopic evidence for previously postulated intermediates Cu–N(=O)–NH<sub>2</sub> and Cu–NO<sub>3</sub> in the NH<sub>3</sub>-SCR deNO<sub>x</sub> mechanism and for the role of [Cu<sup>2+</sup>(OH)]<sup>+</sup>. These results therefore help in building towards a more comprehensive understanding of the reaction mechanism which to date has only been postulated *in silico*. The article was published in *Chem. Sci.*, 2020, 11, pages 447-455, <https://doi.org/10.1039/C9SC04905C>

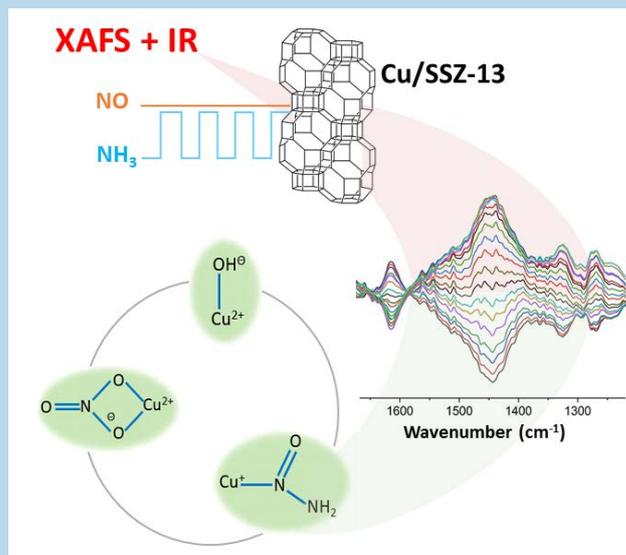


Image by Miren Agote-Arán. *Chem. Sci.*, 2020, 11, 447-455

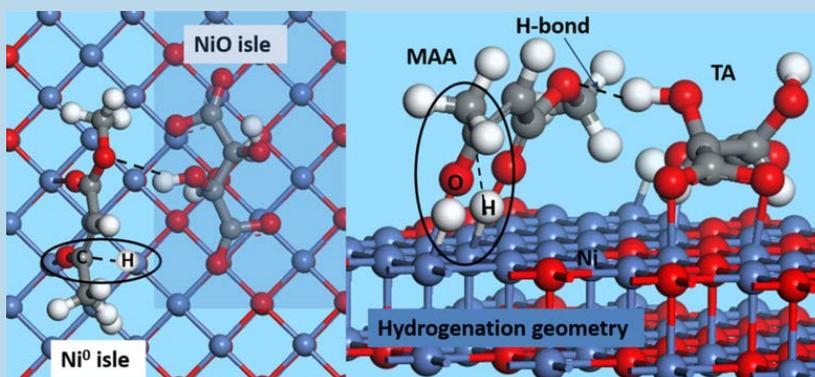


Image by Rosa Arrigo and Matteo Aramini.

### Influence of Synthesis Conditions on the Structure of Nickel Nanoparticles and their Reactivity in Selective Asymmetric Hydrogenation

An article was published by members of the UK Catalysis Hub including; Dr. Rosa Arrigo Simone Gallarati Dr. Manfred E. Schuster Jake M. Seymour Dr. Diego Gianolio Dr. Ivan da Silva

Dr. June Callison Haosheng Feng Dr. John E. Proctor Dr. Pilar Ferrer Dr. Federica Venturini Dr. David Grinter and Prof. Georg Held.

Unsupported and SiO<sub>2</sub>-supported Ni nanoparticles (NPs) were synthesised via hot-injection colloidal route using oleylamine (OAm) and trioctylphosphine (TOP) as reducing and protective agents, respectively. By adopting a multi-length scale structural characterization, it was found that by changing equivalents of OAm and TOP not only the size of the nanoparticles is affected but also the Ni electronic structure. The synthesized NPs were modified with (*R,R*)-tartaric acid (TA) and investigated in the asymmetric hydrogenation of methyl acetoacetate to chiral methyl-3-hydroxy butyrate. The comparative analysis of structure and catalytic performance for the synthesized catalysts has enabled us to identify a Ni metallic active surface, whereby the activity increases with the size of the metallic domains. Conversely, at the high conversion obtained for the unsupported NPs there was no impact of particle size on the selectivity. (*R*)-selectivity was very high only on catalysts containing positively charged Ni species such as over the SiO<sub>2</sub>-supported NiO NPs. This work shows that the chiral modification of metallic Ni NPs with TA is insufficient to maintain high selectivity towards the (*R*)-enantiomer at long reaction times and provides guidance for the engineering of long-term stable enantioselective catalysts. The article was published online in *Chem Cat Chem.*, <https://doi.org/10.1002/cctc.201901955>

## Publications cont:

### Synergistic ultraviolet and visible light photo-activation enables intensified low-temperature methanol synthesis over copper/zinc oxide/alumina

An article was published in *Nature Communications* authored by members of the UK Catalysis Hub including; Bingqiao Xie, Roong Jien Wong, Tze Hao Tan, Michael Higham, Emma K. Gibson, Donato Decarolis, June Callison, Kondo-Francois Aguey-Zinsou, Michael Bowker, C. Richard A. Catlow, Jason Scott and Rose Amal.

A high-pressure hybrid photothermal catalytic system was employed in CO<sub>2</sub> hydrogenation to methanol, exhibiting 32% increase in methanol yield only under full spectrum (300-800 nm) irradiation. Irradiation of UV-rich (200-500 nm) light and visible (420-800 nm) light resulted in enhanced CO production. The synergistic nature of UV and visible light irradiation is attributed to the dual catalytic sites of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub>, where Cu:ZnO perimeter interface is the main active site. The improved catalytic performance originated from the photoenhanced CO<sub>2</sub> activation on ZnO surface under UV irradiation and H<sub>2</sub> activation on Cu surface under visible light irradiation. The roles of ZnO and Cu are revealed by DRIFTS, XAS, XPS, and DFT, showing a more dynamic change in ZnO as well as stronger orbital overlapping in the valence band spectrum. The simultaneous irradiation of UV and visible light successfully decreases the reaction temperature by 50°C without sacrificing methanol yield and selectivity. The present work also provides a new perspective on catalyst design by manipulating the valence band electronic structure. This work was completed in collaboration with UNSW Sydney during the visit of Roong Jien Wong as Visiting Research Fellow, with direct contribution from Emma Gibson, June Callison, Michael Higham, Donato Decarolis, Prof Michael Bowker, and Prof Richard Catlow.

The article was published in *Nat Communications*, 11, 1615 (2020). <https://doi.org/10.1038/s41467-020-15445-z>

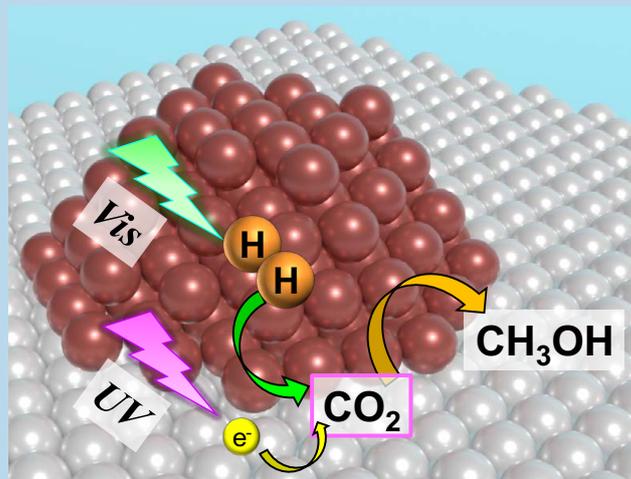


Image by Roong Jien Wong

## Let us know about your publications:

The UK catalysis Hub wants to hear your news. Please contact the Office Manager to contribute to the research highlights and publications in our newsletter.

Office Manager:  
Corinne Anyika  
[corinne.anyika@rc-harwell.ac.uk](mailto:corinne.anyika@rc-harwell.ac.uk) or call (01235) 567870

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## Upcoming Events



### UK Catalysis Hub Conference

7 - 8 December 2020  
Harwell Campus, Oxfordshire

After careful consideration of the rapidly evolving situation with COVID-19 we decided it was best to postpone the UK Catalysis Hub annual summer conference that was due to take place in July.

Our conference will now take place on the **7th and 8th of December 2020**. The Conference will take

place on the Harwell Campus in Oxfordshire. The conference will start at lunchtime on the 7th and the main conference will conclude at lunch on the 8th. There will be a dinner on the evening of the 7th of December. The event will also include a poster session showcasing work from the Hub postdocs and the presentation of the **JMT medal for catalysis**.

Visit <https://ukcatalysishub.co.uk/catalysis-hub-conferences/> for more information and to register for free.



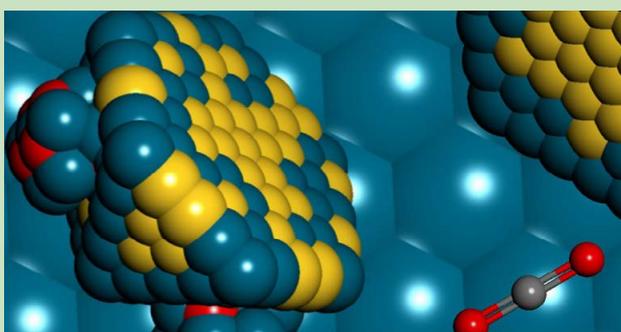
### New UK Catalysis Hub Webinars

Cooperative Catalysis with Prof.  
Duncan Wass (Director, Cardiff  
Catalysis Institute)

Thu, 23 April 2020, 15:00 – 16:00

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 will discuss 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. Register at <https://www.eventbrite.com/e/webinar-cooperative-catalysis-with-prof-duncan-wass-tickets-102171381352> to join us for this FREE webinar.



## Call for UK Catalysis Hub projects

**Due to the Current situation and research climate the UK Catalysis Hub has made the decision to extend the deadline for Proposals from May 8th to July 31st. This is to allow fruitful discussions between industry and academics and to allow academics to adjust to the additional complexities of moving to remote teaching and assessment. We will continue to assess this new deadline as the situation unfolds.**

**The Call will now close on the 31st July at 12.00.** Please send a 2 page (A4, Arial 11 point, margins 2.0 cm) proposal for these projects to The Project Co-ordinator, Josie Goodall [josie.goodall@rc-harwell.ac.uk](mailto:josie.goodall@rc-harwell.ac.uk) before 12.00 noon on the closing date. Please use the Subject line: '**Application for New Call 2020**'

This call is for up to two years of PDRA time (projects of 18 months are particularly encouraged) to work on collaborative multidisciplinary, multi-institution projects that coordinate, promote and advance the UK catalysis research portfolio within the areas of catalysis as represented by the 3 themes of the Catalysis Hub. The hub strongly encourages projects to have up-front funding from industry.

It is expected that successful projects will be announced in the autumn and will start in the second half of 2020 or early 2021, except where they are following directly on from an existing project (e.g. the core PDRAS in science 1) The scientific research themes of the UK Catalysis Hub Phase II are

**Science 1:** Optimising, Predicting and Designing New Catalysts

**Science 2:** Catalysis at the Water Energy Nexus

**Science 3:** Catalysis for the Circular Economy and Sustainable Manufacturing

For more information on the Catalysis Hub, the themes, existing projects, please go to the website - <https://ukcatalysishub.co.uk/>

### Please note:

#### Contracts

All Universities receiving funds will have to sign up an Accession agreement to the Collaboration Agreement as it stands. Any projects involving institutions who

have not already signed an accession agreement will need to seek agreement to sign from their contracts departments prior to submitting a project.

### Budget

The budgets for Hub projects have been set by what EPSRC has granted and, as such, are fixed. Please contact Josie Goodall if your research office would like these figures for the relevant theme. No PI time was granted by EPSRC – the funds will purely cover the PDRA time. It is the responsibility of the applicant to ensure their finance office agrees to these budgets in advance of application. Additionally, please note that the Science 1: Optimising Predicting and Designing new Catalysis (OPDNC) theme is based at Harwell to take advantage of facilities and the location so Projects involving the science 1 theme will need to be located at the Research Complex at Harwell.

### CORE PDRAS

In the OPDNC theme the 4 areas were designated Strategic: Synchrotrons, Neutrons, Lasers and Modelling. PDRAS in these areas have been hired for 5 years, though they will be available to work on projects in these areas from the new call. If you are developing Projects in these areas we strongly suggest you talk to the PI of the theme (Prof. Catlow) and involve the PDRA in the development of the Project

### The PDRAS are

**Donato Decarolis** – Synchrotrons and XAFS - [DecarolisD@cardiff.ac.uk](mailto:DecarolisD@cardiff.ac.uk)

**Santosh Matam** – Neutrons [santhosh.matam@rc-harwell.ac.uk](mailto:santhosh.matam@rc-harwell.ac.uk)

**Yesid Willington Hernandez** – Lasers [HernandezEncisoW@cardiff.ac.uk](mailto:HernandezEncisoW@cardiff.ac.uk)

**Matthew Quesne** – Modelling [QuesneM@cardiff.ac.uk](mailto:QuesneM@cardiff.ac.uk)

Please email [josie.goodall@rc-harwell.ac.uk](mailto:josie.goodall@rc-harwell.ac.uk) for more information, or for a copy of the accession and collaboration agreement or the budgets available.

### Industrial Support

The Hub is encouraging applicants to seek industrial engagement and support for their projects prior to application. The nature of the project should reflect the UK Catalysis Hub ethos. Please note it is important to agree IP arrangements in advance. These agreements should reflect the nature of the project. Most UK catalysis Hub projects are TRLs 1-3 and range from fundamental to applied catalysis but all scientifically excellent proposals will be considered. Please also note that any Hub projects are funded by UKRI (EPSRC) and thus results must be publishable after IP protection.

**Further information and the criteria for proposals can be found at <https://ukcatalysishub.co.uk/new-call-for-uk-catalysis-hub-projects-open/>**

## Opportunities



### Experimental Officer position in Catalysis and XAFS

We seek to recruit an enthusiastic highly motivated scientist with proven intellectual and technical abilities to work on X-ray Absorption Spectroscopy techniques as applied to catalysis research as part of the UK Catalysis Hub. The post is through Cardiff School of Chemistry, Cardiff University and will be based on the Harwell Campus at the Research Complex at Harwell (RCaH), Oxfordshire.

The overall focus of the post is to manage the Block Allocation Group Access to the B18 beamline at the Diamond Light Source, running X-ray absorption fine structure (XAFS) measurements on a variety of homogeneous and heterogeneous catalysis projects from the Hub network, and to contribute to the activities and running of the Catalysis Hub Laboratories at Harwell.

Applicants must hold a Degree/NVQ 4 or equivalent Professional membership/experience, and ideally a Postgraduate degree at PhD level in a related subject area or relevant industrial experience.

Further information on the Cardiff School of Chemistry and Cardiff Catalysis Institute (CCI) may be found at: <http://www.cardiff.ac.uk/chemistry> and <http://www.cardiff.ac.uk/research/cardiff-catalysis-institute>

For informal enquiries about the role, the School and the CCI, please contact Professor Graham Hutchings, PI of the Core theme of the UK Catalysis hub: [Hutch@cardiff.ac.uk](mailto:Hutch@cardiff.ac.uk); Tel. +44 (0)29 208 74059.

For further details about working for Cardiff University and at the RCaH, please contact Dr Josie Goodall project manager for the UK Catalysis Hub: [GoodallJ@cardiff.ac.uk](mailto:GoodallJ@cardiff.ac.uk).

This position is full-time (35 hours) and is available from 1 May 2020 until 30 November 2023.

**Closing date: Thursday, 16 April 2020**

Visit [https://krb-sjobs.brassring.com/TGnewUI/Search/Home/HomeWithPreLoad?partnerid=30011&siteid=5460&PageType=searchResults&SearchType=linkquery&LinkID=11#jobDetails=1658768\\_5460](https://krb-sjobs.brassring.com/TGnewUI/Search/Home/HomeWithPreLoad?partnerid=30011&siteid=5460&PageType=searchResults&SearchType=linkquery&LinkID=11#jobDetails=1658768_5460) for more information and to apply.

## 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 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 Manager - Dr. Josie Goodall 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.

Project Manager:

Dr Josie Goodall

Josie.goodall@rc-harwell.ac.uk  
or call (01235) 567870

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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](mailto:corinne.anyika@rc-harwell.ac.uk) with your profile summary.