



CENTRE FOR DOCTORAL TRAINING

Annual Report 2022





Loughborough



UNIVERSITY^{of} BIRMINGHAM





Engineering and Physical Sciences Research Council



Sustainable Hydrogen Centre for Doctoral Training (SusHy CDT) established 2019.

The Centre is the only UK hydrogen energy CDT, selected through the £45million CDT call from the Engineering and Physical Sciences Research Council (EPSRC) aimed at tackling pressing global challenges.

SusHy CDT has four partner universities – Nottingham, Loughborough,

Birmingham and Ulster – and four overarching Centre objectives (see Vision below).

We're looking to recruit 67 talented individuals (2023 will be the last recruitment year) and provide high quality, multi-disciplinary training to achieve mass uptake of hydrogen technologies in the UK and beyond. Our October 2022 entry will be the fourth cohort of PhD students recruited; working in hydrogen combustion, distribution, production, safety, storage, systems and upgrade. The CDT is supported by the EPSRC and over 40 Stakeholder partners.



Our Vision

In-line with the UK's commitment to reduce emissions by **78% by 2035** and achieve **Net Zero by 2050**, we're developing hydrogen technologies facilitating deep-decarbonisation.

Sustainable Hydrogen CDT's objectives:

- Deliver high quality trans-disciplinary training covering fundamental science, applied engineering, and systems issues and build an appreciation of societal barriers to innovation.
- Through innovation opportunities, build initiative and stimulate an entrepreneurial mindset.
- Deliver 'industry ready' doctorates, who have a comprehensive skill set and experiences.
- Co-create research ideas and undertake, in partnership with our stakeholders, cutting edge investigations of hydrogen-based solutions to deep decarbonisation of the energy system.

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Director's Report By Professor Gavin Walker

It's good to see interest in sustainable hydrogen increasing, with the UK Government doubling 2030's hydrogen generation capacity target to 10 Gigawatts (GW), 50% of that being green hydrogen.

This complements the 40 GW offshore wind target by 2030, acknowledging the expected increased energy storage need. This year we've seen the launch of the H100 Fife project – Fife Council's 100% hydrogen-to-homes heating network, demonstrating hydrogen for domestic heating and hot water - and a variety of other projects developing hydrogen for transport (road, rail, aviation and marine).

Thankfully, decreasing Covid disruption this year allowed more in-person delivery of the taught course, and students the opportunity to visit CDT partner universities.

Cost of living was raised as an issue by our students. The Engineering and Physical Sciences Research Council will increase its basic studentship stipend by 10%. The SusHy CDT is working with partners providing match funding to ensure all students receive the 10% increase for the remainder of their PhD.

I'm pleased to report our students continue to successfully deliver on their PhDs. Cohort 1 are entering their final year of research, Cohort 2 have been making great inroads into research projects as they progress into their third year, Cohort 3 have successfully completed their taught modules and can now focus on research. Cohort 3 benefited from the 'Buddy Scheme' ('thanks' to Mickella Dawkins for instigating this), which helped them adjust to life on an Integrated PhD degree programme.

Recruitment over the past year went well overall. The SusHy CDT commitment to recruiting diverse teams has been very successful, encouraging applications from a wide social cross-section; with our advertising giving candidates from under-represented groups the confidence to apply. This has been accomplished without compromising on academic excellence, as the highly talented set of individuals in Cohort 4 show. Our latest cohort has 36% of students identifying as from ethnic minority communities and 55% identifying as female. Although we've always met our ethnic minority recruitment target (18%), it's the first year we've met our gender target (50%); a significant achievement considering the UK Engineering sector has only around 12% women in the workforce. Examples of the SusHy CDT's efforts to create a supportive and inclusive environment for students can be found in this 2022 Annual Report.

Our recruitment successes have been achieved during one of the most difficult years for PhD recruitment I've ever seen. UK Doctoral programmes have struggled to recruit, as fewer graduates show interest in pursuing a PhD; probably a combination of the UK's buoyant graduate labour market and, possibly, graduates' difficult university experience during the pandemic dissuading them from remaining in academia. Despite this, 11 students were recruited, slightly below our target. We've a challenging final year of recruitment, with 22 places to fill across four universities. Again, we won't compromise on candidate quality during recruitment but aim to fill places by starting early (applications welcome now) and having flexible 2023 start dates (January and October).

The CDT ran a varied 2021/22 events programme. Stakeholder workshops at Loughborough (Oct 2021) and Nottingham (April 2022) attracted speakers from Arup, Shell, GeoPura, European Marine Energy Centre and ORE Catapult. In our first Stakeholder Challenge (hosted by Longcliffe Quarries, Matlock) students identified how hydrogen could help the firm meet 2027 Net-zero targets. On September 13th our first SusHy CDT Conference, at Nottingham's Trent Bridge Cricket Ground, saw Cohorts 1 and 2 give oral and poster research presentations, with Cohort 3 judging. Prior to the conference, students and staff enjoyed archery and laser tag at an Away Day on September 12th.

I'd also thank students for running an excellent LGBTQ+ Researchers' June seminar at the University of Birmingham. I look forward to the CDT supporting other student-led initiatives (more on the seminar in this Report). Looking ahead, 2022/23 will be the first time the CDT has students at all stages of their four year PhDs. We've built a strong base on which to successfully recruit our fifth and final cohort. I look forward to another year of SusHy CDT events.

Sustainable Hydrogen CDT 2021-2022: The Year in Numbers



55% of students recruited to CDT's **Cohort 4** identify as female.

2021/22 target = 50%



36% of students recruited to CDT's **Cohort 4** identify as part of **Ethnic Minority community**.

2021/22 target = 18%



411 PhD applications made to the CDT in 2021/22





Sustainable Hydrogen CDT 2021-2022: The Year in Numbers





Student training 2021/22, circa. 13,000 hours



Presentations & publications by students in 2021/22 - **27**





44 Stakeholder interactions in 2021/22

Equality, Diversity and Inclusivity (EDI)



We recruit amazing individuals from a diverse talent pool

- SusHy CDT knows teams reflecting societal diversity are more successful, which is why we've put EDI at the heart of our operations. Our social media recruitment posts reflect CDT gender and cultural diversity, and back relevant theme days/weeks/months, e.g: June Pride Month, International Women in Engineering Day (June 23rd), Black History Month (October), etc.
- Our revised Recruitment Strategy is working; showing increased interest from female applicants, with **29%** of 2021/22 applicants identifying as female. Interview procedures have been altered to better take into account students' different neurodiversity needs.

The CDT's programme aims to train the energy leaders we need to meet the Net Zero global challenge, which will require leading successful innovation teams informed by diverse perspectives.

We create a more inclusive environment with:

- Our **Student EDI Forum** and the **EDI Student Representatives** at Management Board meetings, give students direct influence on CDT EDI policy and opportunities to deal with issues.
- The **'Buddy Scheme'**, an idea from CDT student Mickella Dawkins, matches current with new intake students, to ease any stresses around beginning a PhD and address concerns.
- The **EDI Access Fund** financially assists students if they have disability, mobility or domestic (child care) needs, which might otherwise prevent participation in activities.
- Direct support for 2021/22 student activities included funding for their June 27th **LGBQT+ Researchers' Seminar**, University of Birmingham, and students attendance on an online 'Effective Mentoring' course with Leadership Coach Jeffrey Wotherspoon.
- In July (2022) CDT Director Prof. Gavin Walker spoke on its Recruiting Diverse Teams Strategy, at the *Women in Research: Let's Thrive Together* event, by University of Nottingham Women's staff Network.
- The CDT is a proud partner of the **Women's Engineering Society** (WES) and **Women Into Science and Engineering** (WISE), and provides free membership for students.



Examples of cohort diversity are reflected in following:

We seek to provide and improve on a supportive environment, where everyone feels equally valued and able to achieve their full potential. Recruitment aims are for a student community reflecting UK diversity; including LGBTQ+, disability, neurodiversity and socio-economic background. Among the diversity figures we pay close attention to are:

Ethnic Minorities

2021/22 recruitment target (18%) exceeded -36% of Cohort 4 identify as part of Ethnic Minority community

Across ALL CDT Cohorts (1-4) these students now account for

36%

of all students (at Oct 2022)

Gender parity

2021/22 recruitment target (50%) exceeded -55% of Cohort 4 identify as female

Across ALL CDT Cohorts (1-4) these students now account for

32% of all students (at Oct 2022)

SH

SusHy CDT Team



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CDT Management Board











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Professor **Gavin Walker** Director: SusHy CDT



Professor **Deborah Kays** Co-Director:



EDI Support

Dr Sanliang Ling

Student Engagement

Co-Director:





Professor

David Saal

Co-Director





Dr Rafael Orozco Co-Director

Lynne Macaskie

Co-Director: EDI Support

Professor

Co-Director

Professor

David Book



Dr Daniel Reed Co-Director: Student Engagement



Professor Vladimir Molkov









Our Students

Combustion	Production	Storage	Systems
Distribution			
Safety			Upgrade



Stakeholders



We work with 40-plus partners and stakeholders including energy providers, researchers, UK government and engineering consultancies. Such links are vital as the CDT pursues its four overarching objectives; particularly, delivering 'industry ready' doctorates and co-creating research ideas in collaboration with stakeholders. A Stakeholder list is at: www.sustainablehydrogen-cdt.ac.uk/stakeholders/stakeholders.aspx

Regular SusHy CDT **Stakeholder Events** (**see below**) enable partners to network with CDT staff and students, and speakers to raise awareness of their work before an informed audience. In **Stakeholder Challenges** partners give students real sector issues to work on:

October 2021 at Loughborough University

The Stakeholder Event keynote was by Dr Mark Neller, Director at Arup sustainable development consultancy. Sessions were on *Production of turquoise hydrogen & its potential for decarbonisation of heating, transport & industry* and *Understanding the potential of hydrogen technologies to decarbonise the heating sector using systems thinking approach.*







November 2021 at Longcliffe Quarries, Derbyshire

The first SusHy CDT Stakeholder Challenge, hosted by Longcliffe Quarries of Matlock, (**pic below**) had students working to identify hydrogen's role in helping the company meet its 2027 Net-Zero targets.



April 2022 at the University of Nottingham

The Event theme of *The potential for hydrogen in connection with the expansion of offshore renewables* saw speakers from GeoPura, the Electric Power Research Institute, Shell, the Offshore Renewable Energy Catapult, the European Marine Energy Centre and Imperial College London speak at two panels; on *Systems and Transportation of Energy* and *Offshore Hydrogen Opportunities*.



April event talks still available on the SusHy CDT YouTube channel at www.youtube.com/channel/UCo-EpdAHeJH0TINPR-j3S-w

SusHy CDT News and Events 2021-2022

October 2021	The welc stud and dinn fello and Thin	Sustainable Hydrogen CDT comed its third Cohort, of 11 lents. Cohort 3 saw Loughborough Nottingham research facilities, had er with Management Board and w students from Cohorts 1 and 2; attended Team Dynamics, Creative sking and Research Skills training.	A Loughbor featured ke Director at A 'turquoise h in decarbon Stakeholde	ough University Stakeholder Event ynote speaker Dr Mark Neller, Arup consultancy. Sessions were on ydrogen' and hydrogen tech's role ising the heating sector. (See ar page for further details).
November		The first SusHy CDT Stakehol Derbyshire, had students work meet its 2027 Net-Zero targets	der Challenge, hosted by Lon king to identify the future role o s. (See Stakeholder page for	gcliffe Quarries of Matlock, of hydrogen in helping the company further details).
December		Students from all three CDT Cohorts Jordanstown and Belfast Campuses Team-building activity was at giant e sightseeing at Belfast Christmas Ma	s enjoyed a cohort building trip 3' facilities. escape room Prison Island Be rket.	o to Ulster University, visiting
February 2022		CDT students Zoe Pallis and Samir Soares were among CDT students visiting Northern Gas Networks' demonstration hydrogen powered homes, at Low Thornley site, near Gateshead.	Effective mentoring Trainer: Jeffrey Wotherspoon Trainer: Jeffrey Wotherspoon	nts attended an online 'Effective oring' course with Leadership Coach y Wotherspoon, whose clients have ed the British Library and Sony.
April				
	Stakeholder Event, Ur Potential for hydrogen offshore renewables (Cohort building activiti	niversity of Nottingham (pic left), on: <i>in connection with the expansion of</i> see Stakeholder page for details). ies also at Birmingham (pic right).	Courtney Quinn, University o on <i>Protic Ionic Liquids for Wa</i> in collaboration with Queen's Research Centre .	f Nottingham, presented her work <i>iter Splitting</i> , which was completed University Belfast QUILL



SusHy CDT News and Events 2021-2022

May 2022	Students Srinivas Sivaraman, Hazhir Ebne-Abbasi, Mina Kazemi with Dr Dmitriy Makarov, Professor Vladimir Molkov and Dr Sile Brennan (HySAFER, Ulster University) presented at the 10th International Seminar on Fire and Explosion Hazards in Norway. Hazhir received the 'Best Student Presenter' award. The three students also presented at the H2FC Supergen Research Conference , University of St Andrews, in June.	CDT student Will Bowling, University of Nottingham, wrote the Executive Summary for the bp-backed H2Tech Series exhibition at the World Hydrogen 2022 Summit, held in Rotterdam. Summit included 150 speakers and 180 exhibitors.
June	An LGBTQ+ Researcher Celebration event was staged by CDT students during June Pride Month. Speakers at the event (funded by CDT's EDI Fund) at the University of Birmingham included Professor Tom Welton, President of the Royal Society of Chemistry.	Dr Sanliang Ling, CDT Management Board, and University of Nottingham Energy Institute at 18th UK Hydrogen & Fuel Cells Conference.
July	Professor Gavin Walker was a speaker at the W Thrive Together event, held at the Advanced W Campus. Organised by the Women's Staff Network, it was based around gender equality in research. Fund	<i>Yomen in Research - Let's</i> lanufacturing Building, Jubilee s one of a series of workshops ling by Research England.
September	The late Forest, I archery 13th, at and pos	est CDT Away Day was held at Into the Nottingham, on September 12th; featuring and Laser Tag. sHy CDT Conference , on September Trent Bridge Cricket Ground, included oral ter presentations by CDT cohorts.

Current Research

Our Sustainable Hydrogen CDT PhD students, across all four Cohorts, are undertaking hydrogen research in a wide variety of areas.

In this section you will find research profiles for each CDT student researcher; working in areas such as Combustion, Distribution, Production, Safety, Storage, Systems and Upgrade, Safety, .





Sustainable catalysts for low temperature and pressure ammonia synthesis

Ammonia's use as a hydrogen rich energy vector – not just for more efficiently moving energy to different markets but also for direct combustion of ammonia as a fuel decarbonising heavy vehicle use in road freight, rail and marine sectors – is attracting interest. Production of ammonia (via Haber Bosch process) requires high temperatures (300-450°C) and pressure (150-200 bar). This makes the process unsuitable for small scale intermittent ammonia generation, for example via distributed generation coupled with wind or solar renewable energy. More agile ammonia synthesis needs a catalyst operating at lower temperature/pressure. Ruthenium is currently the only catalyst that has acceptable kinetics at low temperatures. Bakhtawar's project will investigate sustainable catalysts, avoiding resource limited platinum group metals.

Supervisors: Professor Gavin Walker, Dr Marcus Adams, Dr Matthew Wadge.







Ruth Atkinson (Cohort 3) School of Chemistry



Designing efficient charge-transfer metal-semiconductors heterojunctions for hydrogen generation

Ruth's project assesses metal-semiconductor combinations for suitability as photocatalysts for the generation of hydrogen from water, replacing current catalysts based on expensive precious metals. Designing efficient charge-transfer metal semi-conductors heterojunctions for hydrogen generation, this project will assess a wide range of metal semi-conductor combinations for suitability as photocatalysts for generating hydrogen from water, replacing catalysts based on expensive precious metals. In particular, Ruth will explore materials based on Nb semiconductors in conjunction with metals such as Co, Cu, Ni or Mo. Materials will be synthesised, fully characterized and tested towards the photogeneration of hydrogen from water.

Supervisors: Dr Anabel Lanterna, Professor Elena Besley.





Experimental study of advanced ammonia-fuelled, heavy duty, internal combustion (IC) engines under low load operation

Will is carrying out an experimental research project looking to utilise advanced combustion techniques such as turbulent jet ignition and dual fuel operation to enable the use of ammonia as a fuel in heavy duty, internal combustion engines; with a specific focus on low load operation, during which the combustion is the most challenged. The project will be formed of two main studies, a fundamental combustion study carried out using a bespoke optical constant volume combustion chamber to understand flame development in a laminar environment; as well as an applied engine study, converting a diesel heavy duty compression ignition engine to operate using ammonia and hydrogen.

Supervisors: Prof Alasdair Cairns, Dr Antonino La Rocca, Dr Richard Jefferson-Loveday.



www.sustainablehydrogen-cdt.ac.uk





Alexandra Brochoire (Cohort 4) School of Chemical Engineering



Proton exchange membrane water electrolysers with thin film nanostructured electrodes

The biggest challenge with current proton exchange membrane water electrolysers (PEMWE) is their poor power performance and durability; which is mainly caused by large mass transfer losses and degradation of the electrode structure, from the random electrode structure from catalyst nanoparticles. Alexandra's PhD project will seek to develop a new generation of catalyst electrodes from aligned IrO2- and metal oxide-based nanowires for PEMWE applications; taking advantage of the high stability of nanowires and the boosted mass transfer characteristics of the unique thin catalyst layers from nanowire arrays. Project aims are substrate surface modification approach to increase surface activity, in-situ nanowire array growing process based on IrO2 and metal oxide materials, surface deposition technique of SrIrO3 on nanowire arrays, and electrode evaluation using half-cell and single cell test.

Supervisors: Dr Shanfeng Du, Dr Neil Rees.



Sustainable electrocatalysts for hydrogen (H2) generation

Jack is carrying out research into the development and use of polyoxometalates (POMs) as electrocatalysts, which facilitate both the oxygen and hydrogen evolution reactions during electrolytic water splitting. He is particularly interested in the development of POM-carbon nanotube composites.

Supervisors: Dr Darren Walsh, Dr Graham Newton, Dr Ming Li.







Harvey Craddock-Monroe (Cohort 2) Department of Chemistry

Odor additives for H ₂	<u>×</u>
 Rationale design Chemical synthesis Benchmarking 	Rapid H ₂ gas detection
Leading to Improved H ₂ safety	Odor oo

Development of odour additives for use in hydrogen technology

The remit of Harvey's project involves the design, synthesis and testing of novel compounds for use in hydrogen storage. A number of potential odorants will be selected and compared with the novel compounds, as well as some odorants present in literature. The tests will consist of hedonic tone and odour character tests, to ensure the suitability of an odorant's scent before fuel cell tests are performed to test which odorants don't poison the catalyst. So far, work on the novel compounds has been fully focused on the bicyclopentane framework, due to its volatility and broad substrate scope.

Supervisors: Dr Marc Kimber, Dr Gareth Pritchard.



Highly efficient molecular hydrogen-evolution catalysts

Molecular hydrogen evolution electrocatalysts allow efficient hydrogen production from water under mild conditions.

Adedayo will research development of fully tailorable molecular clusters based on molybdenum/tungsten and sulfur/oxygen. Systems will be combined with conductive nanocarbon materials to develop highly efficient composite electrocatalysts for the water splitting reaction. The stability and efficiency of these systems will be explored during prolonged electrolysis. We are looking to design a new generation of inexpensive electrocatalysts which could outperform state-of-the-art materials, while allowing atomic control of catalyst structure. The cheap and easy-to-prepare systems are particularly interesting from a commercialisation perspective, given the ease with which their preparation could be scaled-up.

Supervisors: Dr Graham Newton, Dr Lee Johnson.









Dehydrogenation catalysis of mixed metal borohydride ammoniates

Antonia is developing novel catalysts for the dehydrogenation of mixed metal borohydride ammoniates. She is seeking to elucidate the mechanisms involved, in order to improve reaction conditions and selectivity.

Supervisors: Professor Deborah Kays, Professor Gavin Walker.





Mickella Dawkins (Cohort 1) Department of Chemistry



Hydrogen enrichment of natural gas by thermo-catalytic decomposition of methane

The gas network currently supplies natural gas to consumers but could supply gases, such as hydrogen, in the future. Thermo-catalytic decomposition of methane allows enrichment of natural gas with hydrogen, a carbon-free fuel. Mickella's research is focused on the development of this technology and the incorporation of wind energy. Her research looks at the use of iron oxide from a natural source as the catalyst for the thermo-catalytic methane decomposition process.

Supervisors: Dr James Reynolds, Professor Sandie Dann and Professor David Saal.











Renewable electricity and sustainable biomass sources	H ₂		Vehicle manufacture, use,
Natural gas with/ without carbon capture	H2		management
3.	ife cycle greenhou Circular resource	ise gas emission: e management	5
Compe	titiveness with oth	her low carbon o	ptions
U	K policy and fleet-	level implication	15

Quantifying environmental and resource impacts of the future UK hydrogen-fuelled vehicle fleet

Cheryl's project is developing novel Life Cycle Assessment (LCA) models to assess the resource and environmental implications of deploying hydrogen-fuelled vehicles in the UK's light duty and heavy duty road fleets. Cheryl's comprehensive approach will consider the current and future mix of hydrogen production routes, vehicle manufacture and use, and end-of-life vehicle management (e.g. recycling). Beyond more common LCA studies comparing technologies on a vehicular level, this project will consider the turnover of UK vehicle fleet and the uptake of hydrogen technologies, to quantify cumulative resource and environmental implications.

Supervisor: Professor Jon McKechnie.

Stakeholder Collaboration







Emily Dunkerley (Cohort 4) Faculty of Engineering



Advanced hydrogen sensing platform based on functionalised metal-organic frameworks

Developing efficient sensor materials with superior performance for selective, fast and sensitive hydrogen detection is essential for environmental protection and human health. Metal-organic frameworks (MOFs) – crystalline and porous solid materials constructed from metal nodes (metal ions or clusters) and functional organic ligands – are of interest for gas sensing for their large surface area, adjustable pore size, tunable functional sites and intriguing properties; such as electrical conductivity, magnetism, ferroelectricity, luminescence and chromism.

However, selectivity, sensitivity and stability are still major challenges for MOFs-based sensors used in hydrogen detection.

Emily's project aims to fabricate novel multi-functional MOFs with improved sensitivity and stability for hydrogen detection. The rational design of these robust, multi-functional MOFs will be guided by computational predictions; after integrating metal nodes, functional ligands, and guest molecules with different properties, to achieve selective sensing of hydrogen over multiple cycles. Computational modelling delivered in collaboration with Nottingham's Computational Materials Group.

Supervisors: Dr Oluwafunmilola Ola, Professor Gavin Walker, Professor Elena Besley.



www.sustainablehydrogen-cdt.ac.uk





Hazhir Ebne-Abbasi (Cohort 2) Belfast School of Architecture and the Built Environment



Figure: Simulation of a Hydrogen fuelling station. Temperature distribution in a vehicle onboard tank at the end of refuelling.

Assessment and mitigation of hydrogen-fuelled vehicle hazards

Since joining HySAFER (Hydrogen Safety Engineering and Research) at Ulster University Hazhir has contributed to a number of projects, including HyTunnel-CS. He is now focusing on the development and validation of the first of its type CFD model for simulation of complex heat and mass transfer processes during refuelling; through the entire chain of equipment at HRS from a high-pressure tank through piping, pressure control valve, precooler, breakaway, hose, nozzle, etc. to onboard storage tanks.

Supervisors: Dr Dmitriy Makarov, Professor Vladimir Molkov.



Safety strategies and engineering solutions for hydrogen heavy-duty vehicles

Pursuit of a low carbon economy means practical implementation of zero-emission applications, including hydrogen-fuelled heavy-duty vehicles (HDV) such as buses and trucks. Hydrogen's use in public transport implies stringent bus design requirements. Industry and regulators' concerns over HDV design include:

- Development of HDV refuel protocol comparable with fossil-fuel vehicles, without risking onboard compressed hydrogen storage system (CHSS) safety.
- Fire-resistance rating of current CHSS, which may lead to rupture in a fire with catastrophic consequences, i.e. blast wave, fireball and projectiles.

Atish's project will review 'old' and new HDV hazards of different designs and sectors (buses and trucks); identifying and analysing existing prevention and mitigation safety strategies, engineering solutions, knowledge gaps and technological bottlenecks in provision of HDV safety.

Supervisors: Dr Sergii Kashkarov, Dr Dmitriy Makarov, Professor Vladimir Molkov.







Kieran Heeley (Cohort 2) School of Chemical Engineering



Algal biomass to hydrogen: A circular approach for green sustainable processing with enhanced efficiency and minimal waste

Kieran's project investigates hydrothermal conversion of algal biomass to hydrogen-rich gas, in a sustainable circular approach.

It looks at optimising the catalyst, feedstock and operating conditions to increase the hydrogen yield; whilst maximising the nutrient recovery.

Supervisors: Professor Bushra Al-Duri, Dr Rafael Orozco, Professor Lynne Macaskie.



Composite membranes for H2 purification

H2 is a high quality and clean energy carrier. Most hydrogen is produced by steam methane reforming, followed by water-gas shift reaction, with bio-hydrogen production increasing. Before hydrogen is used in fuel cell and other applications CO2 and CH4 resulting from production processes has to be removed. Membrane-based separation technologies are promising alternatives to conventional separation technologies, i.e. pressure swing adsorption, due to low energy consumption.

Many inorganic membranes of zeolites, metal alloys and carbon molecular sieves have been developed but scaling-up difficulties limit applications. Polymer membranes are useful, whilst controlling permeability/selectivity in harsh conditions is challenging. Recently, mixed matrix membranes (MMMs) – where inorganic material is embedded into polymer matrix – have attracted attention; as they combine porous materials' functionality with polymer processability. In this context, metal-organic frameworks (MOFs), comprised of metal ions connected by organic linkers, are most promising; due to their diverse and flexible structure. In addition, MOFs' organic linker typically have greater affinity towards polymer chains; allowing control of the MOF/polymer interface. Void-free MMMs can be prepared without requirement for modification of filler or membrane surfaces. Niko's project will explore development of MOF/polymer MMMs with enhanced H2 selectivity, to enable membrane based H2 purification.

Supervisors: Dr Begum Tokay, Dr Andrea Laybourn.

Stakeholder collaboration







Loughborough University

Edward Jones (Cohort 1) Department of Chemistry



Figure: Recent developments in application of nanomaterials to understanding molecular level processes in cobalt catalysed Fischer-Tropsch synthesis, Phys. Chem., 2014, 16, 5034-5043 DOI:10.1039/C3CP55030C

Neutron spectroscopy of surface intermediates on nanoporous metal catalysts for H2 storage technologies

Ed is using inelastic and quasi-elastic neutron scattering techniques to investigate changes in speciation during ethylene and CO co-adsorption on a model skeletal cobalt catalyst, and the formation of insoluble poorly crystalline layers on metal hydrides during steam hydrolysis.

Supervisors: Dr Simon Kondrat, Professor Sandie Dann, Professor Ian Silverwood

Stakeholder Collaboration





Prevention and mitigation of accidents with hydrogen-powered vehicles in confined spaces

The scope of Mina's doctoral study includes the identification and prioritisation of relevant knowledge gaps, to develop innovative safety strategies to mitigate and prevent hydrogen-fuelled vehicle accidents in confined spaces. The first step is performing analytical and numerical studies to increase hydrogen-powered vehicles' safety, through improving TRRDs design; to prevent pressure peaking phenomenon and blow-off phenomenon, which would both lead to hydrogen deflagration or detonation and catastrophe in confined spaces.

Supervisors: Dr Sile Brennan, Dr Dmitriy Makarov, Professor Vladimir Molkov.







Thomas Liddy (Cohort 4) **School of Chemistry**



Insights on metal nanoclusters (MNCs) (de)hydrogenation for onboard hydrogen storage application using electron microscopy and spectroscopy techniques

Development of volumetric efficient solid-state hydrogen storage materials is crucial for transport sector decarbonisation. Magnesium hydride nanoparticles are among the most promising H₂ storage materials, due to high H₂ storage capacity (7.6 wt.%) and low cost (\$3/kg). However, slow kinetics and high working temperature (ca. 250 °C) limit commercial application for onboard H₂ storage. To improve its properties (higher kinetics, lower temperature) Thomas's project will utilise metal nanoclusters (MNCs); which are fundamentally different compared to more widely used metal nanoparticles (diameters >2 nm), where the majority of metal atoms remain 'hidden' within the lattice and are excluded from participation in useful chemistry. In contrast, the majority of atoms in MNCs are fully accessible for physicochemical processes, while new functional properties (inaccessible in bulk metals or nanoparticles) can emerge as result of confinement in MNCs. Theoretical calculations predict nano-tuning could reduce (de)hydrogenation reaction energy when NCs of Mg/MgH2 are used, reducing working temperature [JACS, 2005, 127, 16675-80]. This would substantially reduce onboard H₂ storage cost. Supervisors: Dr Jesum Alves Fernandes. Professor David Grant.

Stakeholder collaboration







Samuel Lines (Cohort 3) **Faculty of Engineering**



Computational modelling of solid-state hydrogen storage materials

Sam's project aims to understand the composition-structure-property correlations of solid-state hydrogen storage materials, through accurate density functional theory simulations of both existing and hypothetical materials.

The most promising candidate materials discovered from the computational simulations will be synthesised and characterised, and their hydrogen storage properties will be validated by experiments.

Supervisors: Dr Sanliang Ling, Professor Gavin Walker, Professor David Grant.



Loughborough University

Stephen Marr (Cohort 2) Department of Chemistry



Development of techniques and methods for sampling, calibration and testing of hydrogen purity for fuel cell vehicles

Measurement challenges for hydrogen fuel cells are preventing the overall sector from growing. Stephen's project is looking at ways of developing a cylinder passivation technology, which would provide temporal stability data for the 14 trace contaminants outlined in ISO (International Organization for Standardization) 14687-2.

Supervisors: Dr Ben Buckley, Professor Upul Wijayantha, Dr Paul Holland.

Stakeholder Collaboration





Base metal catalysis of acceptorless alcohol dehydrogenation for hydrogen storage

Catalytic acceptorless alcohol dehydrogenation is an atom-economical approach for alcohol oxidation, without need for an oxidant. Reversible dehydrogenation/hydrogenation catalysis from this reaction provides a route to the use of organic molecules derived from biomass as liquid organic hydrogen carriers (LOHCs). Alcohols such as ethylene glycol, glycerol and the C4-C6 analogues erythritol, xylitol and sorbitol are considered to be potentially useful biomass-derived feedstocks; derived from agricultural or lumber resources, including waste streams and gravimetric hydrogen storage capacities, meeting targets set by the EU and the US Department of Energy.

This chemistry has long been dominated by the platinum group metals (PGMs); however, low PGMs abundance means high economic and environmental cost, and their high toxicity means their removal from products can produce significant waste streams. Researchers are looking to other catalysts for industrial processes; with obvious candidates being base metals exhibiting low cost, high natural abundance, uniform global distribution and low toxicity.

Isabelle's project will investigate a range of low coordinate and pincer complexes of the first-row transition metals in order to achieve the acceptorless dehydrogenation reactions and, with appropriate candidates, investigate the possibility of undertaking the reverse reaction with addition of H₂.

Supervisors: Professor Deborah Kays, Professor Peter Licence.







Alex McGrath (Cohort 2) Faculty of Engineering

Binary alloys: SEM images in secondary electron (SE) and back scatter electron (BSE) mode presented for alloys with the following binary compositions: *TiCr* **1.55** *TiCr* **1.71** *TiCr* **2.35**



Synthesis and characterisation of metal alloys for hydrogen storage and related applications

Alex's project aims to experimentally synthesise new metal alloys shortlisted by computational screening; and characterise their physical, chemical and structural nature along with their thermodynamic and kinetic properties, during hydrogenation and de-hydrogenation. He is investigating synthesising new metal alloy compositions which will have improved hydrogen storage properties, forming their hydrides and characterising their microstructures.

Supervisors: Professor David Grant, Professor Gavin Walker, Dr Sanliang Ling, Dr Kandavel Manickam.

Stakeholder Collaboration 👢





Loughborough University

Adam McKinley (Cohort 1) Department of Chemical Engineering **Figure**: Schematic example of 3-electrode configuration for electrochemical cell. A standard hydrogen electrode was used in this example. In this research a Mg/MgO or Ag/AgCl would be used instead. S. Bebelis, Thermodynamics and Kinetics of Electrochemical Reactions (2013).



Catalyst development for low-cost, large-scale sustainable hydrogen production from seawater and renewable energy

Adam is looking at the oxygen evolution and hydrogen production, via water and seawater splitting, driven by renewable energy. He is interested in the production and utilisation of low-cost, highly efficient and highly selective catalysts for the process. Adam is currently investigating the performance of Ruthenium and Palladium (Ru and Pd) nanoparticle-based electrodes for the hydrogen evolution reaction at varying temperatures. He aims to explore the prospect of a bifunctional catalyst capable of efficient and consistent performance, in both the hydrogen evolution reaction and oxygen evolution reaction (HER and OER).

Supervisors: Professor Wen-Feng Lin, Professor Jin Xuan, Dr Darren Walsh.



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Modular additive manufacturing for next-generation hydrogen storage

Compact hydrogen storage is a major challenge for hydrogen powered vehicles, with current state-of-the-art storage vessels being too large and operating at dangerously high pressures. Solid state Metal Hydrides (MH) can store large (relative to gaseous storage) quantities of hydrogen in much smaller volumes and at lower pressures; however, current suitable candidate metals that reversibly store hydrogen are characterised by poor thermal conductivities, which is detrimental to refuelling rates. To improve heat transfer into the powdered metal, Yassin's PhD research aims to exploit the benefits and design freedom that Additive Manufacturing (AM) offers, by incorporating lattice structures into the vessel's internal architecture. This project will involve cell selection, lattice generation, mechanical design, numerical analysis and experimental validation.

Supervisors: Dr Ian Maskery, Professor Gavin Walker.



Photocatalytic covalent organic frameworks for hydrogen production and storage

Jai undertakes research into the use of covalent organic frameworks (COFs) for hydrogen production and storage, as opposed to the popular metal organic frameworks (MOFs) alternative.

His project involves the synthesis of new molecules which can be functionalised onto the surface of COFs; creating photocatalytic and size-specific channels which will permit hydrogen production from water and selective ingress, storage and egress.

Supervisors: Dr Iain Wright, Dr Simon Kondrat.







Figure: Schematic for High Definition Neural Network used in Oliver's Research.



Hydrogenation of storage materials

Oliver is undertaking research into the use of Machine Learning Potentials (MLPs), models that use machine learning to approximate the potential energy surface; with particular focus on High-Definition Neural Networks (HDNNs). With sufficient training data, MLPs enable large-size and long timescale, accurate molecular dynamics simulations, which are unattainable via conventional methods.

Oliver has used MLPs to simulate a variety of Magnesium-Hydrogen systems, including hydrogenation of magnesium clusters.

Future simulations, with larger atom counts and timescales, will be used to gain insight into the process of hydrogenation and may inform the selection of improved hydrogen storage materials.

Supervisors: Dr Sanliang Ling, Professor Gavin Walker, Professor David Grant.





Mulako Mukelabai (Cohort 3) Centre for Renewable Energy Systems Technology Wolfson School of Mechanical, Electrical & Manufacturing Figure: Schematic of renewable hydrogen production processes, hydrogen storage, distribution, and utilisation in a hydrogen cooker. M. D. Mukelabai, U. K. G. Wijayantha, and R. E. Blanchard, 'Renewable hydrogen economy outlook in Africa, *Renew. Sustain. Energy Rev.*, vol. 167, no. October 2022, p. 112705, Oct. 2022, https://doi.org/10.1016/ j.rser.2022.112705



Renewable hydrogen production to transition to clean cooking

Mulako's project aims to develop technical and business models, and processes which will enable hydrogen produced from renewable energy to be utilised for cooking.

Though this process is understood, the system needs not just the right technology but also development of the right business model, human capacity and social acceptance to bring about the transformation of traditional cooking practices.

Supervisors: Dr Richard Blanchard, Professor Upul Wijayantha, Dr Alastair Livesey.







Una O'Hara (Cohort 2)

School of Metallurgy and Materials

Figure: Raman equipment, University of Birmingham.



Development of high-performance complex hydrides

Una is investigating thermodynamic tuning of boron and nitrogen-based complex metal hydrides (CMHs), synthesised by chemical and mechano-chemical routes.

Nano-structuring by encapsulation in mesoporous-frameworks seeks to enhance cyclic stability, discharge and recharge rates; whilst maintaining storage capacity. The materials will be characterised using a wide range of techniques to assess electrical, thermal and hydrogen storage properties.

Supervisors: Dr Daniel Reed, Professor David Book.





Katarina Pegg (Cohort 3) School of Chemical Engineering



The role of green hydrogen in the West Midlands Combined Authority local energy system

Green hydrogen production from weather dependent low carbon generation is an area of growth signposted in the UK Committee on Climate Change's 6th Carbon Budget (published December 2020); which provides UK Government Ministers with advice on the volume of greenhouse gases the UK can emit during the period 2033-2037. Katarina's research will focus on the advantages and disadvantages of green hydrogen generation at a local level, specifically within the West Midlands Combined Authority area.

Supervisors: Dr Grant Wilson, Professor Bushra Al-Duri.







Patrick Powell (Cohort 3) School of Metallurgy and Materials



The use of hydrogen as a processing gas to produce rare earth magnets

Hydrogen is used in the conventional production of sintered (rare earth) neodymium-iron-boron magnets and in the recycling of these materials. In recent years new methods to manufacture rare earth magnets based on a process called the Hydrogen Ductilisation Process have been found.

This process reduces the number of processing steps, reduces waste and could give a significant economic advantage to magnet manufacture. However, the process is far from optimised and the aim of Patrick's project will be to develop this process.

Supervisors: Professor Allan Walton, Dr Richard Sheridan, Professor David Book.





High capacity single and mixed metal borohydrides ammoniates for hydrogen energy storage applications

Jacob is researching the synthesis and characterisation of single and mixed metal borohydrides ammoniates (MBA/MMBAs), to increase the hydrogen storage performance of these materials and elucidate the reaction mechanisms of the decomposition process.

He is assessing the influence of metal charge density, electronegativity, additional metal cations and the number of ammonia ligands on the hydrogen storage performance.

Supervisors: Professor Gavin Walker, Professor David Grant, Dr Kandavel Manickam.





School of Chemistry



Sustainable hydrogen evolution catalysts

Courtney is working in collaboration with the QUILL (Queen's University Ionic Liquid Laboratories) Research Centre on the development of ionic liquid electrolytes for the production of green hydrogen. The ionic liquids allow for the investigation of higher operating temperatures than conventional electrolytes, which improves reaction kinetics; thus diversifying the range of materials which may be studied as catalysts and electrodes.

Research will then be undertaken to explore the stability and efficiency of these systems during prolonged electrolysis.

Supervisors: Dr Graham Newton, Dr Darren Walsh, Dr Lee Johnson.



High-throughput cycling coupled X-ray photoelectron spectroscopy (XPS) of hydrogen storage materials

Chris's research looks into the application of X-ray photoelectron spectroscopy (XPS) to samples after reactions at elevated pressures. Chris is designing a sample transfer device that enables rapid XPS analysis of samples after reactions at elevated pressures. The device will soon be used to investigate various solid-state hydrogen storage materials, with a particular focus on their change in performance with increasing hydrogen cycles.

Supervisors: Dr James O'Shea, Professor Gavin Walker, Professor David Grant.







Aryamman Sanyal (Cohort 3) Department of Engineering



Reactor design and performance optimisation for catalytic hydrogen production from methane

Aryamman's project aims to design, develop and test a hydrogen generation reactor suitable for advanced catalyst; demonstrating high H₂ yield and efficient carbon separation.

Natural gas into hydrogen and graphite has the potential to be highly disruptive, and could be of substantial value if the process can be scaled-up to commercial quantities.

Supervisors: Professor Weeratunge Malalasekera, Professor Upul Wijayantha.





Jack Shacklock (Cohort 2) Department of Chemistry



Lowering the H₂ cost in methane cracking technology by using solid carbon as an energy storage material

Jack's research is designed to investigate the systematic alteration of process conditions to obtain value-added solid carbon, specifically for energy storage, whilst still maintaining a high yield of hydrogen. Initial studies have been conducted to improve the methane cracking process to increase yield and longevity. By-product carbon has separated in batch processes and been studied in electrochemical supercapacitors, demonstrating a high rate of performance compared to commercial carbon used for supercapacitor manufacturing. These results suggest lowering the cost of turquoise hydrogen, by finding applications for by-product carbon, is promising. Further studies are currently underway to separate by-product carbon in real-time operation (as opposed to batch process) and evaluate their performance in applications. **Supervisors**: Professor Upul Wijayantha, Dr Niladri Banerjee.



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Srinivas Sivaraman (Cohort 3) Belfast School of Architecture and the Built Environment



Safety of using ammonia in the hydrogen economy

Owing to characteristics such as high energy density and the experience of the use of ammonia in industries; its transportation around the globe offers practical, cost-effective means of storing and transporting large quantities of hydrogen. Using ammonia as a hydrogen carrier and in fuel applications calls for a reassessment of hazards and risks. Srinivas's project aims to develop safety strategies and engineering solutions for the handling of large quantities of ammonia, used as a hydrogen carrier during transport and storage onboard, and the use of relevant infrastructure. His project will analyse the hazards – including toxicity effects, existing prevention and mitigation safety strategies – and perform comprehensive quantitative risk assessment for safe utilisation of ammonia as a hydrogen carrier.

Supervisors: Dr Dmitriy Makarov, Professor Vladimir Molkov, Dr Volodymyr Shentsov.



Optimising decarbonised energy system usage for a rural community using metal hydride hydrogen storage

Samir is developing an understanding of rural energy requirements to develop a decarbonised rural energy model, assessing the viability of multi-vector hydrogen including metal hydride storage. Also developing a representative demonstrator green hydrogen model.

Supervisors: Professor Mark Gillott, Professor Gavin Walker.









Efficient hydrogen separation using proton-conducting ceramic membranes and electrochemical cells

Most hydrogen used today is produced from fossil fuels (e.g., through steam reforming of natural gas, coal gasification). Product gases consist mainly of H₂ and CO₂, and other impurity gases (CH₄ and CO). Energy efficient and low-cost hydrogen separation constitutes a crucial process to move towards a hydrogen economy. Luke's project aims to achieve energy efficient and low-cost hydrogen separation using proton-conducting ceramic membranes for hydrogen rich streams, generated through reforming of natural gas, as well as onsite purification of hydrogen close to the point of end use for dilute hydrogen streams; distributed through natural gas pipelines using ceramic proton electrochemical cells (hydrogen pumps). Dense ceramic membranes made of mixed protonic-electronic conductors (MPECs) are capable of separating hydrogen from gas mixtures with 100% selectivity, reduced energy penalty and cost, compared to well-established techniques such as pressure swing adsorption technique.

Supervisors: Dr Ming Li, Dr Begum Tokay, Professor David Grant.





Optimisation of Polymer Electrolyte Membrane (PEM) electrolyser balance of plant operation and maintenance, to maximise performance and resilience of key infrastructure

It is obviously desirable to maximise the performance of hydrogen plants, not just for economic reasons, but to deliver the best customer experience. Salim's project seeks to optimise plant operation, where planning preventative maintenance can help reduce disruption to service and improve the commercial case of a plant.

Supervisors: Dr Rasa Remenyte-Prescott, Professor Gavin Walker, Dr Matt Lees, Dr Philip Wilson

Stakeholder collaboration (•) ITM POWER







Amit Verma (Cohort 2) School of Business and Economics **Figure**: Hydrogen Pathways in an Energy System (Hydrogen Council 2021)



Understanding the potential of hydrogen technology adoption in a complex challenging energy system

Amit's project will identify relevant policy interventions necessary to achieve successful adoption of hydrogen technologies, within the existing energy system. His research focus is decarbonisation of the heating sector, and he aims to understand how to size and where to locate hydrogen infrastructure to minimise system costs under different scenarios relating to the uptake of hydrogen. He is looking at existing energy systems and potential hydrogen technologies on economic, technological, and engineering grounds; to evaluate their potential for successful adoption. He will also analyse how they support or hinder development of these technologies and give an understanding of what needs to change. His research will lead to the development of a framework to categorise hydrogen technologies and provide strategic insights into the key factors (economic, regulatory, technological, social and political) which influence stronger adoption of these technologies. **Supervisors:** Professor Monica Giulietti, Professor David Saal, Professor Upul Wijayantha.





Zak Waite (Cohort 2) Faculty of Engineering **Figure:** Temperature profiles in CFD model of micro-hydrogen partial premixed bluff body (PPBB) burner.



To a 100% hydrogen domestic boiler

Zak's project seeks to redesign the domestic boiler so that hydrogen can be used as a network fuel. At the moment because methane, which is currently used, burns quite differently from hydrogen our existing domestic boilers cannot utilise hydrogen gas.

Supervisors: Dr Donald Giddings, Professor David Grant, Professor Robin Irons.



Stakeholder collaboration



Joseph Walton (Cohort 4) School of Chemical Engineering

Business cases for green hydrogen

It is generally agreed that hydrogen employed in sustainable and emission-reducing projects needs to be sourced from 'green' feedstock and energy. Nevertheless, the vast majority of hydrogen sold today is 'black' and produced by steam reforming of natural gas. Obviously, there are cost issues. Joseph's work will look into how green hydrogen can be costed, so that it is more compatible with today's energy system. This will include analysing business cases, high-value applications, externalities and options to sell 'greened' products; based on green hydrogen application. Research aims to deliver cost model fully established, environmental pricing added to cost model, business model development concluded; and dialogue with industry, with validation of models and approaches.

Supervisor: Professor Robert Steinberger-Wilckens.

Stakeholders supporting PhD projects

Sustainable Hydrogen CDT gratefully acknowledges those stakeholders collaborating on students' PhD projects, ensuring our research is answering those questions the hydrogen sector needs to further develop. Stakeholder collaborators include:

nationalgrid

Marketing and Social Media Report

Sustainable Hydrogen CDT - Year in Pictures

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